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Marcin Hojny

Modeling Steel Deformation in the Semi-Solid State

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Modeling Steel Deformation in the Semi-Solid State

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Nomenclature

σ_{ij}	Stress tensor components
σ_{kk}	Mean stress
δ_{ij}	Kronecker delta
σ_p	Yield stress
$\dot{\epsilon}_i$	Effective strain rate
$\dot{\epsilon}_{ij}$	Strain rate tensor components
(v_r, v_θ, v_z)	Components of vector of velocity in the cylindrical coordinate system
r, θ, z	Position vector components in a cylindrical coordinate system
W_σ	Work of plastic deformation
W_λ	Work related to the condition of mass conservation
W_t	Friction work
W	Work functional
σ_i	Effective stress
ϵ_{ij}	Strain tensor components
ϵ_i	Effective strain
$\dot{\epsilon}$	Strain rate
ϵ	Strain
m	Friction factor
λ	Thermal conductivity coefficient
T	Absolute temperature
Q	Heat generation rate for volume unit
c_p	Specific heat
ρ	Density
τ	Time
r	Radius
i, j	Particle index
W	Smoothing kernel
h	Smoothing length
m_j	Mass of particle j
ρ_j	Density of particle j

G	Derivative of the kernel function W
$\mathbf{v}$	Velocity
p	Pressure
$\mathbf{F}$	External force
θ	Second-order tensor containing τ_{ij} stresses
$\bar{c}_{ij}$	Mean speed of sound of particle i and j
$\bar{\rho}_{ij}$	Mean density of particle i and j
T_l	Liquidus temperature
T_s	Solidus temperature
NST	Nil strength temperature
NDT	Nil ductility temperature
DRT	Ductility recovery temperature
T_d	Deformation temperature (physical and computer simulation)
V_{ch}	Cooling rate
R_f	Fracture resistance indicator
G	Temperature gradient before the crystallisation front
D	Diffusion coefficient of admixture atoms
ΔT_0	Difference between the solidus and liquidus temperatures
V_c	Critical crystallisation front speed
V_n	Tool stroke rate in the Gleeble 3800 simulator system
F_{max}	Maximum measured force
$\tau_{melting}$	Remelting time
f_s, f_l	Solid- and liquid-phase shares
$\aleph_1, \aleph_2$	Distances between the primary and secondary dendrite branches
A_{dend}	Dendritic structure area
$\mathbf{n}$	Vector of the shape function
$\mathbf{n}^T$	Transposed vector of the shape function in the heat transfer model
$\mathbf{H}$	Main matrix of the discrete form for the steady heat flow
$\mathbf{p}$	Vector of free terms for the steady heat flow
$\bar{\mathbf{H}}$	Main matrix of the discrete form for the transient heat flow
$\bar{\mathbf{p}}$	Vector of free terms for the transient heat flow
$\mathbf{M}$	Matrix of thermal capacity
q	Density of heat flux on the heat transfer zone surface
$\mathbf{T}$	Vector of the temperature nodal values
T_0	Initial temperature
T_{env}	Temperature of medium in contact with the area concerned
α	Heat transfer coefficient
S	Boundary surface
V	Volume of medium analysed
λ	Vector of thermal conductivity distribution function
n_r, n_z	The direction cosines of normal to the outer surface
$\mathbf{T}_1$	Vector of temperature nodal values at the beginning of the time step
$\mathbf{T}_2$	Vector of temperature nodal values at the end of the time step
$\mathbf{f}$	Vector of free terms

$\hat{H}$	Enthalpy
ρ_s	Density of solid phase
ρ_l	Density of liquid phase
$\underline{\mathbf{v}}$	Displacement vector
$\mathbf{A}$	Nodal displacement vector
ξ, η, ζ	Coordinates of the consecutive Gauss points in the local coordinate system
$\mathbf{C}^T$	Transposed unit vector
$\mathbf{B}$	Shape function derivative matrix
$\underline{\underline{\boldsymbol{\varepsilon}}}$	Strain rate vector
$\underline{\boldsymbol{\varepsilon}}$	Strain vector
$\mathbf{D}$	Unit matrix
v_0	Grip velocity $\mathbf{v}$ Nodal velocity vector

Abstract

This monograph presents selected aspects related to the broadly understood modelling of steel deformation both at very high temperatures and in the conditions in which the liquid and the solid phases coexist. Issues of modelling steel deformation with its simultaneous solidification, due to their specificity and complexity, are amongst the most difficult in the metal processing field.

With regard to industrial applications and the development of new integrated continuous casting and rolling processes, the issues related to modelling are growing in importance. Numerous industrial tests, which are necessary when traditional methods are applied to design the process of continuous casting immediately followed by rolling, are expensive. Therefore, the idea has arisen to develop a concept of modelling characterising physical effects occurring during the process of deforming steel with the semi-solid core.

Comprehensive tests were applied to solve problems related to the deformation of steel with a semi-solid core. The tests covered both physical tests using specialist laboratory instruments (thermo-mechanical simulator Gleeble 3800, computer tomograph NANOTOM 180N, testing machine Zwick Z250, 3D systems of blue light scanning) and advanced mathematical modelling (finite-element method (FEM), smoothed particle method (SPH), cellular automata method (CA)). The approach integrating the physical and computer simulation areas with a full or partial information exchange between these areas was the basis for the developed modelling concept of steel deformation in the semi-solid state presented in detail in this monograph.

Chapter 1

Introduction

As of yet, continuous steel casting practices have been little investigated, and as a rule they concern a limited group of steel grades. Very often quality problems occur when casting new steel grades. The reasons for failures related to the casting of special steel grades include the occurrence of temperature ranges with a reduced ductility. If the surface or edge temperature is within the steel reduced ductility range during the cast strand straightening operation, the likelihood of crack initiating increases. Another reason for diminished steel quality, in particular for alloy steels, is the tendency of segregation of alloying elements. Thermomechanical stresses play a significant role in the process of crack initiating in a continuously cast strand. Immediately after leaving the mould, the cast strand shows the presence of an internal liquid zone, with a conical shape. In the secondary cooling zone, the cast strand surface is subjected to complex cycles of temperature and mechanical load changes resulting from intensive water cooling, a cyclical pressure of guide rolls, and for special continuous casting installations, the pressure of the so-called “soft reduction” rolls. If the stress and strain state meets specific conditions, and the material shows reduced ductility, cracks nucleate and propagate on the surface and inside the cast strand. As the limit values depend both on the chemical composition of the steel, and on the casting parameters and parameters of straightening after casting, the determination of the mechanical properties of the material at increased temperatures is vital for the selection of the optimal parameters for the continuous casting process.

The first attempts to design the aforesaid processes only utilised the knowledge obtained by experiments. The thermo-mechanical simulators of the Gleeble series, which are used for this purpose, enable a process, e.g. of continuous casting of steel, to be physically simulated. The essence of simulation is the reconstruction—in laboratory conditions—of the temperature, strain and stress changes to which the material is subjected in an industrial process. Instead of actual products, only small samples made of the same material that is used in the production process are tested. The evaluation of the mechanical properties of the samples subjected to various simulation variants is the basis for developing the “process map”, which enables the

optimal parameters of equipment operation to be determined, e.g. of a continuous casting machine during the casting of a specific steel grade. Special diagrams are constructed where the areas with limited ductility are marked. A thorough knowledge of these areas allows the casting process parameters to be adjusted (casting speed, cooling rate in the primary and secondary zones) so as to avoid the potential threat of cracks. As may be concluded from the above description, each steel grade requires separate research.

The process of numerical modelling of steel deformation when the solid and liquid phase coexist, due to its specificity and complexity, is among the most difficult processes in metal processing. A comprehensive numerical model of semi-solid steel deformation should include the effects related to the steel solidification or the effects related to the flow of liquid steel within the solidified skeleton. Also the lack of constitutive equations allowing the plastic behaviour of steel at extra-high temperatures to be determined affects the result of a computer simulation—for the semi-solid state deformation, as well as above the melting temperature (the solidus temperature). Thermal effects (heat transfer to the environment, heat generation and flows) or the formation and cumulation of internal stresses during a change of the state of aggregation are other important aspects. The mere complexity of the numerical modelling process stems from:

- the complex nature of the model, requiring the application of partial models—mechanical, thermal, fluid mechanics, density changes, and microstructure development,
- lack of data concerning fundamental material properties,
- difficulties in carrying out the experiment because of the very high process temperature,
- impossibility of carrying out direct industrial measurements to verify models.

This monograph summarises the author's research in the context of developing a modelling concept for steel deformation in the conditions where the liquid and solid phase coexist. The research involved the use of advanced methods of physical and computer simulation.

It consists of a few fundamental parts. This chapter presents the outline of the conducted research as regards industrial applications.

Chapter 2 is the description of the art of physical and computer modelling over the last dozen years or so.

Chapter 3 contains the formulation of the thesis of the study concerning the possibility of simulation of steel deformation in the conditions of the liquid and solid phase coexistence. Also the research objective and the adopted methodology is presented here.

Chapter 4 describes an original advanced FEM simulation system called DEFFEM, based upon numerical models presented in Chaps. 5 and 6. This tool has been created with a big effort, and it constitutes an integral part of the developed concept of modelling of semi-solid steel deformation. A short history of the software

development was presented, as well as its current capabilities and the implementation work scope in progress, along with planned further development tendencies.

Chapter 7 constitutes an extensive introduction to the very problem of physical simulation. The physical simulation method allows us to determine the material characteristics very accurately. The knowledge of those characteristics is necessary to develop new techniques, and most of all, it allows us to determine the relationships between the structure state and the mechanical properties of the material, as well as the plastic deformation conditions. However, sometimes problems related to the interpretation of results of physical simulations carried out at a temperature close to the solidus line appear. These are caused by the impossibility of conducting strength tests under constant temperature conditions, and ensuring the homogeneity of plastic deformations in the whole sample volume. They stem from physical conditions and therefore they are difficult to avoid. In such cases, the only solution is to apply a computer analysis of the obtained results, based upon complex numerical models of the processes and using the inverse analysis. Then, this approach requires two factors: an advanced physical simulation system and a dedicated computer simulation system constituting an integral part of the experimental procedure.

Examples of model application results are presented in Chaps. 8 and 9. Chapter 8 presents thorough tests, and the discussion of findings concerning the steel sample heating and remelting process itself. The proposed axially symmetrical numerical model and the adopted research methodology allow the temperature distribution within the sample volume to be correctly determined. The conducted tomography tests and their in-depth analysis complement the whole research project. Chapter 8 is supplemented by research methodologies of the determination of stress-strain curves on the basis of tensile and compression tests. The proposed approaches, along with the prepared methodology of verification of the findings, allow us to determine the strain-stress relationship within a broad range of both temperatures and strain rates.

Chapter 9 presents examples of physical and computer simulation results on the basis of the modelling concept based upon full 3D solutions. The application of full 3D models combined with the capabilities of cellular automata allowed the shape and size of the mushy zone to be reconstructed. The findings constitute the foundation of a new hybrid modelling concept using the capabilities and advantages of the finite element method and particle method.

The paper closes with a section containing a summary of tests conducted and a number of additional conclusions that occurred during the tests. The most important procedures written in the Fortran/C++ language, selected by the author constitute an additional part of the monograph. They may be utilized by a reader during implementation work of their own solutions.

Chapter 2

State of the Art

Contemporary engineering sciences are strictly related to the broad application of computer technologies and methods. The finite difference method (FDM), the boundary element method (BEM) and the finite element method (FEM) are the most popular computational methods. The FEM is certainly the most widely used, which is proven by the numerous computing systems based on this method that are applied in engineering practice. Attempts are being made to model not only changes occurring within the material being processed, but also within the forming tool, which enables a final product of very good quality to be obtained. Such attempts are possible, first and foremost, thanks to the use of mathematical modelling for the occurring physical phenomena. Mathematical models combined with the finite element method provide great possibilities for the modelling of metal deformation processes even for complicated shapes of the deformation zone and complex thermal conditions [23, 69, 88]. They may also be applied for effects that occur during the semi-solid steel deformation process. In actual metal working processes, a number of effects occur in parallel, such as the metal flow, metal temperature changes, heat generation as a result of plastic deformation work, friction force work, heat discharge as a result of contact between the metal deformed and the tool, or heat discharge to the environment by radiation and convection. For hot plastic working, the metal mechanical properties considerably depend on the temperature. A substantial irregularity of deformation in some processes leads to uneven heat generation, and consequently to an uneven structure and metal properties. In addition, the contact of the hot metal with a cold tool causes that high temperature gradients develop in the vicinity of the contact surface [69]. Phase transformations, both in the liquid and the solid state, are additional, temperature dependent factors which may influence the process. They may significantly influence both the deformation resistance and the grain size, as well as the metal properties after the plastic working. At present, there are many mathematical models and computer simulation programmes for processes occurring within the temperature range typical of the cold and hot working. An example of a solution, assuming a rigid-plastic model of the body deformed, may be found in publications concerning rolling

[25–27], upsetting [24, 89], or drawing [104]. Only in recent years have solutions to the semi-solid deformation problem appeared in literature. They primarily concern non-ferrous metals and their alloys [1, 2, 8–11, 15, 17, 22, 40, 42, 44, 46, 52–56, 59–61, 66, 68, 74, 77, 90, 94, 99, 102, 111, 112, 114, 118–120]. The authors of these papers considered a number of aspects related to the deformation of samples with various contents of the liquid and solid phases, starting with equations and computer simulations of heating, and ending with attempts to determine constitutive equations and preliminary computer simulations of deformation of the materials analysed [14, 19, 75, 87, 105]. However, there are no solutions concerning the modelling of the steel solidification with its simultaneous plastic deformation.

Choi, in his paper [11], analysed the influence of the holding time of aluminium samples at the last stage of upsetting and selected the optimum holding time on the basis of the final product shape. The experimental research was conducted in laboratory conditions on an MTS (Material Testing Systems) machine, which enabled the maximum load of up to 25 tonnes to be applied, and induction heating of the material tested to be carried out. Cylindrical samples with a diameter of 44 mm and a length of 65 mm, made of the A356 aluminium alloy were used as the input material for the tests. The experiment included the measurement of temperature changes over time. Appropriately arranged thermocouples were applied for the temperature measurements. Computer simulations of the heat transfer between the sample and tools were made with Fourier's transient heat conduction equation using apparent integration with respect to time. Experiments and computer simulations combined with optimisation techniques allowed the authors of the paper [11] to determine the heat transfer coefficients between the sample and tools. The authors of the paper [15], based upon prior experimental research, conducted a series of compression tests of aluminium alloy samples using their original programme SFAC2D with various tool strokes. In the program, a rigid-viscous-plastic model of the body deformed was used for the solid phase skeleton, combined with the solution of Darcy's equation for the liquid phase. Also attempts to determine the constitutive equations were made. Kang, in his studies [52, 53] of the deformation of aluminium alloys in the di-phase range—liquid and solid—proposed an equation relating to the strain rate, strain degree and the temperature to the fraction of the liquid phase share. Like the authors of the paper [15], for the computer simulation he used a rigid-viscous-plastic model of the body deformed for the solid phase skeleton, combined with the solution of Darcy's equation for the liquid phase. The initial temperature distribution in the volume of the material analysed is a very important factor, which substantially influences the strain and stress state in the deformation process. In research aimed at the computer simulation of such processes, many authors have tried to tackle a number of problems that occur when heating a sample to a desired temperature. The induction heating method was the prevailing method in laboratory conditions [12, 49, 50, 57, 82, 95]. Choi and the authors of the study [12] tested the impact of induction heating on the aluminium alloy microstructure. By using various heating variants and implementing a holding stage at a specific temperature when heating, the changes of temperature at the sample centre and its faces were analysed. The experiments, combined with various

variants of input and output power, allowed the authors to select the optimal parameters of induction heating. The authors of the study [82] used the regression method and neural networks to determine the relationship between the conditions of the induction heating process and the solid phase fraction on the basis of the experiment series for the selected aluminium alloys. Parameters such as the holding time at a specific temperature, re-heating after the holding and the time of such re-heating or the power of induction heating significantly influenced the final quality of the obtained samples. The conditions in which they obtained the minimum grain size and the maximum average temperature measured with four thermocouples in the sample volume [82] were the optimum process conditions. Jung dealt with similar issues in his studies [49, 50]. He analysed the influence of heating conditions on obtaining a homogeneous temperature distribution and a uniform structure across the cross-section of a sample. Also the aluminium alloy was analysed. Kang's studies [57] had a similar nature. Based on Jung's experimental findings and the heating curves developed by Jung [49, 50], he carried out computer simulations of induction heating and compared the results with the experimental findings. A commercial programme ANSYS, which enables induction heating combined with complex thermal conditions to be simulated, was used for the simulations. From the perspective of this monograph subject area, the publication [96] turned out to be very interesting. The authors conducted a few series of resistance heating tests of samples made of aluminium alloy A357 in laboratory conditions. They analysed a number of aspects related to the simulation of resistance heating, e.g. the influence of the initial value of the pressure force between the sample and the electrode on the electric conductivity or the influence of the heating power on the final temperature distribution. Most physical parameters that influence the solidification process are strictly related to temperature changes. Temperature fields in most cases are determined using the solution of Fourier's generalised diffusion equation with the finite element method. For the completeness of the solution, Fourier's equation must be complemented with Neumann-Hankel boundary conditions. Material constants, which are necessary for a model of steel deformation in the semi-solid state, in most cases must be determined experimentally. They are functions of temperature associated with the liquid and solid state of aggregation. The results of computer simulation of the temperature changes in the metal solidification process with the full 3D model presented in the paper [76] may be shown as an example. Generally the modified theory of plasticity is used to analyse the flow of metal in which we can distinguish a mushy zone. This classic theory does not cover such effects as irregularity arising from substantial metal porosity or the relationships between the stress and strain states at very high temperatures. Therefore the modelling of the process of semi-solid metal deformation requires supplementing the model with effects related to the behaviour of the material within the temperature range in which the state of aggregation changes. Recently, thermo-mechanical models of porous material deformation have appeared in literature, including a change in the material density within the temperature range specific to the classic plastic working. The paper [41] in which the authors made an

attempt at mathematical modelling of the forging process of these materials may serve as an example. In this case the constitutive equation includes the relative density of the physical continuum referred to a solid material. Also the material state, where its deformation resistance decays, is an important parameter. Applying the formulated constitutive equation to model forging of porous steel rings allowed the authors of the study [41] to obtain good results of the computer simulation that complied with the experiment. The presented approach may be used for the modelling of metal flow in the semi-solid state if one can determine the relationship between strain and stress for the semi-solid and solid material at very high temperatures. The stress state must be computed for the solidified outer layer with a thermo-elastic-plastic model, taking into account the temperature changes of the solidifying steel and the δ/γ transformation. These computations are conducted in line with the variation formulation and after adopting a discretisation specific to the finite element method. A solution like this is presented in the publication [16]. When applying the presented model to the issues discussed, the main problem is a lack of relationship between strain and stress within the temperature range of the state of aggregation change. The problem of determining the stress-strain relationship for a material in the semi-solid state is much more complex than in the case when this material is deformed at lower temperatures and has been plastically deformed before. Solid materials were subjected to comprehensive tests many times in order to determine the stress-strain relationship at increased temperatures. The paper [117] by Wray, who tested carbon steels, may be used as an example. It is much more difficult to model the behaviour of steel and other alloys within the temperature range in which they transform from liquid to solid. As many effects accompany the solidification, it is difficult to determine precisely the plastic and strength properties of the forming semi-solid structure, which changes its density as a result of strain, temperature changes and the δ/γ transformation. The implementation of Gleeble series thermo-mechanical simulators allowed us to conduct appropriate experimental research to determine those parameters. Those simulators are basically the only units, described in literature and available in the market, which allow similar tests to be performed. Examples of tests with Gleeble simulators are presented by the authors of the papers [71–73], who analysed the conducted experiments with deforming nickel and aluminium alloys. They showed that not only changes in the dependence of stress on strain were very strongly related to temperature, but also depended on the cooling rate within the temperature range between the liquidus and solidus lines. The papers [72, 73] also reveal a linear dependence of the stress causing material destruction on the size of grain which forms during the material solidification. Other than at lower temperatures, for an equiaxial structure the stress causing material destruction is directly proportional to the grain size [72]. The authors explain this effect by the melting of grain boundaries. It results in the need to track changes in the size of the forming grain. During the solidification, the material changes its state of aggregation and at a certain temperature it becomes mechanically strong. Even though it is believed [116] that at increased temperatures the carbon content in steel has a minimal impact on its

deformation resistance, it influences the nil strength temperature [97]. For low carbon steels, the material shows some deformation resistance even at a 60 % fraction of the solid phase. High carbon steels recover their strength only at a solid phase fraction over 80 %. However, the material is brittle and its temperature must decrease so that it can be deformed. Generally, it is believed that although the temperature at which the material loses its strength depends on the carbon content in the steel, the solidifying material becomes plastic at the temperature at which the solid phase fraction is about 98 % and its dependence on the percentage of carbon is minimal. The authors of the article [97], when carbon steel properties were tested, found that the plastic behaviour of low and high carbon steels differs at very high temperatures. They tested a low (0.12 %C), a medium (0.41 %C) and a high carbon steel (0.81 %C). They found that these steels recovered their tensile strengths at temperatures of 1505, 1455 and 1404 °C respectively, and the increase in this strength along with the decrease in temperature had a similar nature, close to linear. However, these steels demonstrated different behaviour regarding ductility changes when cooled. Medium and high carbon steels recovered their ductility at temperatures of 1374 and 1314 °C, and showed a substantial increase in their ductility when the temperature decreased. Low carbon steels recovered slight ductility at a temperature higher than other steels. For instance, for steel containing 0.12 %C the temperature of ductility recovery was 1475 °C. Yet initially the increase in ductility was slow. A faster growth in the ductility of this steel was only observed at a temperature of 1438 °C. This effect was caused by the occurring δ/γ transformation, which started during the solidification at a temperature of 1486 °C, and ended below the solidus line exactly at 1438 °C. A local decrease of the specific volume of steel as a result of the δ/γ transformation causes a strain, which when superimposed on the thermal strain causes the possibility of faster cracking and is the reason for a decrease in the material ductility. Below the transformation temperature the low carbon steel demonstrates a rapid increase in its ductility. The paper [97] also presents a quantitative description of the changes of the parameters discussed. The authors presented a number of relationships which allow the critical stress, i.e. the point at which cracks appear in the steel, to be determined. They showed that the dependence of the yield stress on the temperature and strain rate may be described with the following relationship:

$$\dot{\epsilon}_p = A \exp\left(-\frac{Q}{RT}\right) (\sinh(\alpha\sigma))^{\frac{1}{m}} \quad (2.1)$$

where:

- $\dot{\epsilon}_p$ plastic deformation rate,
- T absolute temperature,
- σ yield stress,
- Q plastic deformation process activation energy,
- R gas constant,
- A, α, m material constants.

The authors [97, 98] described the critical stress to initiate a crack within the range in which phases γ and δ coexist with the following formula:

$$\varepsilon_c = \left(\frac{\varphi}{\dot{\varepsilon}_p^m \Delta T_B^n} \right) \quad (2.2)$$

where

$\dot{\varepsilon}_p$ plastic deformation rate,
 φ, m, n material constants,
 ΔT_B the temperature range of reduced ductility.

On the basis of the quoted papers one may conclude that despite serious experimental difficulties, the application of the foregoing mathematical formalism to describe the mechanical properties of the material in the semi-solid state gives very good results. It needs to be stressed that the research quoted in the papers [97, 98] was made with an old type of Gleeble simulator.

There are many papers concerning the determination of strain–stress curves in the available literature, largely for non-ferrous metals [4, 20, 28, 63, 67, 70, 78, 93, 97, 103]. In recent years also, attempts to describe similar relationships for steels and attempts to deform in the semi-solid state have appeared [14, 19, 43, 45, 47, 48, 51, 62, 64, 75, 79–81, 87, 98, 101, 105, 109, 110]. The main reason for the numerous tests and the determination of constitutive equations for non-ferrous metals is the fact that the liquidus and solidus temperatures for non-ferrous metals are lower than for steels. This fact allowed preliminary tests to be conducted, usually in laboratory conditions, in which samples were melted and deformed slowly. On the basis of test results computer simulations were conducted to verify the findings. When Gleeble simulators were implemented, the technical and research possibilities increased. Whereas the development of continuous steel casting practices in recent years has been very intensive, the research work in this field carried out with new units may constitute the research foundation for the development of new practices. In most papers, to describe changes of stress as a function of strain, the authors used equations combining the strain rate, strain degree and temperature. The fraction of the solid or liquid phase was an additional parameter taken into account in the equations. Kang's studies [52, 53] may be used as an example. He described the dependence of the yield stress on the temperature and strain rate with the following relationship:

$$\sigma = K \dot{\varepsilon}^m \exp\left(\frac{Q}{RT}\right) (1 - \beta f_l)^{\frac{2}{3}} \quad (2.3)$$

where

K, m material constants,
 T absolute temperature,
 β equilibrium factor,
 Q plastic deformation process activation energy,
 f_l liquid phase fraction.

The curves were determined on the basis of compression tests, at a 50 % fraction of the liquid phase and small strain rates under 1 s^{-1} . The obtained dependences became the basis for procedures simulating the deformation of aluminium alloys in the semi-solid state. In his study [63] Kopp conducted a series of compression tests of samples made of the Sn-15 %Pb alloy for two variants with the solid phase fraction of 0.55 and 0.65. On the basis of the conducted tests, the strain–stress curves were determined. Using the commercial FEM software, they made a series of computer simulations for various parameters of the constitutive model. The conducted simulations allowed them to evaluate the formulated constitutive model. The evaluation included a comparison of force parameters obtained during the experiment and by computer simulation, where good compliance of the analysed parameters was obtained.

Other examples may be found in papers [3, 4, 20, 28, 47, 48, 64, 67, 70, 78, 85, 86, 92, 103, 109] concerning primarily non-ferrous metals. A paper by Lewandowski deserves attention [70], where the author presents a number of aspects related to the compression test modelling and determining flow curves for the aluminium alloy 718. Deformation experiments were conducted at very low strain rates of 0.001 s^{-1} . Tests on steels were published in the following papers: [47, 48, 98, 109]. Tseng in his study [109], like Lewandowski in his [70], presented a number of aspects related to the compression test modelling and determining strain–stress curves for the selected carbon steels. By analysing the impact of the solid phase content, he conducted a few series of deformation tests at low speeds ($<0.012 \text{ s}^{-1}$) and obtained curves for various fractions of the solid phase in the sample volume. In publication [98] the authors presented their findings concerning the determination of flow curves for steels in the temperature range between 1100 and 1450 °C. Experimental work was conducted to determine the impact of the temperature and strain rate on the plastic behaviour of two types of carbon steel. The first one containing 0.137 % of carbon was subjected to tensile tests at temperatures of 1100, 1200 and 1300 °C and was used for determining flow curves for austenite. In order to examine similar relationships for ferrite δ , a steel containing 0.0026 % of carbon was selected and was deformed at temperatures of 1400 and 1450 °C. The tests were conducted with a Gleeble simulator. The authors proved the full suitability of Garofalo's model [5] modified by Han to describe the flow curves of the tested steels, dependent on the temperature and strain rate:

$$\dot{\varepsilon}_p = A \exp\left(-\frac{Q}{RT}\right) (\sinh(\beta K))^{\frac{1}{m}} \quad (2.4)$$

$$\sigma = K \varepsilon^n \quad (2.5)$$

where

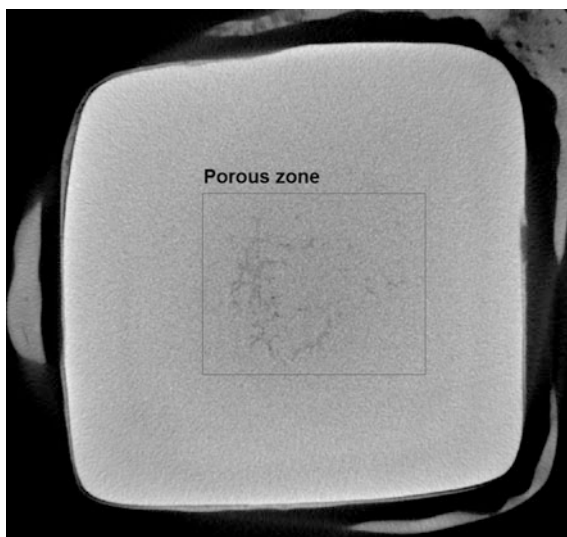
$\dot{\varepsilon}_p$	plastic deformation rate,
T	absolute temperature,
σ	yield stress,
Q	plastic deformation process activation energy,

K strength coefficient,
 n strain hardening exponent,
 A, β, m material constants.

The steels were tested at very high temperatures. This model was used to analyse the deformation of porous materials at lower temperatures, not exceeding 1200 °C and showed its full suitability [41]. The Han relationship can also serve as the basis for the constitutive equation for high temperatures. In paper [98], very good compliance of the obtained experimental findings with the values computed with this model was shown. However, the main objective of the authors was to investigate flow curves for strain rates from 0.0001 to 0.01 s⁻¹ and very small plastic deformations, not exceeding 0.1. For the cases of plastic deformation of semi-solid steel, experimental research should be conducted to determine the material constants for a much broader range of strains and strain rates. One of the most topical publications is Jing's paper [48] concerning primarily the determination of flow curves for steel 304. The curves were determined on the basis of compression tests. The liquidus and solidus temperatures were 1450 and 1390 °C respectively. The deformation temperature range for samples with a diameter of 12 mm and a height of 12 mm was between these two temperatures. During the experiment, the force and the base elongation of the sample were measured, as well as the temperatures read from the thermocouple indications. At the first stage the sample was heated to the deformation temperature within the range between the liquidus and solidus lines according to a set temperature schedule. At the final stage it was deformed at strain rates from 0.5 to 10 s⁻¹.

The tests carried out by the authors of the papers [47, 48, 98, 109] may constitute the research foundation for modelling and designing new continuous steel casting practices. To be competitive in the market one should aim at obtaining products with consistent and good quality. Unfortunately, steel tests at very high temperatures are still very expensive. For business and technological reasons they cannot be conducted under industrial conditions. The Gleeble simulators and computer tomographs (CT scanners), more and more widely available, may provide an alternative. A Gleeble 3800 simulator enables the steel continuous casting process to be physically simulated. The main purpose of the simulation is to use a small sample to reconstruct the changes of temperature, strain and stress that the material undergoes in the industrial process. The evaluation of the mechanical properties of samples subjected to various simulation variants provides the basis for developing the so-called "casting map", which enables the optimal parameters of the continuous caster operation when casting a specific steel grade to be determined. In practice, time-temperature-reduction (TTR) diagrams similar to TTT diagrams are constructed. These diagrams show areas with a limited ductility, and a thorough knowledge of those areas allows us to adjust the casting process parameters, such as for instance the casting speed, so as to avoid the potential threat of cracks in the strand. The Gleeble simulator provides a rare—from an experimental point of view—opportunity to combine the simulation of continuous casting with the plastic deformation applied during or immediately after the solidification of the working

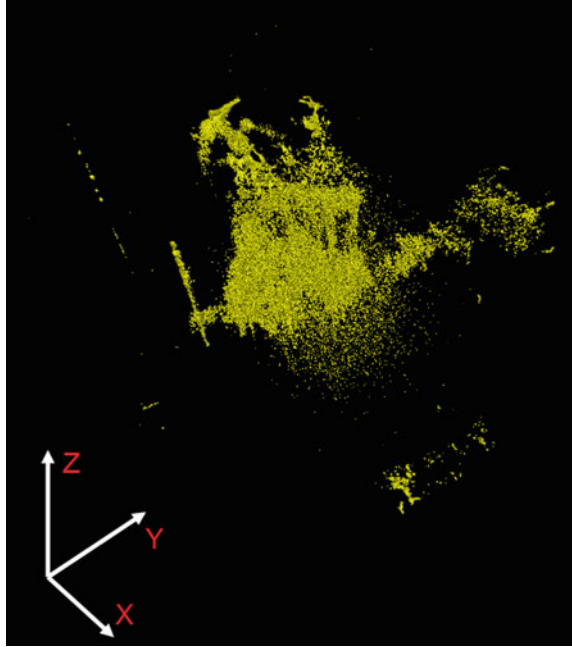
Fig. 2.1 A virtual cross-section of a sample with a visible porous zone (carbon steel)



part of the sample. In both processes, i.e. the solidification and the plastic deformation, in order to determine the impact of process parameters on the microstructural changes, the sample may be cooled with gas (argon, compressed air), a water and air mixture, or water, or cooled with a rate typical of the simulated production process. Increasing availability of modern equipment, such as computer tomographs, allows the medium tested to be analysed without destroying it. The analysis of the remelting zone and the ability to make a virtual cross-section for determining the area of the formed porous zone (Fig. 2.1), or the possibility of the 3D separation of the whole porous zone (Fig. 2.2) are examples from the original research of the author.

Additionally, thanks to the use of specialist dedicated software to analyse the findings, results and information, impossible with other methods, can be obtained. The obtained findings may be the basis for the verification of the adopted model assumptions in the context of numerical modelling. Examples of the application of the computer tomography in high-temperature research are shown in papers [6, 7, 21, 58, 81, 106]. The authors of [81] used the tomographic analysis method to directly analyse the deformation zone of a steel sample deformed with a solid phase share of 55–65 %. On the other hand, the paper by [21] is very interesting from the perspective of this monograph. The scope of the performed tests covered physical simulations with a Gleeble 3500 simulator and numerical simulations of the deformation of an Al–Cu alloy. Everything was complemented by methodology aided by the computer tomography for determining the function describing changes in stress versus strain, strain rate and temperature. To describe, the authors used the following equation form [21]:

Fig. 2.2 A 3D view of a separated porous zone (carbon steel)



$$\sigma(\varepsilon, \dot{\varepsilon}, T) = K(\varepsilon, \dot{\varepsilon}, T) \varepsilon^{m(T)} \dot{\varepsilon}^{n(T)} \quad (2.6)$$

where σ is the stress, ε is the plastic strain, $\dot{\varepsilon}$ is the strain rate, K is the flow stress coefficient, m is the strain hardening factor and n is the strain rate sensitivity factor.

The development of the continuous casting practice, in particular of the twin-roll strip casting process, which is the most important for the industry, continues [13, 18, 29–39, 65, 83, 84, 100, 107, 113, 115]. The development of the continuous casting practice is focused on the manufacturing of near net shape products. This tendency is conditioned by business considerations and competition in the market, and indirectly obviously by advantageous environmental impact. Many factors influence the internal state of the strip cast in the continuous process. The most important are: the degree of superheating, casting speed, characteristics of heat flow between the solidifying shell and the rolls, characteristics of the flow of the liquid metal feeding the mould [98]. Physical conditions, in which the cast strand solidification process occurs, very strongly determine its future state, including such features as the share of individual crystalline zones, the distance between dendrite branches, the austenite grain size, microsegregation and macrosegregation degree, and also the type and arrangement of cracks, or the level of internal stress. These features significantly influence the product quality. Therefore, they must be controlled by the appropriate selection of process parameters, and by the impact on the liquid steel during the process. By focusing on the secondary cooling zone effects, vital for the formation of the cast strand quality parameters, one can find that—from

a mechanical point of view, and also due to the heat flow nature—it is the most complex stage of the process. Within a cast strand we can distinguish the solidified outer layer (shell), the partially solidified mushy zone and the central liquid area, which are characterised by diversified physico-chemical properties. In these conditions the plastic behaviour of the medium considerably differs from the one that is commonly observed, for instance in the hot working processes. The prerequisite for numerical simulations of the changes in the temperature field and stress in a cast strand is to have functions describing the dependence of the thermophysical constants on temperature and the stress–strain relationship for diversified strain conditions. Without this data the numerical simulation of the casting and rolling process cannot be conducted with sufficient accuracy. In this case, it is necessary to apply a simplified approach to continuous casting physical simulation problems—to set linear functions of temperature changes versus time—developed approximately on the basis of temperature measurements carried out at continuous casting facilities [108].

In recent years many companies worked on the development of the rolling process with a semi-solid core. Whilst thin strip casting combined with subsequent rolling is a simple, improved method of the conventional rolling process, rolling a strip, in which both the solid and the liquid phases coexist, is a new process. Cold rolling following simple strand casting is a long process and it is not cost-effective because of energy reasons. For the technological reasons the process should be developed to simplify or eliminate some operations, which would drastically reduce the energy costs. It also involves beneficial environmental impact, due to the reduction of gas emissions. Processes of casting immediately followed by rolling have various versions, which depend on the applying companies and differ with details of industrial installations. A few concepts have been developed by such companies as SMS Demag AG, VAI (Voest Alpine) or Tippins Incorporated. The selected installations include [91]:

- CSP (Compact Strip Production),
- LCR (Liquid Core Reduction),
- ISP (Inline Strip Production),
- AST (Arvedi Steel Technology),
- CONROLL (Continuous thin casting Rolling Technology),
- TSP (Tippins Samsung Process),
- CONROLL (Continuous thin casting Rolling Technology),
- CPR (Casting Pressure Rolling),
- DSC (Direct Strip Casting),
- “Danieli” (Thin slab caster),
- QSP (Quality Strip Production),
- UTHS (Ultra Thin Hot-Strip),
- SMI (Sumitomo heavy industries and Mitsubishi heavy Industries),
- ESP (Endless Strip Production).

The presented state of the art indicates shortage of mathematical models describing comprehensively the process of deformation of strands with a semi-solid core. However, the need of controlled rolling of cast strands is pointed out. Therefore, the results of a computer simulation or physical simulation of the analysed process will be useful to control the process parameters. Creating the modelling concept integrating the physical and computer simulation areas with simultaneous full or partial information exchange between those areas is pioneering in terms of theory.

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Chapter 3

Aim of the Study

The conducted literature analysis concerning the current state of experimental and modelling research on the steel deformation processes in conditions of solid and liquid phase coexistence indicates that there is a considerable interest in these issues. The continuously growing demand for high quality products obtained by metal working forces us to look for new manufacturing processes, providing top quality products while minimising manufacturing costs, including the costs of preparation of new procedures of integrated casting and rolling of strands with a semi-solid core. The study carried out by the author on both physical and computer simulation of steel deformation within the range of the liquid and solid phase coexistence, allows one to propose the following thesis of the study:

The formulated mathematical models of the steel deformation process in conditions of liquid and solid phase coexistence, based upon the results of physical simulations allow one to predict their mechanical properties, and to theoretically design new processes of integrated casting and rolling of strands with a semi-solid core.

On the basis of the following thesis, the main objective of the study was formulated. It is: *to develop innovative modelling concepts integrating areas of physical and computer simulation and at the same time to provide full or partial exchange of information between those areas.*

The accomplishment of the assumed objective was carried out by:

1. Developing the model concept of experimental research methodology for the possibilities of determining the material characteristics, and physical simulations of industrial processes of integrated casting and rolling, with a modern thermo-mechanical Gleeble 3800 simulator. The research was combined with macrostructural and microstructural tests.
2. Developing advanced thermo-mechanical models of deformations of steel samples with a solidifying core, to predict plastic flow kinetics, changes in strains and temperature during deformation under conditions of liquid and solid phase coexistence.

3. Developing the ONEDES (**ONEDE**cision**S**oftware) concept and designing the advanced DEFFEM simulation system, which implements the developed mathematical models. The simulation system was equipped with interactive pre- and post-processing, including an advanced visualisation of the obtained results in the form of vector and scalar fields.
4. Developing fundamental research methodology with the use of the Gleeble 3800 simulator for the purposes of identification of the model parameters and verification of the formulated mathematical models. The research was combined with macro- and micro-structural tests, and with tomographic tests for analysis of the obtained shape of the porous zone.
5. Developing the DIM (Direct Identification Methodology) and NIM (Numerical Identification Methodology) for determining the parameters of a function describing the dependence of stress on strain. The developed methodologies use the capabilities of modern thermo-mechanical Gleeble series simulators and the developed simulation system DEFFEM.
6. Experimental verification of the developed numerical models for predicting the strain and temperature fields, and evaluation of the possibilities for application of the developed models in future research and development projects.

Chapter 4

Integration of Physical and Computer Simulation

This chapter presents main assumptions and component modules of a concept integrating physical and computer simulation areas. The proposed approach utilizes capabilities of modern thermo-mechanical simulators of Gleeble 3800 series in the modelling of steel deformation processes in the semi-solid state [1, 2], as well as in the modelling of integrated casting and rolling processes of flat strands with a solidifying core. Other components, which are necessary and unique in the global scale, are mathematical models including a hybrid-analytical model of steel deformation in the condition of the liquid and solid phase coexistence for the axially symmetrical state, which constitutes the main foundation of the developed modelling concept, and mathematical models in the form of 3D solutions. The whole modelling approach is complemented by the utilization of modern testing and measurement instruments to verify the formulated mathematical models, or to obtain additional information that cannot be obtained with traditional methods.

4.1 Characteristics of the Integrated Modelling Concept

The continuous development of computer technologies has brought about the common access to professional simulation systems [1]. The quality of the obtained simulation results depends on two main factors: the software quality and the user experience. For the former, the accuracy of the adopted mathematical model and the method of its solution is an essential aspect. For the latter, the correct selection of boundary and initial process conditions, and the appropriate selection of parameters, which control the numerical model operation, are vital. Lack of the user experience regarding the evaluation of the simulation course often causes very low quality results. Computer simulations require also a profound knowledge of the process modelled. This knowledge allows one to concentrate on the most important factors and the evaluation of their impact on the process course. The diversity of the commercial software for metal forming or heat transfer simulations that is available

in the market causes difficulties in the selection of appropriate software. Based on the author experience the selection itself is often a trade-off between the functionality of a given simulation system and its capabilities [1]. It is for instance the analysis of steel deformation processes under conditions where its solidification process has not been fully completed yet. A number of practices known jointly as Integrated Strip Casting and Rolling Processes are processes of this type. Such processes, integrating steel strand casting with their subsequent plastic working, constitute one of the modern trends in the steel product manufacturing process development. The solution of the most important engineering problems related to the integrated casting and rolling process of flat strands with the solidifying core is related to the need for determining the course of basic material characteristics, which substantially differ from the ones we deal with at lower temperature ranges. Changes in the steel condition, which occur during steel casting and its direct reduction are so rapid, that they require thorough research of the impact of temperature and strain rate on the mechanical properties of the material. In addition, by utilizing the capabilities of modern thermo-mechanical simulators it became possible to carry out an appropriate experiment, even though it is not simple [2]. However, the test result interpretation is one of the serious problems. It is so, because strength tests cannot be conducted while maintaining a constant temperature and a strain field uniform in the whole area of the sample. Moreover, it is often difficult to determine even the shape of the strain zone itself. A compressed sample shows strong barrelling of central regions (for compression tests) or strong necking (for tensile tests), while the contact areas with the tool are virtually undeformed. It is caused by an extremely strong dependence of the yield stress on the temperature in the conditions of the solid and semi-solid phase coexistence. The results of an experiment like this can only be interpreted with the participation of computer simulation of strength tests performed with the Gleeble 3800 simulator. The concept of modelling integrating the physical and computer simulation areas with simultaneous full or partial information exchange between these areas is presented in Fig. 4.1.

The concept structure consists of six main layers (Fig. 4.1). The layer no.1 is the foundation. This is a hybrid-analytical numerical model, enabling axi-symmetrical samples to be deformed at extra-high temperatures, and in the semi-solid state as well. It is also an important component of the developed NIM (Numerical Identification Methodology) methodology, focused on the complete identification of parameters of the function describing changes of stress versus strain for steel deformed in the semi-solid state.

As the “semi-solid state” hereinafter we refer to the material state able to transfer loads (where within a cohesive solid phase skeleton also the liquid phase coexists).

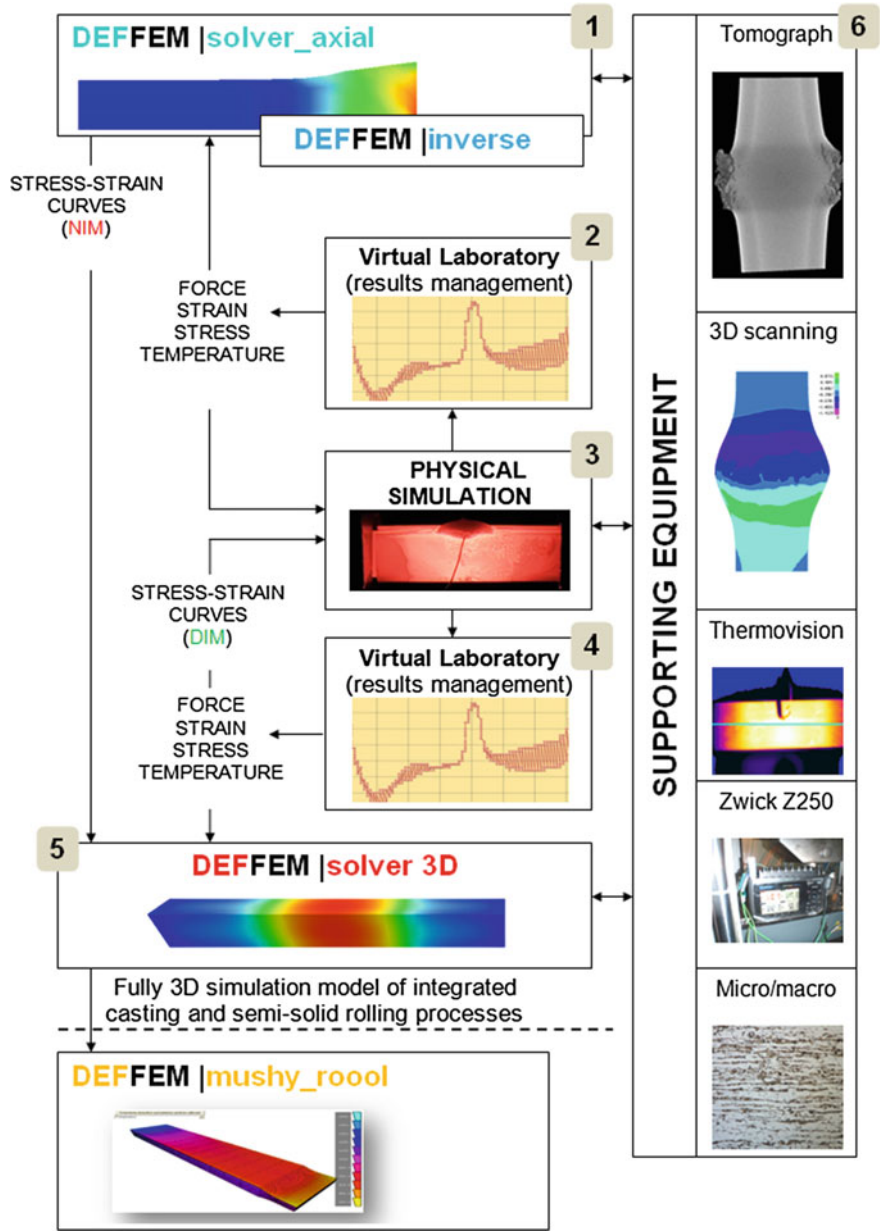


Fig. 4.1 A stratified diagram of the modelling concept (computer simulation, physical simulation)

The Virtual Laboratory constitutes the second and fourth layer intermediary between the mathematical models and the physical simulation layer. The system was designed and adapted to work both online and offline in the web [3–5]. By

using appropriate rooms the user has access to various functions available as part of the developed system. The original assumption was to create the internet system to facilitate physical simulation result management and their easy processing, including experimental data filtration. As shown by tests presented in the Chap. 7, results of physical simulations feature a fairly large scatter of experimental data. Direct utilization of the obtained change courses, e.g. stress-strain curves in the DEFFEM simulation system is impossible. Therefore as part of the project data approximation algorithms and three data filtration algorithms were implemented:

1. Moving arithmetic average filter.
2. Arithmetic average filter.
3. Median filter.

The moving arithmetic average method is applied to smooth stationary time courses. The advantage of this method is the systematic elimination of data values significantly diverging from the neighbouring data. The moving average method assigns more significance to newer data, so that only N of last data is significant, whereas other earlier data are insignificant. Therefore, it was assumed that the last N data is relevant in this case. The moving average MM at time T may be determined on the basis of arithmetic average of N last data, where N is the data frame. The moving average is just the arithmetic average of N data. It is however important that the number of data that we take into account is constant, while the item from which the tests are significant changes. This can be presented as follows:

$$MM = \frac{y_T + y_{T-1} + y_{T-2} + \dots + y_{T-N+1}}{N} \quad (4.1)$$

The arithmetic average method is a modified moving average method, enhanced by a mechanism of averaging of data, which are next taken into account. Thus the data amount is reduced proportionally to the size of the frame we take into account. On the other hand, the median filter is a non-linear filter, which selects the central value of an ascending sequence of values of the process point and its neighbourhood. The filter is applied to remove points significantly diverging from the average value of the tested area, which are completely omitted when a new point value is created. Figure 4.2 presents examples of effects of operation of the implemented data filtration algorithms on the basis of a test actual data set obtained from the Gleeble 3800 simulator (Fig. 4.2a).

The Virtual Laboratory also contains a room with the modelled virtual Gleeble 3800 simulator (Fig. 4.3), coupled with a check sheet generator for the DEFFEM simulation system [1]. With this solution we can interactively prepare the structure of the input file for the needs of the computer simulation. The further development of the Virtual Laboratory is focused on coupling solvers included in the DEFFEM package with the virtual simulator and the possibility of direct online simulation [6].

Analysing the diagram presented in Fig. 4.1 we can indicate three more layers within the developed modelling concept. The layer no.3 is the physical simulation area. This area includes the determination of a number of material characteristics,

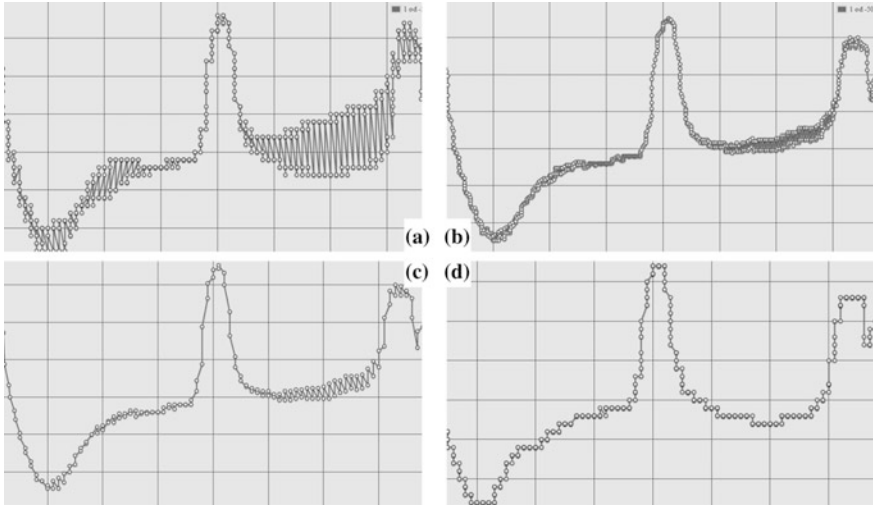
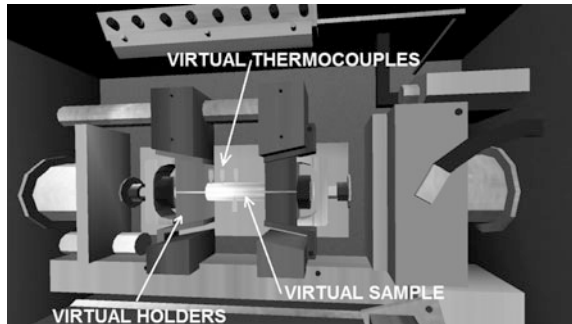


Fig. 4.2 The Gleeble 3800 simulator data before filtration (a), data after filtration with the moving arithmetic average algorithm for the area value $N = 5$ (b), data after filtration with the arithmetic average algorithm for the area value $N = 5$ (c), data after filtration with the median algorithm for the area value $N = 8$ (d)

Fig. 4.3 Virtual thermo-mechanical simulator Gleeble 3800



physical simulations of integrated casting and rolling of strands with a semi-solid core, simulations of heating combined with melting or simulations of deformation of samples with a semi-solid core by compression and tension. This area may also be supported with information obtained both from layer no.1 (hybrid model), as well as layer no.5 (3D model). For instance, utilizing the developed resistance heating model for a 3D space, one can analyse the obtained remelting zone, and thus estimate the shape of 3D mushy zone on the basis of various temperature heating/remelting programmes. On the other hand, information obtained by physical simulation allows us to assess the numerical modelling suitability (as well as to

verify the developed numerical models). The final layer no.6 is the modern additional instrumentation supporting the modelling work, e.g. a computer tomograph enabling samples to be non-destructively analysed for determination of estimated shape and size of the porous zone and its qualitative analysis in terms of determination of the selected characteristics. The simulations are additionally complemented by micro- and macrostructural tests, and 3D scanning systems for their application among others to validate the developed mathematical models.

4.2 Hybrid Analytical-Numerical Model of Mushy Steel Deformation

A mathematical model of the compression and tension process is based on the theory of plastic flow [7]. The principle of the upper assessment [8], calculus of variations [9], approximation theory and optimization methods [10, 11] and numerical methods for solving partial differential equations [12], including the finite element method [13], were used. The mathematical model of the compression and tension process is based upon a number of assumptions [1, 2, 14, 15]. The mathematical model itself contains three main sub-models: a resistance heating model for predicting temperature changes within the sample volume, a compression or tension model and an empirical density change model. The correct definition of boundary and initial conditions of the process analysed is an intrinsic component of the mathematical model. For the case concerned the boundary and initial conditions are adapted on the basis of physical tests carried out with a Gleeble 3800 thermo-mechanical simulator as well as Zwick Z250 machine [1].

It was assumed that the strain and stress state is axi-symmetrical.

This assumption will be correct provided that the physical simulations are performed in order to obtain the deformation zone (also in the case of temperature field for a thermal model) as close to the axially symmetrical state as possible.

Next, we assume the material deformed as isotropic and the material model as rigid-plastic. The relationships between the stress tensor and the strain rate tensor were determined from the Levy-Mises law. This dependence is presented with the following equation:

$$\sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij} = \frac{2}{3} \frac{\sigma_p}{\dot{\epsilon}_i} \dot{\epsilon}_{ij} \quad (4.2)$$

Transition into the plastic state is defined by the Huber-Mises condition:

$$\sigma_{ij}\sigma_{ij} = 2\left(\frac{\sigma_p}{\sqrt{3}}\right)^2 \quad (4.3)$$

In Eqs. (4.2) and (4.3) σ_{ij} denotes the stress tensor components, σ_{kk} represents the mean stress, δ_{ij} is the Kronecker delta, σ_p indicates the yield stress, $\dot{\epsilon}_i$ is the effective strain rate, and $\dot{\epsilon}_{ij}$ denotes strain rate tensor components. The rigid-plastic solution is based on the optimisation of the power functional, which consists of three main parts:

$$W[\mathbf{v}] = W_\sigma + W_\lambda + W_t \quad (4.4)$$

In the presented Eq. (4.4) the first term W_σ is the plastic strain power, W_λ is the power being the penalty for not fulfilling the non-compressibility condition for the solid areas of the sample, or the condition of controlled compressibility for the areas being in the semi-solid state, whereas W_t is the friction force power. The solution searched by the functional (4.4) optimisation is the velocity field $\mathbf{v}(v_r, v_\theta, v_z)$ in the cylindrical coordinate system.

A high accuracy in fulfilling the constant or controlled volume condition is required in the proposed solution. This approach arises from the fact, that errors caused by not fulfilling these conditions may be comparable with the volume changes caused by the variable metal density in the mushy zone. Also because of large differences in the yield stress for individual sub-areas of the deformation zone, which in the temperature range in question are caused by even slight temperature fluctuations, and related difficulties in meeting the non-compressibility condition, this condition was included in the analytical form, which makes the solution more complicated, but substantially improves its accuracy.

Therefore, in Eq. (4.4) there is no other component of equation W_λ , and the velocity fields $\mathbf{v}(v_r, v_\theta, v_z)$ are searched for by optimisation of the power functional comprising two terms:

$$W[\mathbf{v}(v_r, v_\theta, v_z)] = W_\sigma + W_t \quad (4.5)$$

For the mushy zone the controlled compressibility condition is described by the following equation [1, 2]:

$$\frac{\partial v_r}{\partial r} + \frac{v_r}{r} + \frac{\partial v_z}{\partial z} - \frac{1}{\rho} \frac{\partial \rho}{\partial \tau} = 0 \quad (4.6)$$

Equation (4.6) assumes also the specific form to define the non-compressibility condition for the solid zones. A situation like this will occur when the derivative in the fourth term of Eq. (4.6) is zero. The first term W_σ of the power functional (4.5) responsible for the plastic strain power is given by the relationship:

$$W_\sigma = \int_V \sigma_i \dot{\epsilon}_i dV \quad (4.7)$$

where σ_i is the effective stress and $\dot{\epsilon}_i$ denotes the effective strain rate. The plastic deformation starts when the rising of the effective stress has reached the yield stress limit σ_p ($\sigma_i = \sigma_p$). The effective strain occurring in Eq. (4.7) is calculated on the basis of the strain tensor components $\dot{\epsilon}_{ij}$ according to following relationship:

$$\dot{\epsilon}_i = \sqrt{\frac{2}{3} \dot{\epsilon}_{ij} \dot{\epsilon}_{ij}} \quad (4.8)$$

The strain rate tensor, strain and material flow at any process time was determined utilizing the following relationships, based upon the previously determined velocity field from the condition of the functional minimum (4.5):

$$\dot{\epsilon}_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \quad (4.9)$$

$$\epsilon_{ij} = \int_0^\tau \dot{\epsilon}_{ij} d\tau \quad (4.10)$$

$$x_i^k = x_0^k + \int_0^\tau v_i^k d\tau k = 1, 2, \dots, n \quad (4.11)$$

The strain rate tensor existing in Eq. (4.9) assumes the following form for the axially symmetrical strain state:

$$\begin{pmatrix} \frac{\partial v_r}{\partial r} & 0 & \frac{1}{2} \frac{\partial v_r}{\partial z} + \frac{1}{2} \frac{\partial v_z}{\partial r} \\ 0 & \frac{v_r}{r} & 0 \\ \frac{1}{2} \frac{\partial v_r}{\partial z} + \frac{1}{2} \frac{\partial v_z}{\partial r} & 0 & \frac{\partial v_z}{\partial z} \end{pmatrix} \quad (4.12)$$

The second term present in functional (4.5) is the term W_t responsible for the friction force power. In order to find the friction power at the contact face of the sample and the deforming tool, the following relationship was utilized:

$$W_t = \int_S m \frac{\sigma_p}{\sqrt{3}} \|\bar{\mathbf{v}}\| dS \quad (4.13)$$

In Eq. (4.13) m is the friction factor, $\bar{\mathbf{v}}$ is the vector of relative velocity of metal and tool $\bar{\mathbf{v}} = \mathbf{v} - \mathbf{v}_t$. For the adaptation of the presented model for the sample deformation simulation with the Gleeble 3800 unit, the friction power term may be neglected, and functional (4.5) may be simplified to the form:

$$W[\mathbf{v}(v_r, v_\theta, v_z)] = W_\sigma \quad (4.14)$$

It arises from the specificity of the main strain setting unit in the Gleeble 3800 simulator system, where cylindrical samples or hexahedral samples proposed by the author as part of the methodology for validating 3D mathematical models are permanently secured in tools. However, in the context of developing a computer-aided comprehensive methodology for determining parameters of functions describing the changes of stress versus strain, the term W_t was included. It is essential for inverse calculations performed on the basis of experimental data determined with a Zwick Z250 testing machine within a temperature range characteristic to hot forming processes. For this unit, cylindrical samples are upset with flat anvils, where the friction impact is relevant in the context of metal flow diagram during the deformation. The obtaining of an accurate velocity field requires application of complex velocity functions with a large number of variation parameters. Determining each component of the velocity field with a single function in the whole deformation area is not advantageous. Such an approach poses difficulties in particular in non-deformed areas, where velocity functions should remain constant. Therefore the solution to the problem of metal flow in the semi-solid state was based upon the method of strand velocity fields proposed by Malinowski in papers [14, 16]. This method assumes that the deformation area is divided into elements and the velocity field is approximated with various polynomials in individual elements.

The stress field model is based upon the solution to the Navier equilibrium equation:

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \quad (4.15)$$

combined with Levy-Mises equations. In turn the temperature field model is based on the solution of the Fourier-Kirchhoff equation, which in general can be presented as follows:

$$\nabla^T(\lambda \nabla)T + \left(Q - c_p \rho \frac{\partial T}{\partial \tau}\right) = 0 \quad (4.16)$$

In Eq. (4.16) T is the temperature, λ is the thermal conductivity, Q is the heat generation rate, ρ is the density, c_p is the specific heat and τ is the time. A detailed

expansion of the hybrid model was presented in a previous monograph co-written by the author [2] and in industry journals [17–19].

4.2.1 Resistance Heating Model

In the cylindrical coordinate system it is possible to determine the temperature field for a heated sample by solving the Fourier equation, which for an axi-symmetrical non-stationary process may be described by the following equation [1, 2]:

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \lambda_r \frac{\partial T}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left(\frac{1}{r} \lambda_\theta \frac{\partial T}{\partial \theta} \right) + \frac{\partial}{\partial z} \left(\lambda_z \frac{\partial T}{\partial z} \right) + Q = \rho c_p \frac{\partial T}{\partial \tau} \quad (4.17)$$

In Eq. (4.17) T is the temperature, λ is the thermal conductivity, Q is the heat generation rate, ρ is the density, c_p is the specific heat and τ is the time. Assuming the axial symmetry of the process:

$$\frac{\partial T}{\partial \theta} = 0 \quad (4.18)$$

and isotropy of thermal properties of the medium:

$$\lambda_r = \lambda_\theta = \lambda_z = \lambda \quad (4.19)$$

in effect we obtain the following equation form:

$$\lambda \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} \right) + Q = \rho c_p \frac{\partial T}{\partial \tau} \quad (4.20)$$

The application of weighted residual method [1, 2] brings Eq. (4.20) to the system of ordinary differential equations:

$$\mathbf{H}T + \mathbf{M} \frac{\partial T}{\partial \tau} + \mathbf{p} = \mathbf{0} \quad (4.21)$$

where:

$$\begin{aligned} \mathbf{H} &= \int_V r \lambda \left(\frac{\partial \mathbf{n}}{\partial r} \frac{\partial \mathbf{n}^T}{\partial r} + \frac{\partial \mathbf{n}}{\partial z} \frac{\partial \mathbf{n}^T}{\partial z} \right) dV + \int_S \alpha \mathbf{n} \mathbf{n}^T dS \\ \mathbf{p} &= - \int_V r Q \mathbf{n} dV - \int_S (\alpha T_{env} - q) \mathbf{n} dS \\ \mathbf{M} &= \int_V \rho c_p \mathbf{n} \mathbf{n}^T dV \end{aligned} \quad (4.22)$$

Assuming the linear temperature change over time $\Delta\tau$ and applying the Galerkin integration method [1, 2] the following relationship is obtained:

$$\bar{H}T_{i+1} + \bar{p} = 0 \quad (4.23)$$

where:

$$\begin{aligned} \bar{H} &= \left(2H + \frac{3}{\Delta\tau} M \right) \\ \bar{p} &= \left(H - \frac{3}{\Delta\tau} M \right) T_i + 3p \end{aligned} \quad (4.24)$$

Expression (4.23) is a system of algebraic equations, allowing the nodal temperature vector values T_{i+1} to be computed with respect to time $\Delta\tau$, with a set temperature vector T_i at the time $\tau = 0$. The accuracy of a solution based on the foregoing model of temperature distribution in the material during heating and cooling depends primarily on the correct determination of the boundary conditions necessary to solve the heat flow problem. Equation (4.20) must be complemented with boundary conditions (see Chap. 8). The next component of the resistance heating model is the method of taking into account the liberated heat resulting from the current flow (see Chap. 8).

4.3 “One Decision Software”—The DEFFEM Package

The continuous development of computer technologies forces the contemporary engineer to use a computer and the appropriate software to support engineering work in designing new practices. Nowadays, the market offers a broad range of software dedicated to both a broad circle of specialists—e.g. ANSYS [20], ADINA [21], and to a narrow group of specialists in specific fields—stamping simulations e.g. DYNAFORM [22]. The launch of the Gleeble series thermomechanical simulators in recent years, which enable deformations to be set in conditions of coexistence of the solid and liquid phase, involves the need to develop computer programs for supporting engineering work with these units [1]. As part of the research and development work conducted by the author of this monograph, an original simulation DEFFEM package was developed and applied in practice, among others, to support engineering work performed with a Gleeble 3800 thermomechanical simulator or a Zwick Z250 testing machine [1].

The proposed ONEDES (**ONEDE**cisionSoftware) approach is based on the assumption that a set of independent tools comprising the DEFFEM package is developed to enable a virtual deformation test to be carried out in a wide range of temperatures, in particular in extra-high temperatures near the solidus line,

as well as in conditions of the solid and liquid phase coexistence, without the need to use any commercial applications. The developed simulation package also provides tools oriented at the full identification of the selected parameters of numerical models on the basis of data from physical simulations.

The very process of modelling with the use of the developed DEFFEM package is based upon the editing modelling process using so-called check sheets [1]. The check sheets are a certain data structure, assumed in advance, defining e.g. a specific material model or checking the integration step. An example of a complete structure based upon check sheets is presented in Fig. 4.4. A check sheet structure

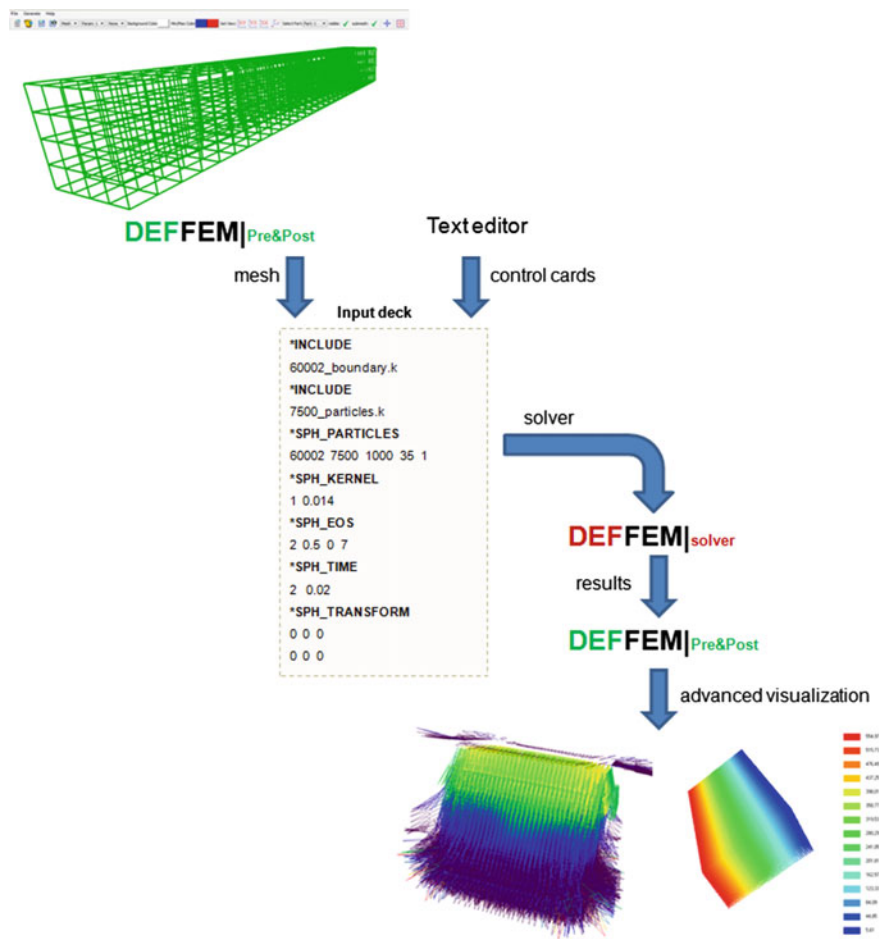


Fig. 4.4 Modelling approach with the DEFFEM package

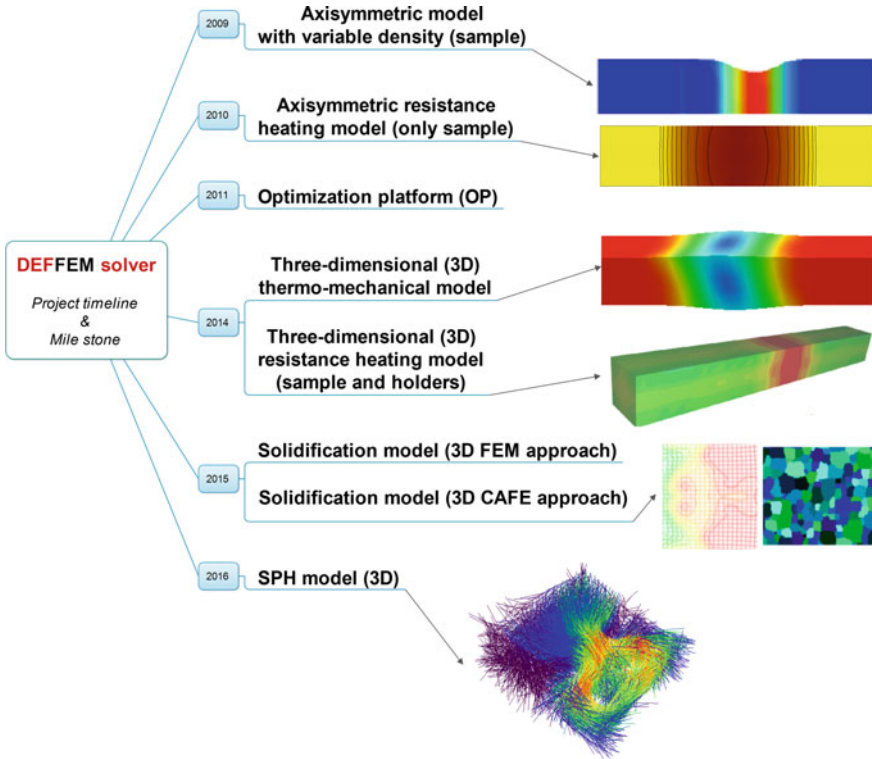


Fig. 4.5 Milestones in the solver development

prepared like this defines the process unambiguously, and constitutes a complete data set, necessary to conduct a simulation. Then, the very process of generating finite element meshes or the visualisation of findings is executed by the Preprocessor and Postprocessor module (Fig. 4.4).

The history of package development goes back to 2009, when work on the first solver version was completed [17–19]. R&D projects conducted in the subsequent years as regards the solver development were oriented at the development of numerical models for elaborating on the behaviour of the medium analysed at various observation levels. The main milestones in the solver development are presented in Fig. 4.5.

In parallel with designing such an advanced simulation tool, the development of visualisation tools and the analysis of findings are being implemented. Advanced numerical algorithms have been developed for plotting the isolines of scalar fields, visualising vector fields, or enabling stereoscopic data to be visualised (Fig. 4.6). Stereoscopy is not a new technology, however during the last few years we have observed a further growth in the interest in these imaging techniques thanks to the development of computer and audio-visual technology.

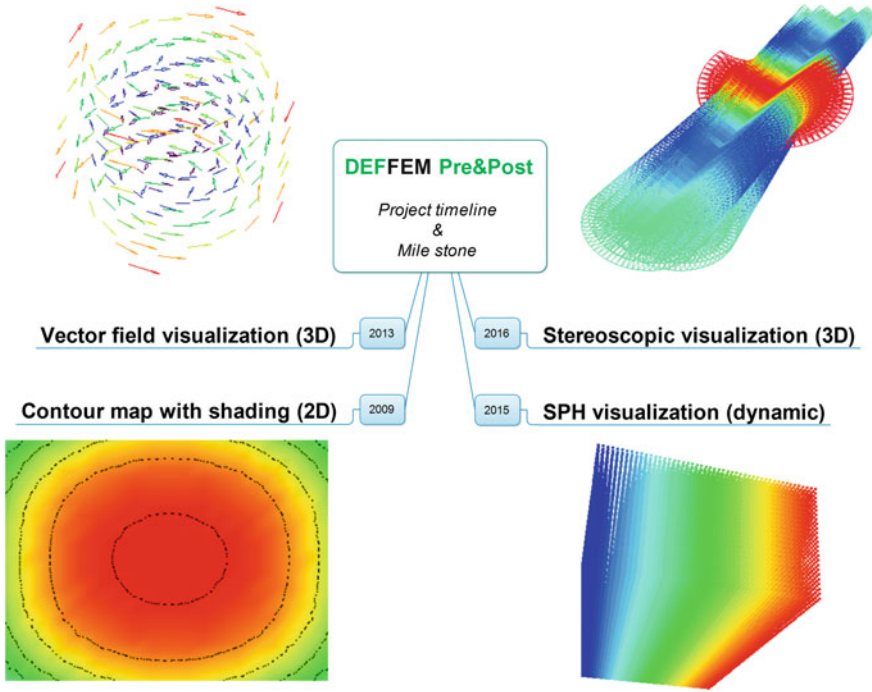


Fig. 4.6 Milestones in Pre&Postprocessor development

Due to the complexity of the problem, this monograph does not cover Pre&Postprocessor engineering. However, from the perspective of the design of dedicated simulation systems, it is a very important issue and must not be neglected. These issues were elaborated by the author in his previous monograph [1]. This monograph includes solutions, which may turn out to be the most interesting from the perspective of the development and efficiency of computer hardware. Issues concerning the visualisation of simulation results with 3D imaging technologies, and the rapid generation of vector fields with the GLSL graphic pipeline programming language, as well as scalar fields using the OpenGL library are presented. The presented technologies and methods for designing modern Pre&Postprocessors, along with the examples of the implementation in the selected programming languages, may be the basis for the independent design and implementation of a simple computer simulation system for the selected physical phenomena.

4.4 Summary

This chapter presents main assumptions of a concept integrating physical and computer simulation areas as well as the ONEDES (**ONEDE**cision**S**oftware) approach, which is the basis for the original computer simulation system oriented at

the processes of deformation in extra-high temperatures, as well as in the conditions of the liquid and solid phase coexistence. The presented DEFFEM package constitutes an integral part of the developed strategies of modelling effects accompanying steel deformation in the conditions of the liquid and solid phase coexistence. All results of numerical calculations and their visualisation within this monograph were performed with the said software.

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Chapter 5

Spatial Solutions Based on the Particle Method

This chapter presents a numerical model of fluid flow simulation on the basis of the smoothed particle method (SPH). The formulated model constitutes the foundation of a new conceptual hybrid model combining the advantages of the finite element method and mesh-free methods. Examples of test simulations were presented, and the implemented model in the DEFFEM system was validated by comparing the obtained simulation results with the analytical solution based on the common laws of physics. The section is concluded with a short summary including a description of the concept of hybrid model development in the context of steel deformation in conditions of liquid and solid phase coexistence.

5.1 Introduction

The SPH method was first developed by [1, 2] to solve astrophysical problems in a three dimensional open space. In recent years, considerable progress in the development of solutions using meshless methods has been achieved, enabling phenomena occurring in many areas, including the description of metallurgical processes such as solidification [3], to be simulated. In many cases, both in industry and science, the issues concern fluid mechanics. The scale of the phenomena studied is very wide, from micro- through meso-, ending at the macro-level. With this approach, it is possible to consider many interesting phenomena that occur at the connection of scales, such as multiphase flows [4] or a turbulent flow [5]. One of the most commonly used methods for simulating the behaviour of fluids and their flow is called the particle method. Smoothed Particle Hydrodynamics (SPH) is a method of this type. In the SPH method [6], the Lagrangian approach is applied to describe the fluid, where calculation points move together with the flowing liquid as opposed to Euler's approach, wherein the calculation points do not change their positions. Simulation of the behaviour of real fluids using computer modelling is of great importance both for industry [7] and for the development of science in many

fields. Research is being conducted on the use of the SPH method to simulate many industrial processes such as: forecasting the metal flow in the process of high-pressure casting of components for the automotive industry [8], aviation [9], as well as the power sector [10]. Another example is the use of the SPH method using commercial software like LS-DYNA to simulate the aluminium flow in a foundry mould [11, 12]. A description of the behaviour of fluids, including multiphase fluids, is extremely important for many technical applications, including those in the metal industry. Such models should take into account the complexity of the simulated systems. Due to their complex nature, systems of this type can cause many problems with the proper simulation of thermodynamic parameters, and the assumption of an adequate flow in systems of vessels with complex shapes. The interesting, and yet at the same time complicated behaviour of fluids is primarily due to the interaction processes. The SPH method, thanks to its high flexibility, is widely used not only for modelling flows (including multiphase) of the liquid, but also to describe the behaviour of solids—heat conductivity, or problems accompanying explosions. Modern models of fluids, which allow the issues concerned to be simulated with acceptable accuracy, due to their high complexity are difficult to design and implement. The use of modern computer architecture and customised algorithms is required to obtain reasonable computing time to enable these methods to be useful. The authors of the publication [13] presented the application of the SPH method to simulate the solidification process. The research was conducted for a single-component fluid and a two-component mixture. After verification of the results for the case of a single-component alloy, an attempt to simulate a two-component alloy was made. The simulation results were verified with the experiment. The SPH method is also used for the modelling of deformation processes such as metal forging, where large deformation of the material occurs, causing serious problems in using mesh methods like the Finite Element Method (FEM). The authors of the publication [14] indicated that the SPH was a useful simulation method that allowed them to obtain information on the deformable material and the flow of material while forging real industrial components. Through the simulation process, the quality of the final product and the impact of process parameters and material properties were established. Also the force needed to sufficiently fill the mould cavity and the effect of the hardening material, which gives the final product its quality, were defined. The method also allowed the prediction of defects such as failure to fill the forging die. The SPH method can thus also be potentially used to assess the quality of forged products.

The authors of the publication [15] successfully applied the SPH method to simulate the fluid flow in an isotropic porous material. The porous structure is defined in the mesoscopic scale by randomly assigning some particles with fixed positions. The designated flow field, calculated at a steady state of the two-dimensional isotropic system, provides information on the macroscopic fluid flow. Meshless methods are widely used in modelling problems with a large deformation or a loss of material cohesion. In the publication [16], the authors use

the SPH method to present a model of material cutting. Preliminary studies for the two-dimensional model have shown the suitability of the method to correctly estimate shear forces, as shown in several examples of the perpendicular cut. Finally, the modelling of cutting forces in a three-dimensional space was performed. In many cases of simulations of complex physical processes, it is reasonable to apply a hybrid method combining the Finite Element Method and meshless methods. To combine both methods, it is required to determine the interactions between the models. The authors of the publication [17] describe several methods of interaction and their combinations in order to obtain satisfactory results. The discussion on the interaction between Lagrangian elements and the particles of the SPH method was included. Sample calculations and the usage of appropriate algorithms were exemplified by a commercial program. In the paper [18], an overview of methods allowing the coupling of the meshless methods with the Finite Element Method was presented. One of them is the coupled master-slave type, wherein the particles are associated with the nodes of the finite element mesh. The coupling, through the interaction of particles with the nodes of the element mesh and vice versa, is satisfactory. Finally, many static and dynamic problems were tested, comparing the results to the experimental data. Another example of coupling of the Finite Element Method with a meshless method is studying the structural resistance to destruction. In the publication [19], to verify the established thesis, the problem of the hydrostatic pressure simulation was also considered. Taking into account the wide use of the SPH method to model phenomena in many fields including metallurgical processes, it is possible to determine the flow of material during the solidification of a slab manufactured in the continuous casting process.

5.2 The Smoothed Particle Hydrodynamics (SPH) Method

The fluid medium in the SPH method is represented by a set of particles that can move freely [20]. Particles can carry some physical properties such as, the speed, the density, the pressure, position or the temperature. The value of any function f at a particle can be approximated by summing up the properties of its neighbouring particles. The SPH interpolation of the function f of particle i at position $\mathbf{r}_i$ is approximated by relationship [20, 21]:

$$\langle f(\mathbf{r}_i) \rangle \approx \sum_{j=1}^N \frac{m_j}{\rho_j} f_j W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (5.1)$$

where:

- m_j and ρ_j are the mass and the density for particle j , respectively,
- W is the smoothing kernel,
- index j corresponds to any neighbouring particle of particle i ,
- f_j is the value of f for particle j ,

- N is the total number of particles,
- h is the smoothing length that defines the radius of influence around the current particle i .

In Eq. (5.1) the value of a function at the position of particle i is given by the weighted sum over the values of the same function at the position of the neighbouring particle j and the sum is weighted by the smoothing kernel W . The gradient of the function f is obtained by differentiating the interpolation Eq. (5.1) which is given by equation [20, 21]:

$$\langle \nabla f(\mathbf{r}_i) \rangle \approx \sum_{j=1}^N \frac{m_j}{\rho_j} f_j \nabla_i W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (5.2)$$

where:

$$\nabla_i W_{ij} = \nabla W(\mathbf{r}_i - \mathbf{r}_j, h) = \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|} G(|\mathbf{r}_i - \mathbf{r}_j|, h) \quad (5.3)$$

and G is the derivative of the kernel function. The definition of the kernel function is represented in:

$$W_{ij} = W(\mathbf{r}_i - \mathbf{r}_j, h) = \frac{1}{h^d} \omega\left(\frac{|\mathbf{r}_i - \mathbf{r}_j|}{h}\right) \quad (5.4)$$

where:

- ω is the function that describes kernel approximation,
- d is the number of space dimensions. There are many kinds of smoothing kernel functions in literature [6, 8, 13, 20, 21]. In the presented implementation, the cubic spline kernel function was chosen [20, 21]:

$$W_{ij} = \alpha_d \begin{cases} \frac{2}{3} - \left(\frac{|\mathbf{r}_i - \mathbf{r}_j|}{h}\right)^2 + \frac{1}{2} \left(\frac{|\mathbf{r}_i - \mathbf{r}_j|}{h}\right)^3, & 0 \leq \frac{|\mathbf{r}_i - \mathbf{r}_j|}{h} < 1 \\ \frac{1}{6} \left(2 - \left(\frac{|\mathbf{r}_i - \mathbf{r}_j|}{h}\right)\right)^3, & 1 \leq \frac{|\mathbf{r}_i - \mathbf{r}_j|}{h} < 2 \\ 0, & 2 \geq \frac{|\mathbf{r}_i - \mathbf{r}_j|}{h} \end{cases} \quad (5.5)$$

where:

- α_d is a constant of normalisation which depends on the number of spatial dimensions [20].

In the presented three dimensional solutions $\alpha_d = \frac{3}{2\pi h^3}$, the radius of influence of this function is $2h$. This means that particle i will not be affected by any neighbouring particles farther than $2h$.

5.2.1 Fluid Model

The governing equations of fluids in the SPH method are based on the Navier-Stokes equations in the Lagrangian form. The main equations are given by [20, 21]:

$$\frac{d\rho}{d\tau} = -\rho \nabla \cdot \mathbf{v} \quad (5.6)$$

$$\rho \frac{d\mathbf{v}}{d\tau} = -\nabla p + \nabla \cdot \boldsymbol{\theta} + \rho \mathbf{F} \quad (5.7)$$

where:

- τ is time,
- $\mathbf{v}$ is velocity,
- p is pressure,
- $\mathbf{F}$ is external force,
- $\boldsymbol{\theta}$ is a second-order tensor containing τ_{ij} stresses.

Equation (5.6) is the continuity equation which describes the evolution of the fluid density over time and Eq. (5.7) is the momentum equation which describes the acceleration of the fluid medium. By employing the SPH interpolation of Eq. (5.2) to (5.6), the SPH representation of the continuity equation can be written as follow [20, 21]:

$$\frac{d\rho_i}{d\tau} = \sum_{j=1}^N m_j (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij} \quad (5.8)$$

Neglecting the friction part $\boldsymbol{\theta}$ and the body forces $\mathbf{F}$ from Eq. (5.7) the momentum equation can be written in the SPH formalism as:

$$\frac{d\mathbf{v}_i}{d\tau} = - \sum_{j=1}^N m_j \left(\frac{p_j}{\rho_j^2} + \frac{p_i}{\rho_i^2} \right) \cdot \nabla_i W_{ij} \quad (5.9)$$

The viscous and body forces (e.g. gravity) can be added to Eq. (5.9) and the momentum equation can be rewritten in the SPH formalism as:

$$\frac{d\mathbf{v}_i}{d\tau} = - \sum_{j=1}^N m_j \left(\frac{p_j}{\rho_j^2} + \frac{p_i}{\rho_i^2} + \Pi_{ij} \right) \cdot \nabla_i W_{ij} + \mathbf{F} \quad (5.10)$$

The viscous force used in this implementation is the viscosity term which was introduced by Monaghan [20] denoted Π_{ij} . Equation (5.10) shows that the change

of the motion of a particle is due to the pressure field, the artificial viscosity and the body forces acting on the fluid. The artificial viscosity Π_{ij} is given by Ref. [20]:

$$\Pi_{ij} = \begin{cases} \frac{-\alpha \bar{c}_{ij} \mu_{ij} + \beta \mu_{ij}^2}{\bar{\rho}_{ij}} & (\mathbf{v}_i - \mathbf{v}_j) \cdot (\mathbf{r}_i - \mathbf{r}_j) < 0 \\ 0 & (\mathbf{v}_i - \mathbf{v}_j) \cdot (\mathbf{r}_i - \mathbf{r}_j) \geq 0 \end{cases} \quad (5.11)$$

where:

- $\bar{c}_{ij}$ is the mean speed of sound of particle i and j ,
- $\bar{\rho}_{ij}$ is the mean density of particle i and j ,

$$\mu_{ij} = \frac{h(\mathbf{v}_i - \mathbf{v}_j) \cdot (\mathbf{r}_i - \mathbf{r}_j)}{(\mathbf{r}_i - \mathbf{r}_j)^2 + \eta^2} \quad (5.12)$$

where:

- $\eta^2 = 0.01h^2$ is a parameter to prevent singularity when $\mathbf{r}_i - \mathbf{r}_j$ goes to zero. The term of Eq. (5.11) associated to produces a bulk and shear viscosity. Coefficients α and β have no physical meaning and they are only used to stabilise solutions and produce a shear force. Monaghan [20] suggests the values be about 2 for β and 1 for α .

An equation of state is required to calculate the pressure in Eq. (5.10). The equation of state used in the presented model is a quasi-compressible form which is calculated by using the density calculation from Eq. (5.8) and is given by Ref. [20]:

$$p = \beta \left[\left(\frac{\rho}{\rho_{ref}} \right)^\gamma - 1 \right] \quad (5.13)$$

where:

- ρ_{ref} is the reference density,
- c is the speed of sound,
- β is the magnitude of pressure and is expressed by:

$$\beta = \frac{c^2 \rho_{ref}}{\gamma} \quad (5.14)$$

where $\gamma = 7$ for liquid steel. The dynamic particle was selected as a definition of boundary conditions [22, 23]. These kind of particles have the same properties as the fluid particles except that the equation of momentum is not solved for them. The time steps can be deduced from the Courant condition, the forces acting on the particles and the viscous forces presented in details by Monaghan [20]. The time integration Runge-Kutta scheme was used for this model.

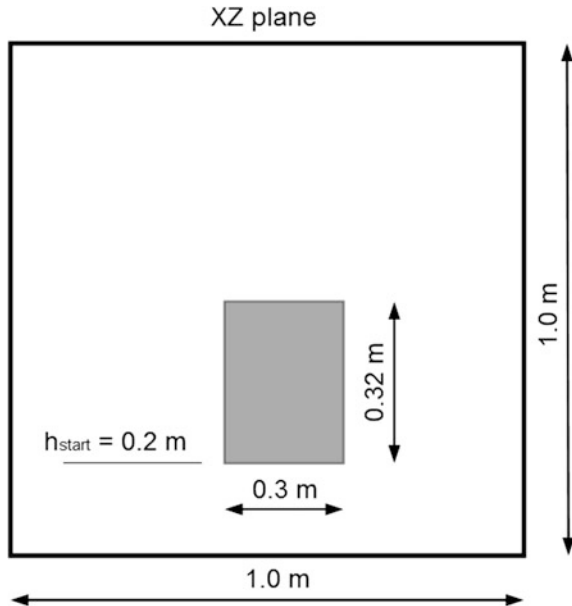
5.3 Test Cases to Validate the Solver

In order to validate the new features of the solver, two test cases were done. The first case of free particles fall was done in order to check the Runge-Kutta integration scheme used in the implementation. The second one is oriented at the structure impact simulation based on dynamic particles. The main return information from this case is: can the dynamic particles handle this kind of boundary condition and the possibility of using such an approach in a mesoscale SPH modelling of the fluid flow in a porous structure.

5.3.1 Free Particles Fall

The scheme of initial geometry in the XZ plane of this problem is presented in Fig. 5.1. The dimensions of the solution domain are given from particle to particle (width = 0.3 m, height = 0.32 m, length = 0.7 m). The solution domain consists of 9792 moving particles. The boundary condition is represented by 60002 dynamic particles as a box given from particle to particle (width = 1.0 m, height = 1.0 m, length = 1.0 m). The initial height h_{start} was set at 0.2 m. Other parameters adopted

Fig. 5.1 The scheme of initial geometry of free particles fall in the XZ plane



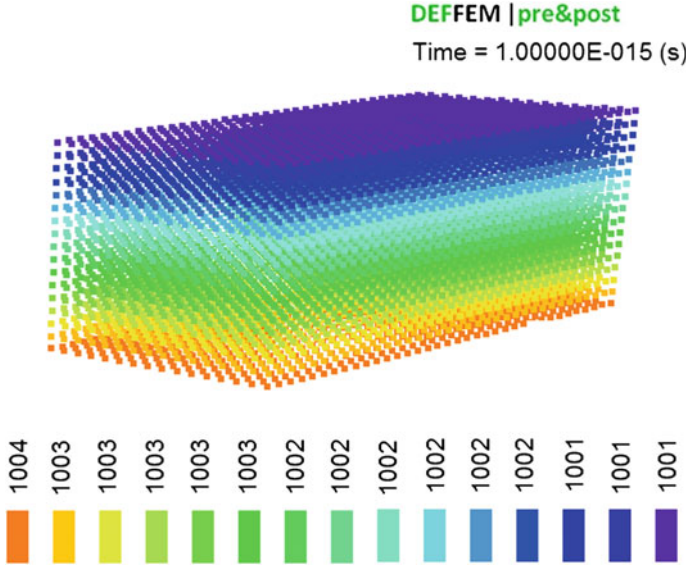


Fig. 5.2 Initial density distribution at the beginning of the simulation (time = 1.0e-15 s)

as: initial smoothing length = 0.024 m, speed of sound 30 m/s, α is equal to 0.5 and the simulation time: 0.65 s.

The initial density distribution is presented in Fig. 5.2. It can be seen that near the liquid surface the density value is smaller. After substituting in Eq. (5.1) ρ as a scalar quantity it leads to a basic formula for the density of the particles i :

$$\rho_i \approx \sum_{j=1}^N m_j W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (5.15)$$

The method for calculating the density according to the above equation is not entirely correct. For example, it can be used for building the initial configuration. This is due to the fact that the number of particles near the surface, which includes the sum in Eq. (5.15), is lower than the number of particles inside the solution domain. Based on Eq. (5.15), it can be seen that the density changes continuously. In real fluids the density changes discontinuously, therefore Eq. (5.8) should be used in the simulations. By using Eq. (5.8) in each time step, the density of the particles is not calculated again, but only the adjustment density is calculated.

In Fig. 5.3 the final density distribution is presented, showing that at the end of the simulation, the fluid and the density stabilise around a given value.

The next example results are presented in Fig. 5.4, where the distribution of vector velocity is shown. The mean particle velocity is around a given value

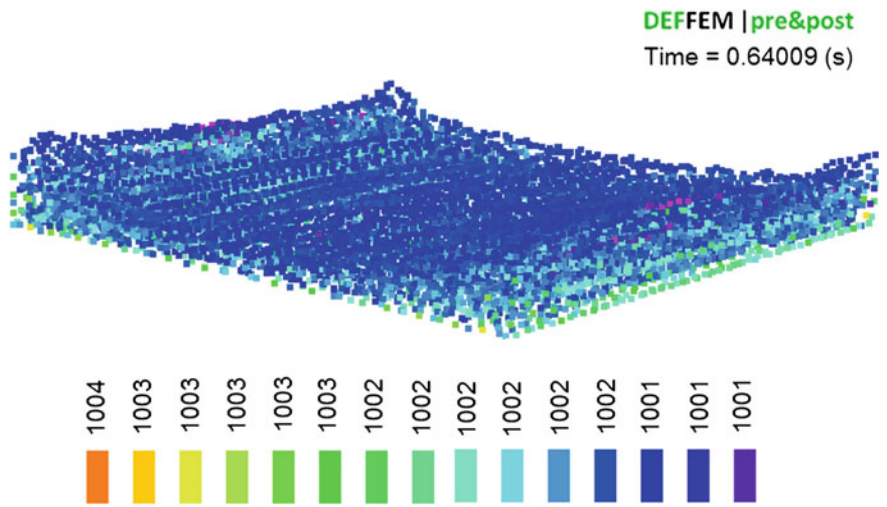


Fig. 5.3 Final density distribution at the end of the simulation (time = 0.64009 s)

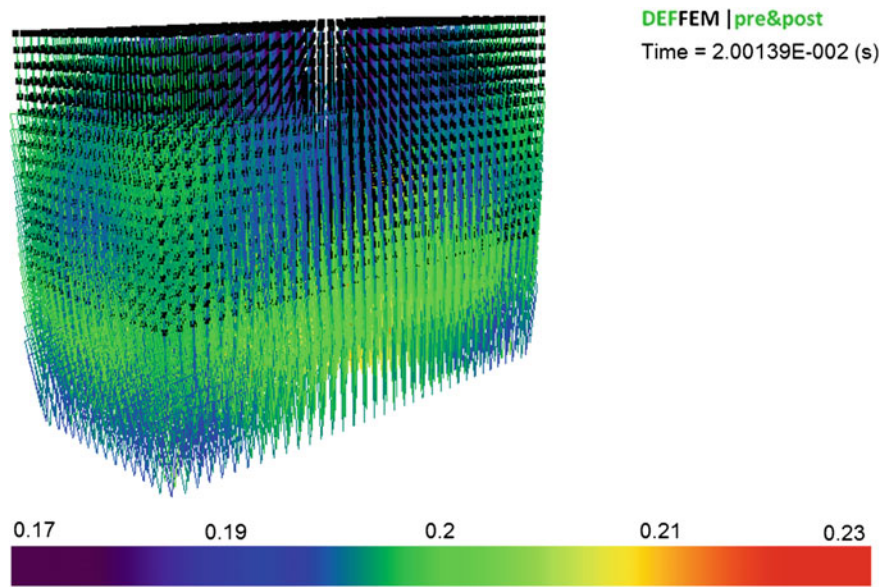
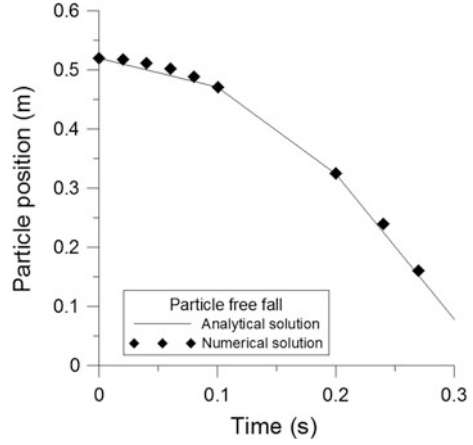


Fig. 5.4 Field of vector velocity (time = 2.00139e-02 s)

Fig. 5.5 Position z of a particle that falls (analytical solutions vs. numerical solutions)



0.19–0.2 m/s. The current velocity very well corresponds to the value expected by the analytical solution given by the equation:

$$V(\tau) = g\tau \quad (5.16)$$

where:

- τ is the current elapsed time,
- $g = 9.81 \frac{\text{m}}{\text{s}^2}$ (acceleration due to gravity).

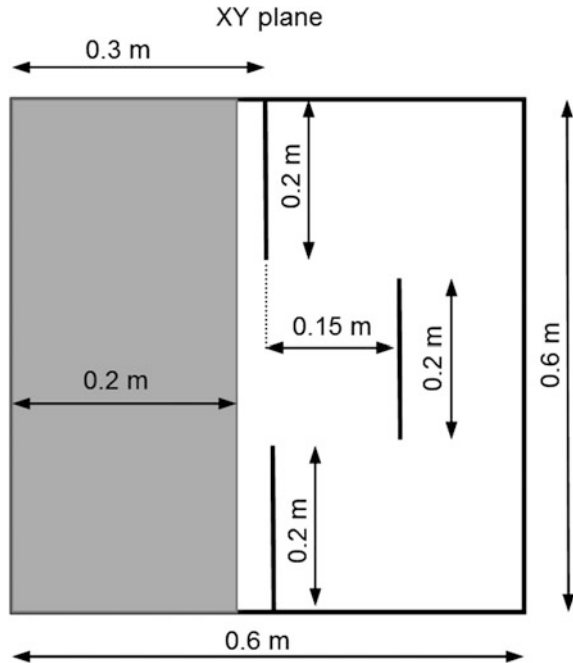
Figure 5.5 summarises that the Runge-Kutta integration scheme used in the implementation works correctly. Analytical solutions and numerical solutions of a particle fall with respect to z position, correspond very well to the value expected by the analytical solution given by equation:

$$h(\tau) = h_0 - \frac{g\tau^2}{2} \quad (5.17)$$

where:

- h_0 is the initial height from which the particle falls,
- τ is the elapsed time,
- $g = 9.81 \frac{\text{m}}{\text{s}^2}$ (acceleration due to gravity).

Fig. 5.6 Start geometry - impact structure (particle $0.22 \times 0.58 \times 0.5$), box $0.6 \times 0.6 \times 0.6$



5.3.2 Structure Impact

The scheme of the initial geometry in the XY plane of this problem is presented in Fig. 5.6. The dimensions of the solution domain are given from particle to particle (width = 0.2 m, height = 0.5 m, length = 0.58 m). The solution domain consists of 7150 moving particles. The boundary condition is represented by 6492 dynamic particles as a box given from particle to particle (width = 0.6 m, height = 0.6 m, length = 0.6 m) together with an additional vertical section as is presented in Fig. 5.6. Other parameters are adopted as: initial smoothing length = 0.024 m, speed of sound 30 m/s, α is equal to 0.2 and simulation time: 1.0 s.

Figure 5.7 presents the selected four stages of a free flow simulation taking into account the fluid-structure interaction. The analysis of the obtained results indicates that the implemented interaction model is correct.

We can observe a greater speed when the fluid passes through the first barrier defined by dynamic particles (Fig. 5.8). Near the second barrier, the velocity is also

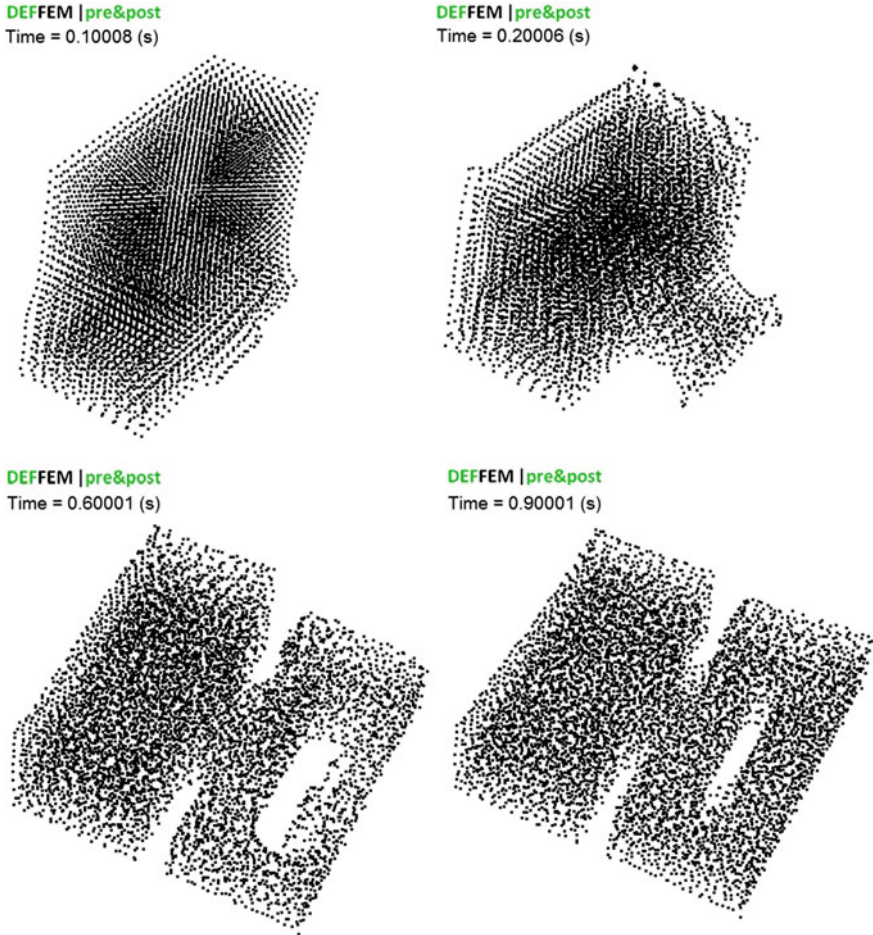


Fig. 5.7 Selected four stages of the simulation of particle impact structure

increased as a high repulsion force is created by the boundary defined by dynamic particles [22, 23]. However, for further detailed verification, more tests for various variants are required. Nevertheless, the first conclusions and the findings indicate that the formulated model may be used to simulate the flow in the area of a porous structure in the meso-scale.

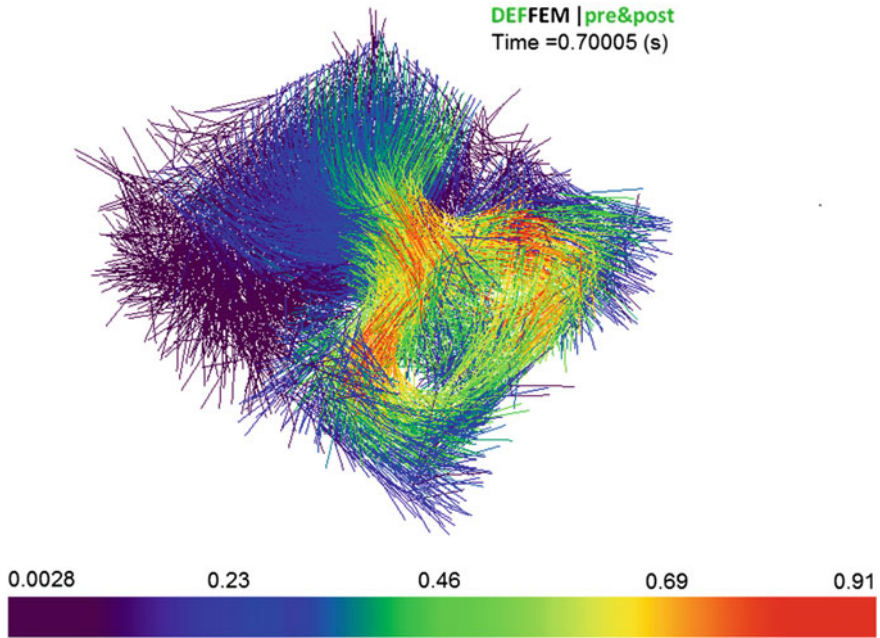


Fig. 5.8 Field of vector velocity (time = 0.7 s)

5.4 Summary

In this chapter the mathematical model based on the particle method for fluid mechanics in Lagrange's description was presented as well as the first test results indicating the correctness of the adopted model assumptions. Further work is focused on theoretical work leading to the construction of a hybrid mathematical model based on combination FEM (finite element method) and SPH (smoothed particle hydrodynamics) describing the phenomena accompanying the deformation at temperatures which are characteristic of direct rolling of continuously cast charge. The new idea requires intensive work on the numerical implementation of mathematical models that constitute the hybrid model. Amongst them, the most important is the implementation of the smoothed particle hydrodynamics method for liquid flow simulation which is presented in the current chapter. The first simulations show that the developed solver complies with the laws of physics. Further implementation work based on the SPH formulation included implementation of: heat transfer and the phase transition model, the liquid-solid interaction model and the plastic deformation model. The numerical model of fluid flow formulated and implemented as part of the DEFFEM package, based upon the smoothed particle method (SPH), enables various problems such as the impact of structures on flows through a barrier to be simulated in multiple variants. The possibility of applying the model to simulate the flow in the area of a porous

structure in meso-scale is particularly promising. After introducing small modifications, it is also possible to conduct a simulation taking into account two types of fluids or a gas and a liquid.

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Chapter 6

Spatial Solutions Based on the Finite Element Method

This chapter presents a 3D solution to the problem of medium deformation in conditions of its simultaneous solidification. The proposed solution consists of four sub-models. These are a mechanical model based upon a rigid-plastic solution, and a thermal model based on the Fourier equation solution. Another key component model is the model of function of stress versus strain change. The developed methodologies of determining the mentioned functions are presented in details in Chap. 8. The whole solution is complemented by the solidification model from the perspective of the finite element method. A multi-scale approach combining the solidification modelling in the meso-scale (use of cellular automata) with a macro model of heat conduction (use of the finite element method) is an alternative development of the model.

The selected aspects related to the numerical implementation of the proposed solutions, along with comments, are presented in separate annexes to this monograph in the form of procedures in C++ and Fortran languages.

6.1 Thermal Model

The determination of the temperature distribution inside a body with a complicated shape, subjected to a deformation process in the state of the liquid and solid phase coexistence, is a very complex problem. The analysis of a flat and spatial heat conduction state requires the application of advanced numerical methods [1–4]. In some cases, for instance for the rolling process, we deal with a strand, the considerable length of which allows the heat conduction state to be simplified to a flat cross-section [5, 6]. In this case the conduction effect in the rolling axis direction is neglected (Appendix C). The finite difference method is a frequently used method of heat transfer analysis. For a simulation of thermal effects coupled with a strain analysis, the finite element method is much better suited than the finite difference method [7]. This method allows us to obtain more accurate results, or to use the

same mesh to analyse the temperature field and the strain field. The temperature field may be determined by solving the Fourier equation:

$$\nabla^T(\lambda \nabla T) + \left(Q - c_p \rho \frac{\partial T}{\partial \tau} \right) = 0 \quad (6.1)$$

where T is temperature, and λ is the vector of heat transfer coefficient distribution function:

$$\lambda = (\lambda_x, \lambda_y, \lambda_z) \quad (6.2)$$

Q present in Eq. (6.1) represents the generation rate of the heat generated as a result of metal plastic deformation or the heat generated as a result of current flow during resistance heating, ρ is the metal density at temperature T , and specific heat c_p represents its thermal capacity at this temperature. Equation (6.1) must meet appropriate boundary conditions. In the proposed solution the mixed Neumann and Hankel boundary condition was applied in the form of [5, 6, 8, 9]:

$$\lambda \frac{\partial T}{\partial n} + \alpha(T - T_{env}) + q = 0 \quad (6.3)$$

In Eq. (6.3), the first summand may be expressed by:

$$\lambda \frac{\partial T}{\partial n} = \lambda \left(\frac{\partial T}{\partial x} n_x + \frac{\partial T}{\partial y} n_y + \frac{\partial T}{\partial z} n_z \right) \quad (6.4)$$

The physical interpretation of the mixed condition (Eq. 6.3) concerns the heat flux q representing the generation rate of the heat resulting from friction at the contact face of the metal with the tool. However, the second term occurring in expression (Eq. 6.3) describes either the heat exchange with the environment, which may be executed by the air or a cooling medium on free surfaces, or heat exchange with the deforming tool—using the heat transfer coefficient α . The application of the finite element method to solve problems related to heat transfer requires replacing the Eq. (6.1) solution, including the boundary condition (Eq. 6.3) by minimising a certain variation formula [5, 6, 8, 9]. Direct implementation of the boundary conditions to the functional is not possible, therefore in practice, this condition is imposed by adding an integral to the functional, in the form:

$$\int_S \frac{1}{2} \alpha (T - T_{env})^2 dS + \int_S q T dS \quad (6.5)$$

Let us consider the issue of heat flux power functional minimization [5, 6, 8, 9]:

$$\chi = \int_V p(x, y, z, T, T_x, T_y, T_z) dV + \int_S \frac{1}{2} \alpha (T - T_{env})^2 dS + \int_S q T dS \quad (6.6)$$

where T_{env} is the temperature of the medium contacting the cooled or heated area concerned, and p is any function of position, temperature and temperature gradient components:

$$T_x = \frac{\partial T}{\partial x}; \quad T_y = \frac{\partial T}{\partial y}; \quad T_z = \frac{\partial T}{\partial z} \quad (6.7)$$

This function is determined in the V area considered, with the edge S . Taking into account a small variation δ_χ of functional (Eq. 6.6):

$$\begin{aligned} \delta_\chi = & \int_V \left(\frac{\partial p}{\partial T} \delta T + \frac{\partial p}{\partial T_x} \delta T_x + \frac{\partial p}{\partial T_y} \delta T_y + \frac{\partial p}{\partial T_z} \delta T_z \right) dV \\ & + \int_S q \delta T dS + \int_S \alpha (T - T_{env}) \delta T dS \end{aligned} \quad (6.8)$$

If:

$$\begin{aligned} \delta T_x &= \delta \frac{\partial T}{\partial x} = \frac{\partial}{\partial x} (\delta T) \\ \delta T_y &= \delta \frac{\partial T}{\partial y} = \frac{\partial}{\partial y} (\delta T) \\ \delta T_z &= \delta \frac{\partial T}{\partial z} = \frac{\partial}{\partial z} (\delta T) \end{aligned} \quad (6.9)$$

Equation (6.8) can be written as:

$$\begin{aligned} \delta_\chi = & \int_V \left[\frac{\partial p}{\partial T} \delta T + \frac{\partial p}{\partial T_x} \frac{\partial}{\partial x} (\delta T) + \frac{\partial p}{\partial T_y} \frac{\partial}{\partial y} (\delta T) + \frac{\partial p}{\partial T_z} \frac{\partial}{\partial z} (\delta T) \right] dV \\ & + \int_S (q \delta T + \alpha (T - T_0) \delta T) dS \end{aligned} \quad (6.10)$$

By differentiating by parts the second, third and fourth of the summands of the first integrand in Eq. (6.10), assuming that $dV = dx dy dz$, we obtain:

$$\begin{aligned}
\int_V \frac{\partial p}{\partial T_x} \frac{\partial}{\partial x} (\delta V) dV &= \int_S \frac{\partial p}{\partial T_x} \delta T n_x dS - \int_V \frac{\partial}{\partial x} \left(\frac{\partial p}{\partial T_x} \right) \delta T dV \\
\int_V \frac{\partial p}{\partial T_y} \frac{\partial}{\partial y} (\delta V) dV &= \int_S \frac{\partial p}{\partial T_y} \delta T n_y dS - \int_V \frac{\partial}{\partial y} \left(\frac{\partial p}{\partial T_y} \right) \delta T dV \\
\int_V \frac{\partial p}{\partial T_z} \frac{\partial}{\partial z} (\delta V) dV &= \int_S \frac{\partial p}{\partial T_z} \delta T n_z dS - \int_V \frac{\partial}{\partial z} \left(\frac{\partial p}{\partial T_z} \right) \delta T dV
\end{aligned} \tag{6.11}$$

where n_x is the directional cosine of the normal to the external surface with respect to axis OX . After substituting the obtained relationships (Eq. 6.11) to Eq. (6.10) we obtain:

$$\begin{aligned}
\delta_\chi &= \int_V \delta T \left[\frac{\partial p}{\partial T} - \frac{\partial}{\partial x} \left(\frac{\partial p}{\partial T_x} \right) - \frac{\partial}{\partial y} \left(\frac{\partial p}{\partial T_y} \right) - \frac{\partial}{\partial z} \left(\frac{\partial p}{\partial T_z} \right) \right] dV \\
&\quad + \int_S \delta T \left(q + \alpha(T - T_0) + n_x \frac{\partial p}{\partial T_x} + n_y \frac{\partial p}{\partial T_y} + n_z \frac{\partial p}{\partial T_z} \right) dS
\end{aligned} \tag{6.12}$$

Equation (6.12) must be satisfied for any variations in δT , therefore the expressions in brackets must be zero:

$$\frac{\partial}{\partial x} \left(\frac{\partial p}{\partial T_x} \right) + \frac{\partial}{\partial y} \left(\frac{\partial p}{\partial T_y} \right) + \frac{\partial}{\partial z} \left(\frac{\partial p}{\partial T_z} \right) - \frac{\partial p}{\partial T} = 0 \tag{6.13}$$

for the whole volume V considered of the body deformed and for its edge area:

$$n_x \frac{\partial p}{\partial T_x} + n_y \frac{\partial p}{\partial T_y} + n_z \frac{\partial p}{\partial T_z} + q + \alpha(T - T_{env}) = 0 \tag{6.14}$$

Therefore, one may state that if Eqs. (6.13–6.14) are satisfied, the functional (Eq. 6.6) reaches its minimum. Therefore, both the formulas are equivalent. The above reasoning solves the so-called Euler problem [5, 6, 8, 9]. Let us assume the following form of function p :

$$p = \frac{1}{2} \left(\lambda_x T_x^2 + \lambda_y T_y^2 + \lambda_z T_z^2 \right) + QT \tag{6.15}$$

where T_x , T_y and T_z are determined by the relationship (Eq. 6.7). By differentiating the function p with respect to subsequently T , T_x , T_y and T_z , we obtain:

$$\begin{aligned}
\frac{\partial p}{\partial T} &= \frac{\partial}{\partial T} \left[\frac{1}{2} \left(\lambda_x T_x^2 + \lambda_y T_y^2 + \lambda_z T_z^2 \right) + QT \right] = Q \\
\frac{\partial p}{\partial T_x} &= \frac{\partial}{\partial T_x} \left[\frac{1}{2} \left(\lambda_x T_x^2 + \lambda_y T_y^2 + \lambda_z T_z^2 \right) + QT \right] = \lambda_x T_x \\
\frac{\partial p}{\partial T_y} &= \frac{\partial}{\partial T_y} \left[\frac{1}{2} \left(\lambda_x T_x^2 + \lambda_y T_y^2 + \lambda_z T_z^2 \right) + QT \right] = \lambda_y T_y \\
\frac{\partial p}{\partial T_z} &= \frac{\partial}{\partial T_z} \left[\frac{1}{2} \left(\lambda_x T_x^2 + \lambda_y T_y^2 + \lambda_z T_z^2 \right) + QT \right] = \lambda_z T_z
\end{aligned} \tag{6.16}$$

and after substituting to relationships Eqs. (6.13) and (6.14) and including dependence (Eq. 6.7), we obtain the following system of equations:

$$\begin{aligned}
\frac{\partial}{\partial x} \left(\lambda_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\lambda_z \frac{\partial T}{\partial z} \right) - Q &= 0 \\
\lambda_x \frac{\partial T}{\partial x} n_x + \lambda_y \frac{\partial T}{\partial y} n_y + \lambda_z \frac{\partial T}{\partial z} n_z + q + \alpha(T - T_{env}) &= 0
\end{aligned} \tag{6.17}$$

For isotropic heat transfer coefficients λ Eq. (6.17) may be written in the form:

$$\begin{aligned}
\nabla^T (\lambda \nabla T) + Q &= 0 \\
\lambda \frac{\partial T}{\partial n} + q + \alpha(T - T_0) &= 0
\end{aligned} \tag{6.18}$$

If we assume that we are dealing with a steady heat flow, i.e. if the temperature derivative with respect to time assumes the value of 0, then Eq. (6.18) are identical with Eq. (6.1) and boundary condition (Eq. 6.3), therefore, based on Euler's reasoning, satisfying Eqs. (6.1) and (6.3) is tantamount to achieving the minimum functional value:

$$\begin{aligned}
\chi &= \int_V \left\{ \frac{1}{2} \left[\lambda_x \left(\frac{\partial T}{\partial x} \right)^2 + \lambda_y \left(\frac{\partial T}{\partial y} \right)^2 + \lambda_z \left(\frac{\partial T}{\partial z} \right)^2 \right] - QT \right\} dV \\
&+ \int_S \left(qT + \frac{1}{2} \alpha (T - T_{env})^2 \right) dS
\end{aligned} \tag{6.19}$$

In the solution, a two-stage solution of Eq. (6.1) was proposed, at boundary conditions (Eq. 6.3). First, the Fourier Eq. (6.19) for the steady heat flow is solved by the finite element method. Next, thus obtained matrix equations are generalized for the case of transient heat flow given by Eq. (6.1), by using one of the residual methods [5, 6, 8, 9].

6.1.1 Discretization for Steady Heat Flow Cases

The finite element method allows Eq. (6.19) to be optimized in a discrete manner only. Therefore, the temperature distribution function should be discretized within the area analysed [5, 7]. For a single element the temperature at any of its points is the product of the shape function vector and the node temperature vector:

$$T = \mathbf{n}^T \mathbf{T} \quad (6.20)$$

On this basis one can determine the values of temperature derivatives with respect to variable coordinates x, y, z :

$$\begin{aligned} \frac{\partial T}{\partial x} &= \frac{\partial}{\partial x} (\mathbf{n}^T \mathbf{T}) = \frac{\partial \mathbf{n}^T}{\partial x} \mathbf{T} \\ \frac{\partial T}{\partial y} &= \frac{\partial}{\partial y} (\mathbf{n}^T \mathbf{T}) = \frac{\partial \mathbf{n}^T}{\partial y} \mathbf{T} \\ \frac{\partial T}{\partial z} &= \frac{\partial}{\partial z} (\mathbf{n}^T \mathbf{T}) = \frac{\partial \mathbf{n}^T}{\partial z} \mathbf{T} \end{aligned} \quad (6.21)$$

After substituting Eqs. (6.20) and (6.21) into Eq. (6.19) we obtain:

$$\begin{aligned} \chi &= \int_V \left\{ \frac{1}{2} \left[\lambda_x \left(\frac{\partial \mathbf{n}^T}{\partial x} \mathbf{T} \right)^2 + \lambda_y \left(\frac{\partial \mathbf{n}^T}{\partial y} \mathbf{T} \right)^2 + \lambda_z \left(\frac{\partial \mathbf{n}^T}{\partial z} \mathbf{T} \right)^2 \right] - Q \mathbf{n}^T \mathbf{T} \right\} dV \\ &+ \int_S \left(q \mathbf{n}^T \mathbf{T} + \frac{1}{2} \alpha (\mathbf{n}^T \mathbf{T} - T_{env})^2 \right) dS \end{aligned} \quad (6.22)$$

To minimize the above functional one should calculate its derivatives with respect to the nodal temperature vector and equate them to zero. Therefore, it becomes necessary to calculate the derivatives from expressions:

$$\begin{aligned} \frac{\partial}{\partial \mathbf{T}} \left(\frac{\partial \mathbf{n}^T}{\partial x} \mathbf{T} \right)^2 &= 2 \left(\frac{\partial \mathbf{n}^T}{\partial x} \mathbf{T} \right) \frac{\partial}{\partial \mathbf{T}} \left(\frac{\partial \mathbf{n}^T}{\partial x} \mathbf{T} \right) = 2 \frac{\partial \mathbf{n}^T}{\partial x} \mathbf{T} \frac{\partial \mathbf{n}^T}{\partial x} \\ &= 2 \mathbf{T}^T \frac{\partial \mathbf{n}}{\partial x} \frac{\partial \mathbf{n}^T}{\partial x} \end{aligned} \quad (6.23)$$

After performing similar differentiations for other summands of Eq. (6.22) we obtain:

$$\begin{aligned} \frac{\partial \chi}{\partial \mathbf{T}} = & \int_V \left\{ \left[\lambda_x \mathbf{T}^T \frac{\partial \mathbf{n}}{\partial x} \frac{\partial \mathbf{n}^T}{\partial x} + \lambda_y \mathbf{T}^T \frac{\partial \mathbf{n}}{\partial y} \frac{\partial \mathbf{n}^T}{\partial y} + \lambda_z \mathbf{T}^T \frac{\partial \mathbf{n}}{\partial z} \frac{\partial \mathbf{n}^T}{\partial z} \right] - Q \mathbf{n}^T \right\} dV \\ & + \int_S [q \mathbf{n}^T + \alpha (\mathbf{T}^T \mathbf{n} - T_{env}) \mathbf{n}^T] dS = 0 \end{aligned} \quad (6.24)$$

Equation (6.24) in the matrix form is:

$$\mathbf{T}^T \mathbf{K} + \mathbf{f}^T = 0 \quad (6.25)$$

where individual matrices present in Eq. (6.25) are written in the form:

$$\begin{aligned} \mathbf{K} = & \int_V \left(\lambda_x \frac{\partial \mathbf{n}}{\partial x} \frac{\partial \mathbf{n}^T}{\partial x} + \lambda_y \frac{\partial \mathbf{n}}{\partial y} \frac{\partial \mathbf{n}^T}{\partial y} + \lambda_z \frac{\partial \mathbf{n}}{\partial z} \frac{\partial \mathbf{n}^T}{\partial z} \right) dV + \int_S \alpha \mathbf{n} \mathbf{n}^T dS \\ \mathbf{f} = & - \int_S (\alpha T_{env} - q) \mathbf{n} dS - \int_V Q \mathbf{n} dV \end{aligned} \quad (6.26)$$

Due to the fact that the matrix $\mathbf{K}$ is a symmetrical matrix, Eq. (6.26) may be written as:

$$\mathbf{K} \mathbf{T} + \mathbf{f} = 0 \quad (6.27)$$

By solving linear Eq. (6.27) by using e.g. Gauss method (Appendix D) with respect to the nodal temperature vector we obtain the temperature distribution in the analysed area at a specific time.

6.1.2 Discretization for Transient Heat Flow Cases

For transient heat flow, Eq. (6.19) after discretization may be presented in the following form:

$$\begin{aligned} \chi = & \int_V \left\{ \frac{1}{2} \left[\lambda_x \left(\frac{\partial \mathbf{n}^T}{\partial x} \mathbf{T} \right)^2 + \lambda_y \left(\frac{\partial \mathbf{n}^T}{\partial y} \mathbf{T} \right)^2 + \lambda_z \left(\frac{\partial \mathbf{n}^T}{\partial z} \mathbf{T} \right)^2 \right] \right. \\ & \left. - \left[Q - c_p \rho \frac{\partial}{\partial \tau} (\mathbf{n}^T \mathbf{T}) \right] \mathbf{n}^T \mathbf{T} \right\} dV \\ & + \int_S \left(q \mathbf{n}^T \mathbf{T} + \frac{1}{2} \alpha (\mathbf{n}^T \mathbf{T} - T_{env})^2 \right) dS \end{aligned} \quad (6.28)$$

The temperature derivative with respect to time present in Eq. (6.28) makes the solution dependent on the flow of time. After differentiating functional (Eq. 6.28) with respect to the nodal temperature vector we obtain an equation analogous to relationship (Eq. 6.24):

$$\begin{aligned} \frac{\partial \chi}{\partial \mathbf{T}} = & \int_V \left\{ \left[\lambda_x \mathbf{T}^T \frac{\partial \mathbf{n}}{\partial x} \frac{\partial \mathbf{n}^T}{\partial x} + \lambda_y \mathbf{T}^T \frac{\partial \mathbf{n}}{\partial y} \frac{\partial \mathbf{n}^T}{\partial y} + \lambda_z \mathbf{T}^T \frac{\partial \mathbf{n}}{\partial z} \frac{\partial \mathbf{n}^T}{\partial z} \right] \right. \\ & - \left(Q - c_p \rho \frac{\partial \mathbf{T}^T}{\partial \tau} \mathbf{n} \right) \mathbf{n}^T \Big\} dV \\ & + \int_S [q \mathbf{n}^T + \alpha (\mathbf{T}^T \mathbf{n} - T_{env}) \mathbf{n}^T] dS = 0 \end{aligned} \quad (6.29)$$

The matrix equation corresponding to system (Eq. 6.29) for the transient heat flow will assume a form analogous to (Eq. 6.27):

$$\mathbf{K} \mathbf{T} + \mathbf{M} \frac{\partial \mathbf{T}}{\partial \tau} + \mathbf{f} = 0 \quad (6.30)$$

where $\mathbf{K}$ and $\mathbf{f}$ are identical as in the steady state, whereas $\mathbf{M}$ is given by the formula:

$$\mathbf{M} = \int_V \rho c_p \mathbf{n} \mathbf{n}^T dV \quad (6.31)$$

For a transient heat flow the temperature values in nodes depend on time. In the proposed solution the Galerkin integration method [5, 6, 8, 9], which allows us, on the basis of knowledge of the temperature vector at the time $\tau = 0$, that is the vector $\mathbf{T}_0$, to determine vector $\mathbf{T}_1$, representing nodal temperatures with respect to time $\Delta \tau$:

$$\left(2\mathbf{K} + \frac{3}{\Delta \tau} \mathbf{M} \right) \mathbf{T}_1 + \left(\mathbf{K} - \frac{3}{\Delta \tau} \mathbf{M} \right) \mathbf{T}_0 + 3\mathbf{f} = 0 \quad (6.32)$$

Expression (Eq. 6.32) is a system of linear algebraic equations that allows the nodal temperature values $\mathbf{T}_1$ to be computed with respect to time $\Delta \tau$, with set temperatures $\mathbf{T}_0$ at the time $\tau = 0$. Apart from the Galerkin method other integration methods are also used, e.g. the Euler method—explicit and implicit, or the Crank-Nicholson method [9]. They differ from one another with constant factors present in Eq. (6.32).

6.2 Solidification Model (FEM Approach)

The solidification process most often occurs within a temperature range or at a constant temperature. If the solidification occurs at a constant temperature, then this process is the so-called Stefan problem or the solidification problem with a zero solidification temperature range [10]. In the Stefan problem there is a clear interface between the liquid and the solidified phase. Both phases touch each other, forming the solidification front. The very process of steel alloy solidification most often occurs within certain temperature ranges, called solidification temperature ranges. In this case, there is no clear interface between the liquid and the solidified phase. Both the phases are separated by the so-called diphasic area, where the liquid and the solid phase exist simultaneously (fuzzy solidification front). The width of the diphasic area depends on the chemical composition of the solidifying alloy and the solidification rate (growth of the solid phase), depending on the heat discharging conditions. The occurrence of the diphasic area and its dynamics in the solidification process then influence the solidified metal microstructure. Both numerical and analytical methods are applied to model solidification processes. The finite difference method and the finite element method are the most often used numerical methods. The most important thermal effect occurring during the solidification is the liberation of the solidification heat. At the same time, it is the effect most difficult to be numerically modelled, also because of the numerical stability of the solution.

The solidification is described by the heat conduction Eq. (6.1) containing the heat source term Q , which is the liberating solidification heat [2]:

$$Q = \rho_s L \frac{\partial f_s}{\partial \tau} \quad (6.33)$$

where ρ_s is the density of the solid fraction, L is the latent heat, and f_s is the fraction of the solid phase. After substituting relationship (Eq. 6.33) into Eq. (6.1) we obtain:

$$\nabla^T(\lambda \nabla T) = c_p \rho \frac{\partial T}{\partial \tau} - \rho_s L \frac{\partial f_s}{\partial \tau} \quad (6.34)$$

Equation (6.34) along with adequate initial boundary conditions forms the basis for the temperature description of the solidification. It is one of the most often used methods, in which the liberating solidification heat is treated as a temperature-dependent heat source. An example of such an approach is presented in detail in this paper [2]. Non-linear Eq. (6.34) is simplified by applying the enthalpy method in which the liberating solidification heat is included in the mathematical description, in a temperature-dependent heat capacity term [10, 11]. The enthalpy methods can be divided into two methods: effective heat capacity depends on the temperature or depends on the enthalpy. By introducing enthalpy, defined as [10, 11]:

$$\widehat{H} = \int_{T_{ref}}^T c_p \rho dT \quad (6.35)$$

and calculating the derivative with respect to the temperature:

$$\frac{\partial \widehat{H}}{\partial T} = c_p \rho = c_{ef} \quad (6.36)$$

where c_{ef} is the effective heat capacity. Assuming heat source $Q = 0$, Eq. (6.1) can be written in the form:

$$\nabla^T(\lambda \nabla T) = c_{ef} \frac{\partial T}{\partial \tau} \quad (6.37)$$

Equations (6.35) and (6.37) form the basis of the thermal description of solidification. When introducing the enthalpy formulation one uses the enthalpy definition as [11]:

$$\widehat{H}(T) = \int_{T_{ref}}^T c_p \rho dT + \rho_s L(1 - f_s(T)) \quad (6.38)$$

Differentiating Eq. (6.35) with respect to τ :

$$\frac{\partial \widehat{H}}{\partial \tau} = c_p \rho \frac{\partial T}{\partial \tau} - \rho_s L \frac{\partial f_s}{\partial \tau} \quad (6.39)$$

Taking into account Eqs. (6.39) and (6.34) may be written in the form:

$$\nabla^T(\lambda \nabla T) = \frac{\partial \widehat{H}}{\partial \tau} = \frac{\partial \widehat{H}}{\partial T} \frac{\partial T}{\partial \tau} \quad (6.40)$$

The derivative $\frac{\partial \widehat{H}}{\partial T}$ present in Eq. (6.40) may be determined by differentiating Eq. (6.38), resulting in:

$$\frac{\partial \widehat{H}}{\partial T} = c_p \rho - \rho_s L \frac{\partial f_s}{\partial T} \quad (6.41)$$

By substituting the obtained relationship Eq. (6.41) into Eq. (6.40) we obtain:

$$\nabla^T(\lambda \nabla T) = \left(c_p \rho - \rho_s L \frac{\partial f_s}{\partial T} \right) \frac{\partial T}{\partial \tau} \quad (6.42)$$

By identifying the expression in brackets as c_{ef} defining the substitute heat capacity we obtain the final form of Eq. (6.37):

$$\nabla^T(\lambda \nabla T) = c_{ef}(T) \frac{\partial T}{\partial \tau} \quad (6.43)$$

The substitute heat capacity c_{ef} is determined from appropriate approximation formulas [10–12].

6.3 Mechanical Model

The mathematical model of the mechanical solution was based upon the following assumptions [7, 13]:

- (a) The principles of the finite element method and advantages arising from assuming a rigid-plastic model of the physical continuum were assumed. The application of the rigid-plastic model is becoming more and more important for very high-temperature processes. As showed by tests under conditions of hot deformation, the share of elastic strain in the strain tensor components is small. For modelling steel deformation processes in the semi-solid state elastic strains are even less important [8].
- (b) The assumed medium model satisfies the Levy-Mises plastic flow rule.
- (c) We neglect the influence of gravity and inertia forces in the medium volume.
- (d) The Lagrange type constant volume condition was assumed.
- (e) The friction model in the presented model is missing. For physical simulations performed with the Gleeble 3800 thermo-mechanical simulator, hexahedral samples are permanently fixed in clamps of the physical simulator and friction does not need to be considered.
- (f) The division of the medium (computational domain) was discretized by hexahedral elements (isoparametric elements).

In the process of deformation of e.g. a hexahedral sample, the shape of the strain zone varies over time. Then we say that we are dealing with a transient process. During the process not only geometrical parameters change, but also physical parameters assigned to individual nodes of the computational domain. In terms of stress and strain state analysis, the most important physical parameters are strain and stress tensor components. In the transient process the components of the mentioned tensors are therefore functions of time and position:

$$\varepsilon_i = \varepsilon(x, y, z, \tau) \quad (6.44)$$

$$\sigma_i = \sigma(x, y, z, \tau) \quad (6.45)$$

For spatial cases the above relationships Eqs. (6.44) and (6.45), due to their complicated forms, are most often approximated with various methods. One approach, similarly applied in the thermal model taking time into account, is the division of the process into two stages [5, 7]:

1. At the first stage we determine the distribution of strain, strain rates and stress inside the deformation zone at a specific time τ . At this stage we assume that the geometric size of the computational domain is steady.
2. At the second stage, based upon a previously determined velocity field, we determine the new shape of the deformation zone after passing the time $\Delta\tau$.

The step $\Delta\tau$ and the selection of its size are crucial from the perspective of the numerical solution stability and accuracy of determination of the physical parameters searched. The assuming of the adequate step value $\Delta\tau$ is most often a trade-off between the computation accuracy and time [5, 6, 8, 9, 13].

6.3.1 Spatial Solution

The deformation zone in accordance with the model assumptions has been divided into hexahedral elements [7]. The sample geometry presented like this is only correct for the beginning of the process simulation $\tau = 0$, where all elements specific to the area analysed are rectangular prisms.

In accordance with the assumptions of the finite element method it will be required to integrate with respect to the volume of the functions that will be included in the power functional of the rigid-plastic solution. Due to the complicated shape of the integration area, as well as the integrands, analytical integration is not possible. In order to perform integration with Gauss's method, the real coordinate system (xyz) needs to be transformed into a local coordinate system ($\xi\eta\zeta$) separately for each element which is transformed into a cube (Fig. 6.1).

The area transformed is limited with planes $\xi = -1$, $\xi = 1$, $\eta = -1$, $\eta = 1$, $\zeta = -1$, $\zeta = 1$ in the local coordinate system ($\xi\eta\zeta$). Nodal velocities $v_1, v_2, v_3, \dots, v_{24}$ do not transform. The application of the shape function N_i allows the element inside to be related to its nodes. This function at any node must be:

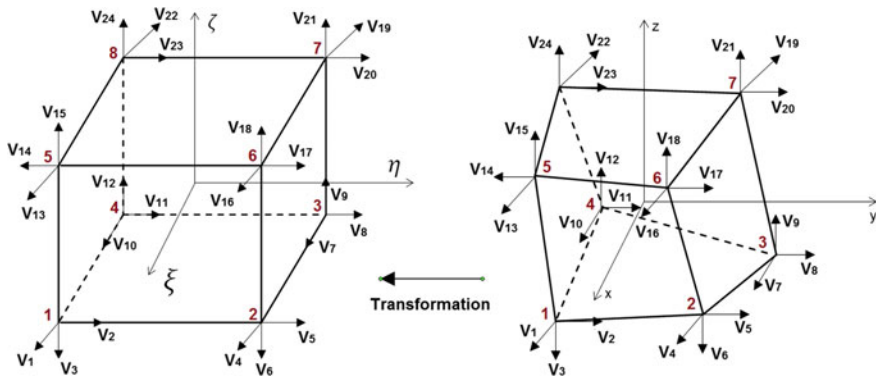


Fig. 6.1 Element transformation

$$N_i(x_k, y_k, z_k) = \begin{cases} 1 & \text{dla } i = k \\ 0 & \text{dla } i \neq k \end{cases} \quad (6.46)$$

In the local coordinate system, each element has its node numeration independent of the entire mesh. Equations (6.47) presents relationships which allow the global coordinate system to be connected to the local system [7]:

$$\begin{aligned} x &= N_1x_1 + N_2x_2 + N_3x_3 + N_4x_4 + N_5x_5 + N_6x_6 + N_7x_7 + N_8x_8 \\ y &= N_1y_1 + N_2y_2 + N_3y_3 + N_4y_4 + N_5y_5 + N_6y_6 + N_7y_7 + N_8y_8 \\ z &= N_1z_1 + N_2z_2 + N_3z_3 + N_4z_4 + N_5z_5 + N_6z_6 + N_7z_7 + N_8z_8 \end{aligned} \quad (6.47)$$

where: N_i , $i = 1, 2, \dots, 8$ are shape functions, connecting the element inside to its nodes. However, $x_1, x_2, \dots, x_8$, $y_1, y_2, \dots, y_8$ and $z_1, z_2, \dots, z_8$ respectively are the node coordinates in the global system. For a hexahedral, eight-node element (Fig. 6.1) used for the formation of the finite element mesh, the shape functions are as follows (Appendix E):

$$\begin{aligned} N_1(\xi, \eta, \zeta) &= 0.125[(1 - \xi)(1 - \eta)(1 - \zeta)] \\ N_2(\xi, \eta, \zeta) &= 0.125[(1 + \xi)(1 - \eta)(1 - \zeta)] \\ N_3(\xi, \eta, \zeta) &= 0.125[(1 + \xi)(1 + \eta)(1 - \zeta)] \\ N_4(\xi, \eta, \zeta) &= 0.125[(1 - \xi)(1 + \eta)(1 - \zeta)] \\ N_5(\xi, \eta, \zeta) &= 0.125[(1 - \xi)(1 - \eta)(1 + \zeta)] \\ N_6(\xi, \eta, \zeta) &= 0.125[(1 + \xi)(1 - \eta)(1 + \zeta)] \\ N_7(\xi, \eta, \zeta) &= 0.125[(1 + \xi)(1 + \eta)(1 + \zeta)] \\ N_8(\xi, \eta, \zeta) &= 0.125[(1 - \xi)(1 + \eta)(1 + \zeta)] \end{aligned} \quad (6.48)$$

where ξ, η, ζ are coordinates of the consecutive Gauss points in the local coordinate system. A point inside an element, movable, will be represented by a displacement vector $\underline{A}$, which is related to the nodal displacement vector $\underline{A}$, with the shape function matrix N in accordance with the equation [5–9, 13]:

$$\underline{A} = \{A_x, A_y, A_z\}^T = N \underline{A} \quad (6.49)$$

The shape function matrix with dimensions 3×24 is as follows:

$$N = \begin{bmatrix} N_1 & 0 & 0 & N_2 & 0 & 0 & \cdots & N_8 & 0 & 0 \\ 0 & N_1 & 0 & 0 & N_2 & 0 & \cdots & 0 & N_8 & 0 \\ 0 & 0 & N_1 & 0 & 0 & N_2 & \cdots & 0 & 0 & N_8 \end{bmatrix} \quad (6.50)$$

Then the nodal displacement vector is presented in the form:

$$\mathbf{A}^T = \{\Delta_1, \Delta_2, \dots, \Delta_{24}\} \quad (6.51)$$

According to the assumptions of the rigid-plastic model it is necessary to record the strain tensor, which is replaced with a six-element strain vector $\underline{\varepsilon}^T = \{\varepsilon_x, \varepsilon_y, \varepsilon_z, \varepsilon_{xy}, \varepsilon_{xz}, \varepsilon_{yz}\}$. Individual components of this vector are compatible with the components of the strain tensor. Derivatives of displacement components with respect to the coordinate system were determined, for example, for displacement in x direction:

$$\varepsilon_x = \frac{\partial \Delta_x}{\partial x} = \frac{\partial}{\partial x} (N_1 \mathbf{A}) = \frac{\partial N_1}{\partial x} \mathbf{A} \quad (6.52)$$

where:

$$\frac{\partial N_1}{\partial x} = \left\{ \frac{\partial N_1}{\partial x}, 0, 0, \frac{\partial N_2}{\partial x}, 0, 0, \dots, \frac{\partial N_8}{\partial x}, 0, 0 \right\} \quad (6.53)$$

The strain vector at any point inside the element will assume the form:

$$\underline{\varepsilon} = \mathbf{B} \mathbf{A} \quad (6.54)$$

In relationship (Eq. 6.54) matrix $\mathbf{B}$ with the dimensions 6×24 is a matrix of shape function derivatives with the following form [5–9, 13]:

$$\mathbf{B} = \begin{bmatrix} \frac{\partial N_1}{\partial x} & 0 & 0 & \frac{\partial N_2}{\partial x} & 0 & 0 & \dots & \frac{\partial N_8}{\partial x} & 0 & 0 \\ 0 & \frac{\partial N_1}{\partial y} & 0 & 0 & \frac{\partial N_2}{\partial y} & 0 & \dots & 0 & \frac{\partial N_8}{\partial y} & 0 \\ 0 & 0 & \frac{\partial N_1}{\partial z} & 0 & 0 & \frac{\partial N_2}{\partial z} & \dots & 0 & 0 & \frac{\partial N_8}{\partial z} \\ \frac{1}{2} \frac{\partial N_1}{\partial y} & \frac{1}{2} \frac{\partial N_1}{\partial x} & 0 & \frac{1}{2} \frac{\partial N_2}{\partial y} & \frac{1}{2} \frac{\partial N_2}{\partial x} & 0 & \dots & \frac{1}{2} \frac{\partial N_8}{\partial y} & \frac{1}{2} \frac{\partial N_8}{\partial x} & 0 \\ \frac{1}{2} \frac{\partial N_1}{\partial z} & 0 & \frac{1}{2} \frac{\partial N_1}{\partial x} & \frac{1}{2} \frac{\partial N_2}{\partial z} & 0 & \frac{1}{2} \frac{\partial N_2}{\partial x} & \dots & \frac{1}{2} \frac{\partial N_8}{\partial z} & 0 & \frac{1}{2} \frac{\partial N_8}{\partial x} \\ 0 & \frac{1}{2} \frac{\partial N_1}{\partial z} & \frac{1}{2} \frac{\partial N_1}{\partial x} & 0 & \frac{1}{2} \frac{\partial N_2}{\partial z} & \frac{1}{2} \frac{\partial N_2}{\partial x} & \dots & 0 & \frac{1}{2} \frac{\partial N_8}{\partial z} & \frac{1}{2} \frac{\partial N_8}{\partial x} \end{bmatrix} \quad (6.55)$$

The strain rate at any point of the element is represented by the strain rate vector $\dot{\underline{\varepsilon}}$, which we determine by differentiating the strain vector with respect to time:

$$\dot{\underline{\varepsilon}} = \frac{\partial}{\partial \tau} \underline{\varepsilon} = \frac{\partial}{\partial \tau} (\mathbf{B} \mathbf{A}) = \mathbf{B} \mathbf{v} \quad (6.56)$$

As presented in the model assumptions, a rigid-plastic model of the deformed physical continuum was assumed in the solution. It is used for the analysis of large plastic deformations and gives good results for complicated areas deformed at a high temperature. It is assumed in this model that prior to yielding the material does not deform. The application of this assumption as a rule forces the use of Levy-Mises plastic flow law, given by equation:

$$\underline{\sigma} = \frac{2}{3} \frac{\sigma_i}{\dot{\epsilon}_i} D \dot{\underline{\epsilon}} \quad (6.57)$$

where matrix D is an identity matrix.

The classic rigid-plastic solution is based upon the optimisation of the power functional [5, 7, 13]. Applying the law of conservation of energy for a certain isolated system, which in the case concerned is the volume of the metal deformed, one can find that the total work performed in the system in a time unit is equal to the energy that this system gains in the same time. The energy balance for the zone deformed, referred to a time unit may be expressed by the relationship:

$$W = \dot{W}_\sigma + \dot{W}_\lambda \quad (6.58)$$

In Eq. (6.58) $\dot{W}_\sigma$ is the plastic strain power, $\dot{W}_\lambda$ is the power necessary to change the body volume in a time unit and W is the power of external forces impacting the system. In the computational process $\dot{W}_\lambda$ it performs the role of a Lagrangian limiting function, superimposed in the volume change. The right hand side of Eq. (6.58) constitutes the power functional:

$$J = \dot{W}_p + \dot{W}_\lambda \quad (6.59)$$

Reaching the minimum for the so-defined functional leads to the determination of the actual nodal velocity field, and thus to determine strain fields, strain rates and stresses in the strain zone analysed. The first component of the functional J (Eq. 6.59) is defined by the equation:

$$\dot{W}_p = \int_V \sigma_i \dot{\epsilon}_i dV \quad (6.60)$$

where: the stress intensity σ_i is expressed by relationship (Eq. 6.61), whereas the strain rate intensity $\dot{\epsilon}_i$ by relationship (Eq. 6.62):

$$\sigma_i = \sqrt{\frac{3}{2} \underline{\sigma}^T \underline{\sigma}} \quad (6.61)$$

$$\dot{\epsilon}_i = \sqrt{\frac{2}{3} \underline{\dot{\epsilon}}^T \underline{\dot{\epsilon}}} \quad (6.62)$$

In the above relationships Eqs. (6.61) and (6.62):

- $\underline{\sigma}$ the stress tensor at any point inside the element,
- $\underline{\dot{\epsilon}}$ the strain vector at any point inside the element.

In fact, the determination of σ_i from dependence (Eq. 6.61) is ineffective and often forces the application of simplifying limitations superimposed on the metal

deformation process model. In practice most often the so-called substitute stress is determined from the flow curve, determined for a specific continuous medium analysed. The strain hardening curve equation is most often a function which relates such parameters as temperature, strain or strain rate. Generally, it can be written as follows [8, 9, 13]:

$$\sigma_i = \sigma(x, y, z, T, \varepsilon_i, \dot{\varepsilon}_i) \quad (6.63)$$

So defined, a mathematical model provides a fair amount of latitude in the selection of the nature of the relationship (Eq. 6.63), and as a result allows a considerable number of analysed process parameters to be considered.

The second term of the power functional J (Eq. 6.59) is determined from the relationship:

$$\dot{W}_\lambda = \int_V \lambda (\dot{\varepsilon}_x, \dot{\varepsilon}_y, \dot{\varepsilon}_z) dV = \lambda \int_V \mathbf{C}^T \dot{\underline{\varepsilon}} dV \quad (6.64)$$

where: $\mathbf{C}^T$ is a vector with the form $\mathbf{C}^T = \{1 \ 1 \ 1 \ 0 \ 0 \ 0\}$. The expression $\mathbf{C}^T \dot{\underline{\varepsilon}}$ describes a momentary unit change in the body volume, so it is a Lagrangian condition, imposed on the process:

$$\mathbf{C}^T \dot{\underline{\varepsilon}} = 0 \quad (6.65)$$

The value of λ for a given element is constant.

By substituting dependences Eqs. (6.60) and (6.64) into the dependence (Eq. 6.59), we define the total power, which is used for deforming the metal:

$$J = \int_V \sigma_i \dot{\varepsilon}_i dV + \lambda \int_V \mathbf{C}^T \dot{\underline{\varepsilon}} dV \quad (6.66)$$

By using dependences Eqs. (6.56) and (6.62) we can record the power functional as:

$$J = \int_V \sigma_i \sqrt{\frac{2}{3}} \mathbf{v}^T \mathbf{K} \mathbf{v} dV + \lambda \mathbf{v}^T \mathbf{Q} \quad (6.67)$$

where:

$$\begin{aligned} \mathbf{K} &= \mathbf{B}^T \mathbf{B} \\ \mathbf{Q} &= \int_V \mathbf{B}^T \mathbf{C} dV \end{aligned} \quad (6.68)$$

The functional (Eq. 6.67) achieves its minimum for the real velocity field. The necessary condition to achieve this minimum is to obtain nil values of power

functional derivatives J with respect to the velocity field parameters, such as the nodal velocity values, and Lagrange multiplier values. By performing necessary differentiations, we obtain the following system of equations [5, 6, 8, 9, 13]:

$$\begin{cases} \left\{ \frac{\partial J}{\partial \mathbf{v}} \right\} = \int_V \frac{\frac{2}{3} \sigma_i \mathbf{v}^T \mathbf{K}}{\sqrt{\frac{2}{3} \mathbf{v}^T \mathbf{K} \mathbf{v}}} dV + \lambda \mathbf{Q} = 0 \\ \frac{\partial J}{\partial \lambda} = \mathbf{Q}^T \mathbf{v} = 0 \end{cases} \quad (6.69)$$

The dependence (Eq. 6.69) is a system of non-linear equations, which can be solved by its linearisation, and then by solving the created system of linear equations with the iterative method. If k is the iteration number, then by expanding each of the Eqs. (6.69) into the Taylor series and neglecting the higher derivatives than of the first order, we will obtain for k iteration a linear equation system with respect to λ and nodal velocity increments Δv_i in the form of:

$$\begin{cases} \left\{ \frac{\partial J}{\partial \mathbf{v}} \right\}_{\mathbf{v}_{k+1}} = \left\{ \frac{\partial J}{\partial \mathbf{v}} \right\}_{\mathbf{v}_k} + \left[\frac{\partial}{\partial \mathbf{v}} \left\{ \frac{\partial J}{\partial \mathbf{v}} \right\} \right]_{\mathbf{v}_k} \{ \Delta \mathbf{v} \} \\ \left. \frac{\partial J}{\partial \lambda} \right|_{\mathbf{v}_{k+1}} = \left. \frac{\partial J}{\partial \lambda} \right|_{\mathbf{v}_k} + \left\{ \frac{\partial}{\partial \{\mathbf{v}\}^T} \left(\frac{\partial J}{\partial \lambda} \right) \right\}_{\mathbf{v}_k} \{ \Delta \mathbf{v} \} \end{cases} \quad (6.70)$$

By differentiating and transforming Eqs. (6.69–6.70) we obtain:

$$\begin{cases} \frac{2}{3} \int_V \frac{\sigma_i}{\varepsilon_i} \left(\mathbf{K} - \frac{2}{3} \frac{\mathbf{b} \mathbf{b}^T}{\varepsilon_i^2} \right) dV \Delta \mathbf{v} + \frac{2}{3} \int_V \frac{\sigma_i}{\varepsilon_i} \mathbf{b} dV + \lambda \mathbf{Q} = 0 \\ \mathbf{Q}^T \mathbf{v} + \mathbf{Q}^T \Delta \mathbf{v} = 0 \end{cases} \quad (6.71)$$

where: $\mathbf{b} = \mathbf{K} \mathbf{v}$. The above Eq. (6.71) may be written in the matrix form for each element in the form of:

$$\mathbf{H}^e \frac{\Delta \mathbf{v}}{\lambda} = \mathbf{P}^e \quad (6.72)$$

where:

$$\mathbf{H}^e = \begin{bmatrix} \frac{2}{3} \int_V \frac{\sigma_i}{\varepsilon_i} \left(\mathbf{K} - \frac{2}{3} \frac{\mathbf{b} \mathbf{b}^T}{\varepsilon_i^2} \right) dV, & \mathbf{Q} \\ \mathbf{Q}^T, & 0 \end{bmatrix} \quad (6.73)$$

$$\mathbf{P}^e = \begin{Bmatrix} -\frac{2}{3} \int_V \frac{\sigma_i}{\varepsilon_i} \mathbf{b} dV \\ -\mathbf{Q}^T \mathbf{v} \end{Bmatrix} \quad (6.74)$$

Individual matrices $\mathbf{H}^e$ and the vector $\mathbf{P}^e$ determined for each element should be incorporated into the matrix $\mathbf{H}$ and the vector $\mathbf{P}$, created for the whole structure concerned. The final effect will be a system of linear equations relating together all nodal values existing in the area deformed. By solving the system of equations we obtain the values of corrections $\Delta \mathbf{v}$ for the velocity field and the Lagrange multiplier

values λ_k for each element. The new, corrected nodal velocity field will, in the k iteration, have the following components:

$$\mathbf{v}_{k+j} = \mathbf{v}_k + \Delta \mathbf{v}_k \quad (6.75)$$

The iterative process of correcting the velocity field is carried out until the norm of the solution is smaller than the accuracy set.

6.3.1.1 Transformation of the Coordinate System and Integration

In the presented model the integration was performed on the basis of the Gauss method [5–9, 13]. After discretization of the area, and then after its deformation, the elements may have an irregular shape, and therefore a number of performed integrations is complicated. The solution to the problem is to introduce a local coordinate system (ξ, η, ζ) , into which, after transformation from the global system, the element is transformed to a cube with sides 2 units long. In the local coordinate system, the element has its node numeration independent of the entire mesh. Equation (6.47) presents relationships which allow the global coordinate system to be connected to the local system. The element in the volume of which the integration operation is performed should be described in local coordinates, which causes an appropriate change in the limits of integration. In addition, the shape functions are defined in local curvilinear coordinates. Therefore, one should determine the method for expressing global derivatives by local derivatives. For the local coordinate system (ξ, η, ζ) and the corresponding global coordinate system (x, y, z) pursuant to partial differentiation rules, one may write the derivative [5–9, 13]:

$$\frac{\partial N_i}{\partial \xi} = \frac{\partial N_i}{\partial x} \frac{\partial x}{\partial \xi} + \frac{\partial N_i}{\partial y} \frac{\partial y}{\partial \xi} + \frac{\partial N_i}{\partial z} \frac{\partial z}{\partial \xi} \quad (6.76)$$

By differentiating with respect to two other directions of the local coordinate system (ξ, η, ζ) , thus established a system of equations may be noted in the matrix form:

$$\begin{Bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{Bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix} \begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix} = \mathbf{J} \begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix} \quad (6.77)$$

The left hand side of the Eq. (6.77) may be calculated if the functions are expressed in local coordinates. The coordinates x, y, z are expressed directly by the relationships:

$$x = [N_i] \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_3 \end{pmatrix}, \quad y = [N_i] \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_3 \end{pmatrix}, \quad z = [N_i] \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_3 \end{pmatrix} \quad (6.78)$$

The matrix $\mathbf{J}$ occurring in Eq. (6.77), also called the Jacobian matrix, is described by equation:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix} \quad (6.79)$$

To determine global derivatives, one should inverse the matrix $\mathbf{J}$:

$$\left\{ \begin{matrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{matrix} \right\} = \mathbf{J}^{-1} \left\{ \begin{matrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{matrix} \right\} \quad (6.80)$$

For transformation of variables and the area with respect to which the integration is performed, one should define the determinant $\det \mathbf{J}$ of matrix $\mathbf{J}$:

$$dx dy dz = \det \mathbf{J} d\xi d\eta d\zeta \quad (6.81)$$

On the basis of expression (Eq. 6.79) we obtain an equation allowing us to find the determinant $\det \mathbf{J}$ of matrix $\mathbf{J}$:

$$\begin{aligned} \det \mathbf{J} = & \left[\frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} \frac{\partial z}{\partial \zeta} + \frac{\partial y}{\partial \xi} \frac{\partial z}{\partial \eta} \frac{\partial x}{\partial \zeta} + \frac{\partial z}{\partial \xi} \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \zeta} \right] \\ & - \left[\frac{\partial x}{\partial \zeta} \frac{\partial y}{\partial \eta} \frac{\partial z}{\partial \xi} + \frac{\partial y}{\partial \zeta} \frac{\partial z}{\partial \eta} \frac{\partial x}{\partial \xi} + \frac{\partial z}{\partial \zeta} \frac{\partial x}{\partial \eta} \frac{\partial y}{\partial \xi} \right] \end{aligned} \quad (6.82)$$

By using dependences (Eq. 6.47) and shape functions (Eq. 6.48), the global coordinates may be determined on the basis of the local coordinate system [5, 6, 8, 9]:

$$\begin{aligned}
x = & 0.125[(1 - \xi)(1 - \eta)(1 - \zeta)]x_0 \\
& + 0.125[(1 + \xi)(1 - \eta)(1 - \zeta)]x_1 \\
& + 0.125[(1 + \xi)(1 + \eta)(1 - \zeta)]x_2 \\
& + 0.125[(1 - \xi)(1 + \eta)(1 - \zeta)]x_3 \\
& + 0.125[(1 - \xi)(1 - \eta)(1 + \zeta)]x_4 \\
& + 0.125[(1 + \xi)(1 - \eta)(1 + \zeta)]x_5 \\
& + 0.125[(1 + \xi)(1 + \eta)(1 + \zeta)]x_6 \\
& + 0.125[(1 - \xi)(1 + \eta)(1 + \zeta)]x_7
\end{aligned} \tag{6.83}$$

$$\begin{aligned}
y = & 0.125[(1 - \xi)(1 - \eta)(1 - \zeta)]y_0 \\
& + 0.125[(1 + \xi)(1 - \eta)(1 - \zeta)]y_1 \\
& + 0.125[(1 + \xi)(1 + \eta)(1 - \zeta)]y_2 \\
& + 0.125[(1 - \xi)(1 + \eta)(1 - \zeta)]y_3 \\
& + 0.125[(1 - \xi)(1 - \eta)(1 + \zeta)]y_4 \\
& + 0.125[(1 + \xi)(1 - \eta)(1 + \zeta)]y_5 \\
& + 0.125[(1 + \xi)(1 + \eta)(1 + \zeta)]y_6 \\
& + 0.125[(1 - \xi)(1 + \eta)(1 + \zeta)]y_7
\end{aligned} \tag{6.84}$$

$$\begin{aligned}
z = & 0.125[(1 - \xi)(1 - \eta)(1 - \zeta)]z_0 \\
& + 0.125[(1 + \xi)(1 - \eta)(1 - \zeta)]z_1 \\
& + 0.125[(1 + \xi)(1 + \eta)(1 - \zeta)]z_2 \\
& + 0.125[(1 - \xi)(1 + \eta)(1 - \zeta)]z_3 \\
& + 0.125[(1 - \xi)(1 - \eta)(1 + \zeta)]z_4 \\
& + 0.125[(1 + \xi)(1 - \eta)(1 + \zeta)]z_5 \\
& + 0.125[(1 + \xi)(1 + \eta)(1 + \zeta)]z_6 \\
& + 0.125[(1 - \xi)(1 + \eta)(1 + \zeta)]z_7
\end{aligned} \tag{6.85}$$

The next step is the determination of derivatives of global coordinates in the local coordinate system: $\frac{\partial x}{\partial \xi}, \frac{\partial x}{\partial \eta}, \frac{\partial x}{\partial \zeta}, \frac{\partial y}{\partial \xi}, \frac{\partial y}{\partial \eta}, \frac{\partial y}{\partial \zeta}, \frac{\partial z}{\partial \xi}, \frac{\partial z}{\partial \eta}, \frac{\partial z}{\partial \zeta}$. Below an example of a derivative determination is presented $\frac{\partial x}{\partial \xi}$: The partial derivative with respect to ξ is as follows:

$$\begin{aligned}
\frac{\partial x}{\partial \xi} = & \frac{\partial N_1}{\partial \xi} x_1 + \frac{\partial N_2}{\partial \xi} x_2 + \frac{\partial N_3}{\partial \xi} x_3 + \frac{\partial N_4}{\partial \xi} x_4 \\
& + \frac{\partial N_5}{\partial \xi} x_5 + \frac{\partial N_6}{\partial \xi} x_6 + \frac{\partial N_7}{\partial \xi} x_7 + \frac{\partial N_8}{\partial \xi} x_8
\end{aligned} \tag{6.86}$$

To calculate the derivative (Eq. 6.86) one should determinate derivatives of the shape function (Eq. 6.48) with respect to ζ :

$$\begin{aligned}
 \frac{\partial N_1}{\partial \zeta} &= -0.125[(1 - \eta)(1 - \zeta)] \\
 \frac{\partial N_2}{\partial \zeta} &= 0.125[(1 - \eta)(1 - \zeta)] \\
 \frac{\partial N_3}{\partial \zeta} &= 0.125[(1 + \eta)(1 - \zeta)] \\
 \frac{\partial N_4}{\partial \zeta} &= -0.125[(1 + \eta)(1 - \zeta)] \\
 \frac{\partial N_5}{\partial \zeta} &= -0.125[(1 - \eta)(1 + \zeta)] \\
 \frac{\partial N_6}{\partial \zeta} &= 0.125[(1 - \eta)(1 + \zeta)] \\
 \frac{\partial N_7}{\partial \zeta} &= 0.125[(1 + \eta)(1 + \zeta)] \\
 \frac{\partial N_8}{\partial \zeta} &= -0.125[(1 + \eta)(1 + \zeta)]
 \end{aligned} \tag{6.87}$$

By substituting the relationships (Eq. 6.87) to Eq. (6.86) we obtain:

$$\begin{aligned}
 \frac{\partial x}{\partial \zeta} &= -0.125[(1 - \eta)(1 - \zeta)]x_0 + 0.125[(1 - \eta)(1 - \zeta)]x_1 \\
 &\quad + 0.125[(1 + \eta)(1 - \zeta)]x_2 - 0.125[(1 + \eta)(1 - \zeta)]x_3 \\
 &\quad - 0.125[(1 - \eta)(1 + \zeta)]x_4 + 0.125[(1 - \eta)(1 + \zeta)]x_5 \\
 &\quad + 0.125[(1 + \eta)(1 + \zeta)]x_6 - 0.125[(1 + \eta)(1 + \zeta)]x_7
 \end{aligned} \tag{6.88}$$

By ordering and assuming notation $x_{ij} = (x_i - x_j)$ we finally obtain:

$$\begin{aligned}
 \frac{\partial x}{\partial \zeta} &= 0.125[(1 - \eta)(1 - \zeta)x_{10} + (1 + \eta)(1 - \zeta)x_{23} \\
 &\quad + (1 - \eta)(1 + \zeta)x_{54} + (1 + \eta)(1 + \zeta)x_{67}]
 \end{aligned} \tag{6.89}$$

We determine the other derivatives $\frac{\partial x}{\partial \eta}$, $\frac{\partial x}{\partial \xi}$ analogous as the derivative $\frac{\partial x}{\partial \zeta}$, bearing in mind that adequate derivatives of the shape function (Eq. 6.48) with respect to η, ξ should be used:

$$\begin{aligned}
 \frac{\partial x}{\partial \eta} &= 0.125[(1 - \xi)(1 - \zeta)x_{30} + (1 + \xi)(1 - \zeta)x_{21} \\
 &\quad + (1 - \xi)(1 + \zeta)x_{74} + (1 + \xi)(1 + \zeta)x_{65}]
 \end{aligned} \tag{6.90}$$

$$\begin{aligned} \frac{\partial x}{\partial \xi} = & 0.125[(1 - \xi)(1 - \eta)x_{40} + (1 - \xi)(1 - \eta)x_{51} \\ & + (1 - \xi)(1 - \eta)x_{62} + (1 - \xi)(1 - \eta)x_{73}] \end{aligned} \quad (6.91)$$

We determine the other derivatives $\frac{\partial y}{\partial \xi}, \frac{\partial y}{\partial \eta}, \frac{\partial y}{\partial \xi}, \frac{\partial z}{\partial \xi}, \frac{\partial z}{\partial \eta}, \frac{\partial z}{\partial \xi}$ for global coordinates y and z in an analogous way as for the coordinate x . For the coordinate y the derivatives present the following relationships:

$$\begin{aligned} \frac{\partial y}{\partial \xi} = & 0.125[(1 - \eta)(1 - \zeta)y_{10} + (1 + \eta)(1 - \zeta)y_{23} \\ & + (1 - \eta)(1 + \zeta)y_{54} + (1 + \eta)(1 + \zeta)y_{67}] \end{aligned} \quad (6.92)$$

$$\begin{aligned} \frac{\partial y}{\partial \eta} = & 0.125[(1 - \xi)(1 - \zeta)y_{30} + (1 + \xi)(1 - \zeta)y_{21} \\ & + (1 - \xi)(1 + \zeta)y_{74} + (1 + \xi)(1 + \zeta)y_{65}] \end{aligned} \quad (6.93)$$

$$\begin{aligned} \frac{\partial y}{\partial \zeta} = & 0.125[(1 - \xi)(1 - \eta)y_{40} + (1 - \xi)(1 - \eta)y_{51} \\ & + (1 - \xi)(1 - \eta)y_{62} + (1 - \xi)(1 - \eta)y_{73}] \end{aligned} \quad (6.94)$$

However, for the coordinate z they have the following relationships:

$$\begin{aligned} \frac{\partial z}{\partial \xi} = & 0.125[(1 - \eta)(1 - \zeta)z_{10} + (1 + \eta)(1 - \zeta)z_{23} \\ & + (1 - \eta)(1 + \zeta)z_{54} + (1 + \eta)(1 + \zeta)z_{67}] \end{aligned} \quad (6.95)$$

$$\begin{aligned} \frac{\partial z}{\partial \eta} = & 0.125[(1 - \xi)(1 - \zeta)z_{30} + (1 + \xi)(1 - \zeta)z_{21} \\ & + (1 - \xi)(1 + \zeta)z_{74} + (1 + \xi)(1 + \zeta)z_{65}] \end{aligned} \quad (6.96)$$

$$\begin{aligned} \frac{\partial z}{\partial \zeta} = & 0.125[(1 - \xi)(1 - \eta)z_{40} + (1 - \xi)(1 - \eta)z_{51} \\ & + (1 - \xi)(1 - \eta)z_{62} + (1 - \xi)(1 - \eta)z_{73}] \end{aligned} \quad (6.97)$$

Using expressions Eqs. (6.89–6.97) one may determine the Jacobian determinant Eq. (6.79), necessary to transform coordinates in the global system into the local coordinate system. After performing calculations in the local coordinate system one should go back to the global system, in order to determine the calculated values in the appropriate nodes of the element mesh. To this end we use relationship (Eq. 6.80), by calculating the inverse matrix to the Jacobian matrix (Eq. 6.79). To determine the inverse matrix one should determine the minor matrix $\tilde{\mathbf{J}}$, and next perform its transposition $\tilde{\mathbf{J}}^T$.

After performing the mentioned operations, the calculated matrix should be multiplied by the converse of the determinant of the basic matrix $\det \mathbf{J}$ specified by Eq. (6.82), according to dependence Eq. (6.98):

$$\mathbf{J}^{-1} = \frac{1}{\det \mathbf{J}} \tilde{\mathbf{J}}^T \quad (6.98)$$

Assuming that the Jacobian matrix can be inverted and if the coordinates are normalized, the calculation of element properties may be reduced to finding an appropriate integral, presented with the expression:

$$\int_{-1}^1 \int_{-1}^1 \int_{-1}^1 [f(\xi, \eta, \zeta)] d\xi d\eta d\zeta \quad (6.99)$$

where: $f(\xi, \eta, \zeta)$ is any integrand.

In the presented solution a two-point integration with the Gauss quadrature method was applied. Assuming more Gauss points considerably increases the computing time, and only slightly improves the solution accuracy. An increase of the number of elements while maintaining the Gauss point number is a more optimal method (Appendix E).

6.3.1.2 Time Problem

The transient process of deformation of a hexahedral sample was treated in the adopted model as quasi-steady. As in the thermal model assumptions, the whole process was divided into a series of subsequent stages. It is assumed for each stage that the velocity field is time independent. The nodal velocity vector $\mathbf{v}_{ke} = \text{const}$, where ke is the number of the subsequent stage. The velocity field obtained during a specific stage remains constant, and therefore irregularities will occur related to the maintaining of the constant volume condition. This condition, which is strictly satisfied at a given time, may be not satisfied for the whole process. The factor decisive to the size of this error is the size of the reduction increment at subsequent steps. The absolute reduction Δh_{ke} at a given step is assumed so that the relative reduction of the sample height is constant:

$$\varepsilon_k = \frac{\Delta h_{ke}}{h_{ke}} = \text{const} \quad (6.100)$$

It ensures, approximately, the same changes in the volume, related to not meeting the condition of constant volume. The time necessary to clear the path Δh_{ke} by the holder in the simulator system is:

$$\Delta t_k = \frac{\Delta h_{ke}}{v_0} \quad (6.101)$$

Figure 6.2 presents approximately the change in mesh node positions for k_e reduction increment Δh_{ke} at the section of the deformation zone by the plane $x = 0$.

A demonstration node identified with the letter P will change its position and will take position P' after time $\Delta \tau_{ke}$. At the same time the strain value at this point will increase. By definition, the size of the strain vector components ε is presented by the relationship:

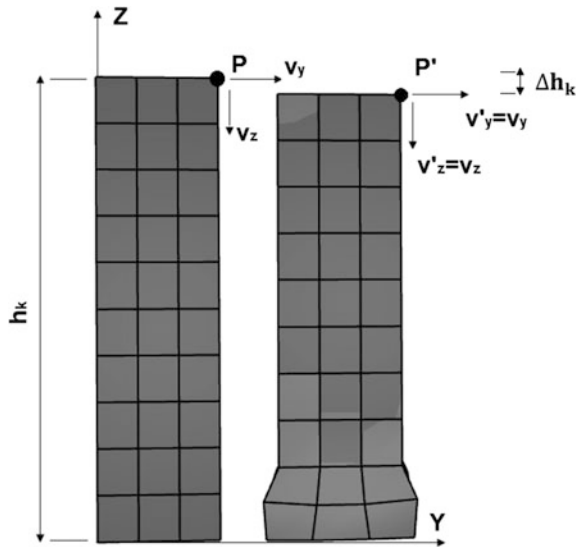
$$\varepsilon = \int_0^{\tau} \dot{\varepsilon} d\tau \quad (6.102)$$

Due to the assumption that at a given deformation step the nodal velocity field and at the same time the strain rate field do not change, the integral (Eq. 6.102) for the assumed model may be replaced with the sum:

$$\varepsilon = \sum_{ke=1}^n \varepsilon_{ke} \Delta \tau_{ke} \quad (6.103)$$

In Eq. (6.103) n is the number of deformation stages. Using the relationship Eqs. (6.56) and (6.101) one may write:

Fig. 6.2 The change in mesh node positions in the k_e step at the intersection of the deformation zone



$$\varepsilon = \sum_{ke=1}^n \mathbf{B}_{ke} \mathbf{v}_{ke} \Delta \tau_{ke} \quad (6.104)$$

Finally, the components of the strain vector at any point of the considered area of the sample deformed are determined with the relationship:

$$\varepsilon = \frac{1}{v_0} \sum_{ke=1}^n \mathbf{B}_{ke} \mathbf{v}_{ke} \Delta h_{ke} \quad (6.105)$$

The procedure that is presented above is a simple solution to the time problem.

6.4 Solidification Model (CAFE Approach)

Approaches to modelling of effects accompanying the solidification with the use of cellular automata method, known from the literature, are fairly diverse and elaborated [10, 12]. The first group of models focuses on microstructure details, including the simulation of single dendritic grains, with the accuracy of at least to the second order branches [14]. The second group of models deals with the grain growth kinetics, and not its shape, which is assumed in advance. The best known model of this type was created by Rappaz and Gandin [15–18]. It was assumed in the algorithm that the grain envelope is a square (a regular octahedron for 3D areas), which is better satisfied when the so-called incubation time of second order branches is shorter. It is possible to present various crystallographic grain orientation by a change in the square position (regular octahedron for 3D areas), with respect to the cellular automata mesh. Models that map the relevant effects primarily quantitatively constitute the last group of models. The transition rules used in these models do not have an explicit physical interpretation, and their main task is to reconstruct the branched structure of dendritic grains. A Brown and Brucet paper [19] is an interesting example. The paper deals with the modelling of three-dimensional dendritic grains of pure metal. Single grains are considered during their free growth in an undercooled liquid. Each cell of the three-dimensional cellular automaton has its temperature and state 1 or 0 assigned, depending on whether the cell belongs to the solid or the liquid phase, respectively. The solid state appears in those cells which have an adequate number of solidified neighbours, and their temperature is below the critical temperature (depending on the number of the solidified neighbours). The effect of the latent heat liberation is presented by increasing the temperature of the solidifying cell to a certain, set value corresponding to the solidification temperature. The heat flow in the area is executed with the following procedure: the average temperature of the six closest neighbours is calculated (von Neumann neighbourhood), and then the temperature of a specific cell is changed towards this average temperature by a value depending on the heat transfer coefficient.

In order to estimate the shape and size of the melting zone a model based on combining the finite element (FEM) and cellular automata (CA) methods was formulated. The formulated model is considered a multi-scale parallel model. A specific classification of multi-scale modelling was presented by Madej in the paper [20]. A brief description of the model is presented here, emphasizing the important features of the coupling between both submodels. The macro model is based on the Fourier equation, simulated using the finite element method described in detail at the beginning of the current chapter. The micro model of the solidification process is based on the solutions developed by Rappaz and Gandin and presented in details in papers [15–18, 21]. The coupling between both sub-models is realized in the solid fraction and latent heat calculation. For each cell (v), the unknown temperature $T_v^{\tau+\Delta\tau}$, and internal volume fraction of solid $f_{s,v}^{\tau+\Delta\tau}$, must satisfy the following relationship [15–18, 21]:

$$\begin{aligned}\delta\widehat{H}_v &= \rho c_p \delta T_v - \Delta H_f \delta f_{s,v} \\ &= \rho c_p [T_v^{\tau+\Delta\tau} - T_v^{\tau}] - \Delta H_f [f_{s,v}^{\tau+\Delta\tau} - f_{s,v}^{\tau}]\end{aligned}\quad (6.106)$$

where ΔH_f is the latent heat of fusion per unit volume. Nucleation and growth of grains in the proposed solution is performed on the basis of transition rules defined as follows:

1. Each CA cell (v) has three possible states: $index = 0$ (liquid zone), $index = 1$ (solid zone) and $0 < index < 1$ (mushy zone).
2. The cell (v) is liquid at time τ . Then, $\delta f_{s,v} = 0$.
3. A liquid CA cell changes its status from $index = 0$ to a positive number during the time step, when the liquid CA cell (v) reaches a predetermined local undercooling temperature $\Delta T_N = T_L - T_N$, where T_L and T_N are the liquidus and nucleation temperatures, respectively, and at least one solid neighbour exists (Moore neighborhood for simulation without deformation and random cellula automata with radius-cut neighborhood for simulations of deformation).
4. After nucleation at a liquid CA cell (v), its solid fraction $\delta f_s = F_s(T_v^{\tau})$ is calculated at the corresponding explicit temperature, where $F_s(T_v^{\tau})$ is function giving the internal volume fraction of solid of the cell (v). T_v^{τ} is the temperature obtained by interpolation at the position of the CA cell (v), of the temperature values T_n^{τ} at the four nodes of the finite element mesh.
5. The cell (v) is mushy $0 < f_{s,v} < 1$ in which case the evolution of the volume fraction of solid is calculated at every CA (v).
6. The cell (v) is fully solid at time τ . Then, $\delta f_{s,v} = 0$.

In the next step, at a finite element mesh, the change in solid fraction $\delta f_{s,n}^{\tau+\Delta\tau}$ is obtained by averaging the values of $\delta f_{s,v}^{\tau+\Delta\tau}$ at all CA cells within current finite volume. Finally, the temperature at a node of the finite element mesh can be updated according to relationship:

$$\begin{aligned}\delta\hat{H}_n &= \rho c_p \delta T_n - \Delta H_f \delta f_{s,n} \\ &= \rho c_p [T_n^{\tau+\Delta\tau} - T_n^{\tau}] - \Delta H_f [f_{s,n}^{\tau+\Delta\tau} - f_{s,n}^{\tau}]\end{aligned}\quad (6.107)$$

and the next FE heat flow calculation can be carried out using these updated temperatures, completing the micro-macro coupling cycle.

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Chapter 7

Physical Simulation of Steel Deformation in the Semi-solid State

A new category has appeared in the experimental research for evaluation of material properties. It is called “physical simulation” and is directly related to a new type of computer controlled testing machine, able to change experiment conditions automatically during the experiment progress according to the assumed programme. It allows the course of industrial processes to be reconstructed in laboratory conditions, and, more precisely, the dynamics of changes in the tested material properties to be reconstructed as in the actual industrial process. So, the laboratory test results may be applied directly for commercial purposes. The rapid development of physical simulations of metallurgical industry processes was caused by the steel manufacturers’ interest in tests, which would allow them to learn the essence of the production processes not only theoretically, as is the case for well-known computer simulations, but also physically. For instance, in physical simulations of plastic working processes, small metal samples undergo strictly controlled temperature changes, and at the same time are deformed in conditions similar to industrial ones. At the same time, the material response to the applied loads is accurately recorded, which is not possible directly during production. The development of physical simulation methods is determined by the capabilities of the testing equipment used. Equipment designers aim at increasing the possibilities of applying the equipment and at the same time ensuring more and more precise measurements. Modern machines (simulators) perform plastic deformations—from quasi-static to as dynamic deformations as the ones that can be found e.g. when rolling bars in fast-stretching passes. These machines enable both the metal creep tests, and fast rolling or forging operations to be carried out.

The only commercial simulator is the Gleeble system, manufactured by Dynamics System Inc. Troy, USA. For over 20 years the company has developed a series of simulators, consisting of models 1500, 2000, 3200, 3500 and 3800. The units setting the deformation in the Gleeble simulator are servo-hydraulic type devices. These simulators are distinguished by a resistance sample heating system. This system enables very uniform temperature distribution within the sample volume to be obtained, while the maximum sample heating rate (with the diameter of

φ10 mm) may reach up to 10.000 °C/s. The 3800 simulator version allows a sample to be deformed by compression or tension; in addition, both deformation types may be alternated. The Gleeble 3800 simulator consists of the following units [1]:

- a work station, to program the experiment course using firmware, and to collect the measurement results,
- a control unit, which consists of electronic control modules and a processor supervising the experiment course,
- a basic unit for setting the strain,
- a versatile multipoint control unit (MCU),
- a Hydrowedge unit.

Hydrowedge is a specialist unit which is used to simulate plastic working processes. The design of this unit ensures that in the experiments, constant strain rates are maintained during the whole deformation, without the need for slowing down the tool to obtain the referred strain value. Then, the testing functions of the versatile multipoint control unit are simulations of welding, continuous casting of steel, steel plasticity tests at increased temperatures, phase transformation tests, and tests of the influence of thermo-mechanical loads in changes of microstructure and the mechanical properties of steel. Both units are connected interchangeably to the basic unit setting the strain. In addition, various experimental systems can be installed in each testing unit to allow various simulation tests to be performed. The course of experiments performed with the Gleeble system is controlled in a closed loop control system, allowing the programmed temperature and mechanical load changes to be very accurately executed. Two types of experiments can be distinguished, namely, the physical simulation of industrial processes and tests to determine material characteristics. The course of the experiment during the physical simulation must very accurately reflect changes in the stress and strain states and temperatures, taking into account non-uniformities of the temperature distribution and changing friction conditions which occur in the industrial processes. Next, there are tests in order to determine material characteristics, for instance the yield stress function; they require that experiments are conducted maintaining as uniform a temperature distribution as possible in the sample, while minimising friction at the contact surface between the tool and the sample. Complex experiment conditions are executed with the Gleeble simulator with various types of testing units and measurement systems.

A specific feature of modern physical simulators is the capability to carry out experiments in conditions which are not applied in the present practices due to theoretical restrictions. For instance, this is the analysis of steel deformation processes occurring at the temperature range in which the steel solidification process has not been fully completed yet. Such processes, integrating steel strand casting with the subsequent plastic working of the strains, constitute one of the modern trends in steel product manufacturing process development. A number of practices known jointly as Integrated Strip Casting and Rolling Processes are an example in

this area. The solution to the most important engineering problems related to the Integrated Plate Casting and Rolling Process is related to the need to determine the course of basic material characteristics, which substantially differ from the ones we deal with at lower temperature ranges. Changes in the steel's condition, which occur during steel casting and its direct reduction, are so rapid that they require thorough research of the impact of the temperature and strain rate on the mechanical properties of the material. The capabilities of physical simulators are sufficient to carry out an appropriate experiment, even though it is not the most simple. However, the test result interpretation is a serious problem, because it is not possible to conduct strength tests maintaining a constant temperature and a strain field uniform in the whole area of the sample. Moreover, it is often difficult to determine even the shape of the actual strain zone.

A compressed sample shows strong barrelling of central regions, while the contact areas with the tool are virtually undeformed. It is caused by an extremely strong dependence of the yield stress on the temperature in the conditions of the solid and semi-solid phase coexistence. The selected results of physical simulations presented in this monograph result from over 15 years of the author's academic collaboration with a team of the Department of Process Simulations of the Institute for Ferrous Metallurgy in Gliwice.

7.1 Material and Test Methodology

Tests related to the steel deformation physical simulation in the conditions of the liquid and solid phase coexistence were conducted for a number of steel grades with diversified chemical compositions. This monograph presents the findings of research carried out on steel S355 and C45 with the chemical compositions presented in Table 7.1, for which comprehensive tests were carried out.

From the perspective of developing the methodology aimed at determining the foundations of the deformation model in the zone where the final phase of material solidification occurs, the temperatures which in this range are characteristic for the test material must be taken into account [1–6]. The liquidus T_l and the solidus T_s temperatures, the nil strength temperature NST , the nil ductility temperature NDT and the ductility recovery temperature DRT are most important. The determined characteristic temperatures allow a thermal process map (TPM) to be developed. The thermal process map allows us, among others, to determine the temperature

Table 7.1 The chemical composition of the tested steel (%)

Steel	S355	C45
C	0.16	0.44
Si	0.26	0.25
Mn	1.26	0.72
P	0.011	0.021
S	0.009	0.012

ranges in which the liquid phase appears or disappears, or the temperature above which the mechanical properties of the medium analysed degrade.

The proposed test methodology covers:

1. Estimating the liquidus T_l and the solidus T_s temperatures by the calculation method (program JMaTPro [7]) and other thermo-physical data necessary for the purposes of numerical process analysis.
2. Determining characteristic temperatures: nil strength NST , nil ductility NDT , and ductility recovery temperature DRT .
3. Developing the thermal process map (TPM).
4. The procedure of deformation within the range of the liquid and solid phase coexistence contains the following stages:
 - a selection of the sample and grip types,
 - heating according to the assumed schedule to a temperature from the $T_l - T_s$ range in order to melt the central sample zone. In the preliminary test phase, this stage is combined with additional tests, such as the analysis of temperature distribution along the heating zone length, and within the sample volume,
 - holding for a short time (10–60 s.) at a constant temperature in order to obtain the optimum melting zone. For configuration of tools for a cylindrical sample, the optimum melting zone length is 10–15 mm. In the variant with a hexahedral sample, the optimum melting zone length is 3–5 mm,
 - execution of the sample deformation process with a set stroke rate (1–100 mm/s),
 - potential cooling combined with compression in order to compensate shrinkage to the nominal temperature of the tensile or compression test, or cooling to the ambient temperature without the deformation process,
 - recording of force process parameters, temperature changes according to readings of the installed thermocouples, or determination of the stress-strain curves (for the tensile test),
 - examinations of the micro- and macrostructure combined with tomographic tests.

7.1.1 Samples and Tools

Tests were carried out on cylindrical samples threaded on both ends with a diameter of 10 mm and a length of 125 mm and hexahedral samples with a base dimension of 10×10 mm and the lengths of 76, 100 and 125 mm. Figure 7.1 presents a view of an example of a cylindrical sample used for the tests [1].

The experiments were carried out with copper grips with a long or a short contact zone, which were dedicated to cylindrical samples (Fig. 7.2a, b). For a hexahedral sample, only grips with a long contact zone were applied (Fig. 7.2c).

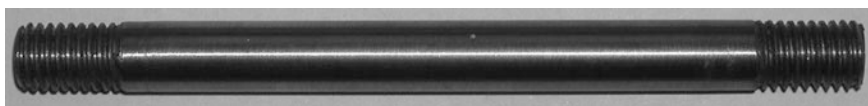


Fig. 7.1 Example of a cylindrical sample used during the physical simulation

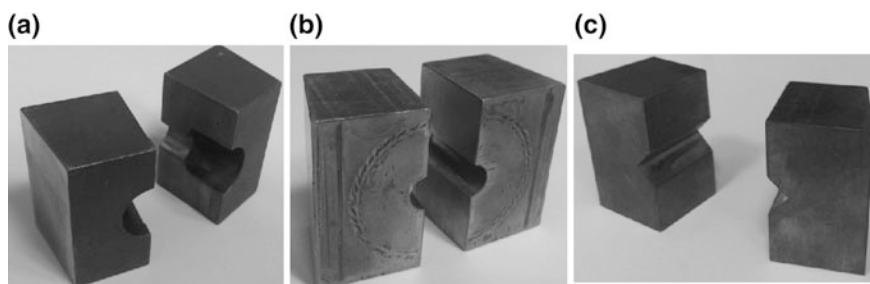


Fig. 7.2 The view of copper grips applied in the physical simulations

Results of the experimental-model tests showing the influence of the type of applied tools on the melting zone width and the temperature distribution in the sample volume are presented in a separate section.

7.1.2 *The Determination of Characteristic Temperatures*

The liquidus T_l and solidus T_s temperatures for the steel grades tested were determined by a calculation method in the program JMatPro [2–7]. JMatPro is simulation software which calculates a wide range of material properties. Using JMatPro we can make the necessary calculations for the purposes of numerical modelling of steel deformation in the semi-solid state. Based on the chemical composition of the investigated steel we can estimate for example:

1. Solidification behaviour and properties.
2. Mechanical properties.
3. Thermo-physical properties.
4. Phase transformations.

The liquidus T_l and solidus T_s temperatures for the steel grades analysed may be easily read, for instance from graphs presenting the fraction of the liquid or solid phase versus the temperature (Fig. 7.3). For steel S355, the liquidus T_l and solidus T_s temperatures were 1513 and 1465 °C respectively.

For steel C45 the liquidus T_l and solidus T_s temperatures were 1495 and 1410 °C respectively [1].

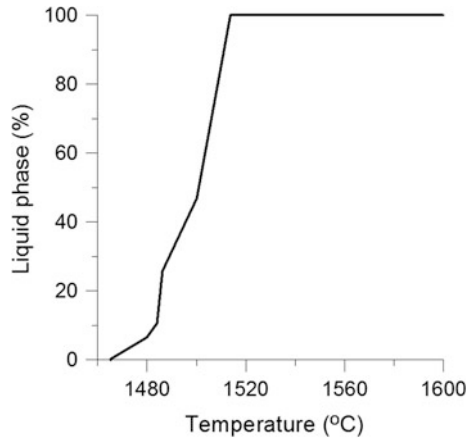


Fig. 7.3 Phase fraction of liquid (S355 grade steel)

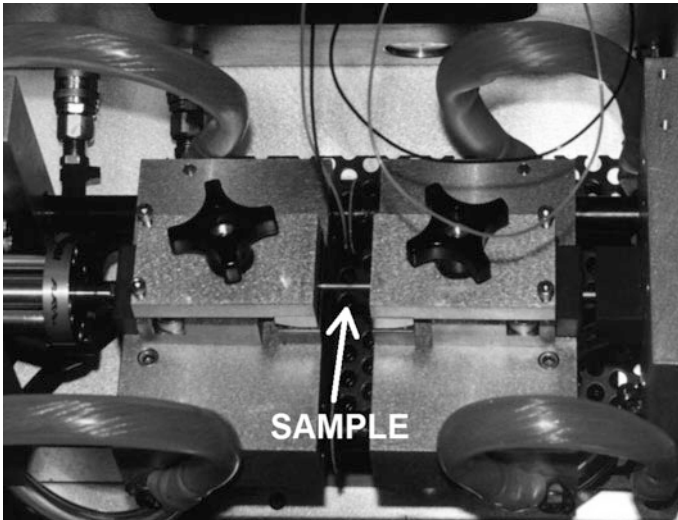


Fig. 7.4 The measurement system for determining the *NST* temperature

The procedure of determining the *NST* temperature is executed with a special measurement system presented in Fig. 7.4. This system ensures that a small load—between 15 and 80 N—is obtained and simultaneously the sample length changes related to thermal expansion are compensated [1, 2].

The experiment course includes [1, 2]:

1. Securing a sample with a diameter of Ø6 mm and a length of 90 mm in the measurement system.

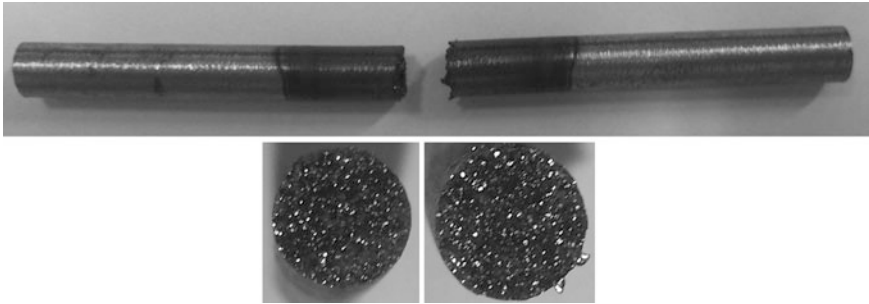
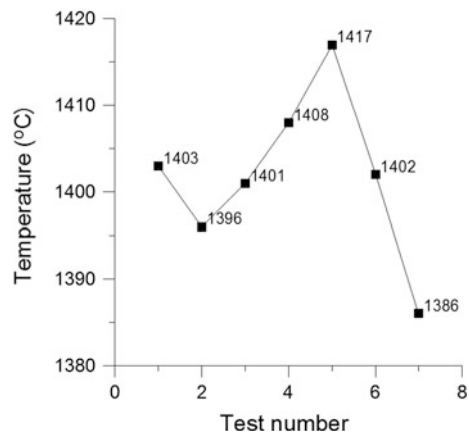


Fig. 7.5 The appearance of the sample fracture after reaching the *NST* temperature (C45 grade steel)

Fig. 7.6 The determined *NST* in the subsequent tests (C45 grade steel)



2. Pre-loading the sample with a small force of about 80 N.
3. Heating the sample to a temperature of $(T_s - 50 \text{ } ^\circ\text{C})$ at a rate between 20 and $50 \text{ } ^\circ\text{C/s}$, and next to the temperature of $T_l + 50 \text{ } ^\circ\text{C}$ at a rate of $1 \text{ } ^\circ\text{C/s}$. When heated, the sample breaks (Fig. 7.5) after reaching the *NST* temperature.

The value of this temperature may be easily read from the temperature change curve for individual tests (Fig. 7.6).

The determined average *NST* temperatures for steels S355 and C45 were 1448 and $1402 \text{ } ^\circ\text{C}$ respectively.

The determination of the *NDT* temperature is carried out with a standard measuring system presented in Fig. 7.7.

The experiment course includes [1, 2]:

1. Securing a sample with a diameter of $\varnothing 10 \text{ mm}$ and a length of 125 mm in the measurement system.

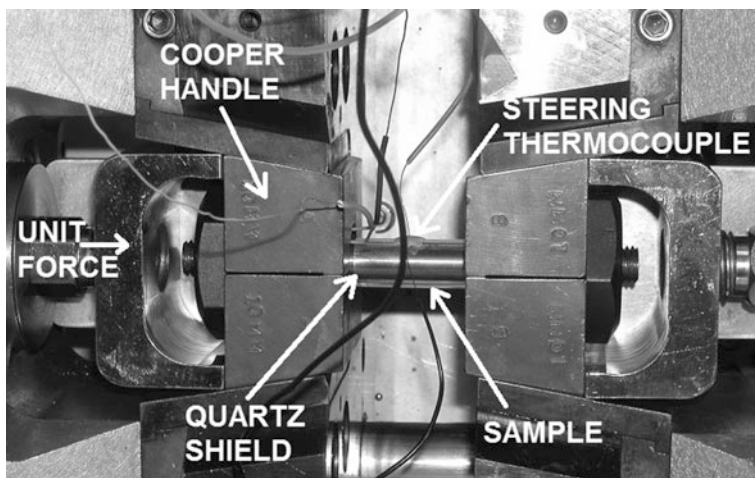


Fig. 7.7 The view of the measurement system for determining the *NDT* temperature



Fig. 7.8 The appearance of the C45 steel samples after reaching the temperature of **a** 1350 °C and **b** 1400 °C

2. Heating the sample, according to the following procedure: to a temperature of $(T_s - 50\text{ }^{\circ}\text{C})$ at a rate between 20 and 50 $^{\circ}\text{C/s}$, and next to a set temperature within the range of $T\text{--}NST$ at a rate of 1 $^{\circ}\text{C/s}$.
3. Holding for a short time (e.g. 5 s.) in order to make the temperature on the fracture level uniform, and to deform until broken (Fig. 7.8).
4. Measurement of the reduction of the area of fracture. The determined value of the *NDT* temperature constitutes the value at which the sample shows no reduction in the area of fracture.

The determined average *NDT* temperatures for steels S355 and C45 were 1420 and 1390 $^{\circ}\text{C}$ respectively.

The *DRT* temperature is determined in a series of experiments, where the sample is heated to the *NST* temperature set at the previous stage, and next it is cooled to various temperatures, and then deformed by tensioning until broken.

The experiment course includes [1, 2]:

1. Securing a sample with a diameter of $\varnothing 6$ mm and a length of 116.5 mm in the measurement system.
2. Heating the sample to the *NST* temperature.
3. Cooling the sample to the tensioning temperature at a rate comparable to the rate in the actual process.
4. Tensioning the sample until broken. Subsequent tests should be made at lowered tensioning temperatures. The *DRT* parameter is defined as the temperature at which the ductility index (reduction of the area at fraction) of the sample is 5 %.

The determined *DRT* temperature for steel S355 was 1385 °C. For steel C45 the *DRT* temperature was not determined.

7.1.3 Thermal Process Map (TPM)

The determined characteristic temperatures allow the process to be divided into stages, for which different physical and mathematical model types must be applied, and also allow the shape and size of the mushy zone to be determined theoretically [1]. Figure 7.9 presents the thermal process map *TPM* with marked characteristic temperatures.

In the conducted research [8–10] and on the basis of observations of the sample microstructure after deformation and intensive cooling, it was found that the *NST* temperature is the temperature under which the residues of the solid phase remain in steel in the form of a coherent skeleton, and above which the solid phase skeleton loses its coherence, and consequently deformation resistance drops to zero.

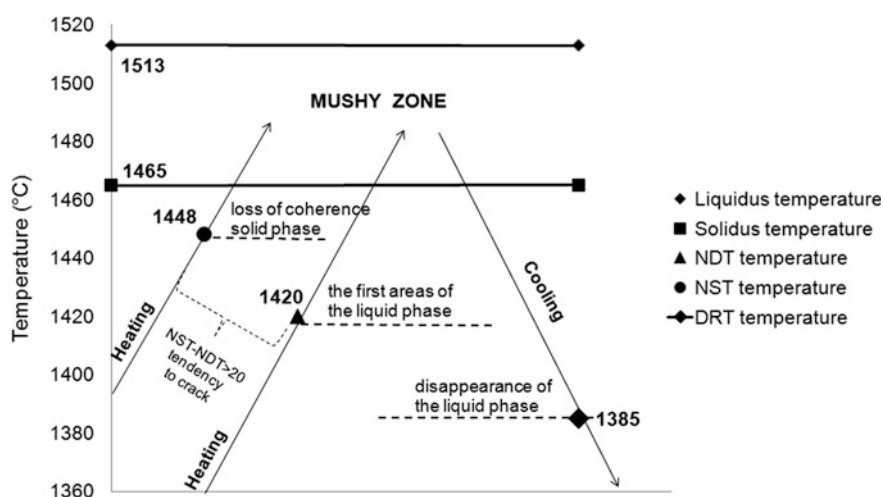


Fig. 7.9 The thermal process map for the deformation process for steel S355

However, the *NDT* is the temperature at which the first liquid phase areas appear in steel. Then the ductility recovery temperature *DRT* is the temperature at which the last liquid phase areas disappear.

The knowledge of characteristic temperatures allows us also to determine the susceptibility of steel to fracture [2–6], which is characterised by the following fracture resistance indicator R_f :

$$R_f = \frac{NST - NDT}{NDT} \quad (7.1)$$

When the condition $NST - NDT < 20 \text{ }^\circ\text{C}$ is met, it is assumed no fracture will occur in steels. For instance, for the tested steel S355, the above condition is not met; it indicates the possibility of the cast strand shell breaking during its formation within the mould and within the secondary cooling zone. Therefore one can suppose, that this steel is characterised by a high susceptibility to fracture.

7.2 Preliminary Experimental Research of Steel Deformation in the Semi-solid State

In preliminary experiments, cylindrical samples with a diameter of $\varnothing 10 \text{ mm}$ and a length of 125 mm were used with a control thermocouple *TC4* installed in the centre of the melting zone (Fig. 7.10).

Six tests were made as part of the pilot research [3–6]. In the first variant (Test no. 1) the deformation process was performed in the melting phase of the sample, during holding at a temperature of $1470 \text{ }^\circ\text{C}$. The maximum temperature achieved in the test was $1476 \text{ }^\circ\text{C}$. The obtained cooling rate within the temperature range $1470\text{--}1385 \text{ }^\circ\text{C}$ (thermocouple *TC4*) was about $78.5 \text{ }^\circ\text{C/s}$. The maximum force achieved in the test was about -137 N , and at the time of the deformation end it was -98 N . In the second variant (Test no. 2) of the experiment, a linear deformation was introduced during the crystallization stage, causing a linear shift of the tool system by 1.5 mm during 800 ms. The deformation was performed during cooling within the two-phase range, that is, in the temperature range $1470\text{--}1385 \text{ }^\circ\text{C}$.

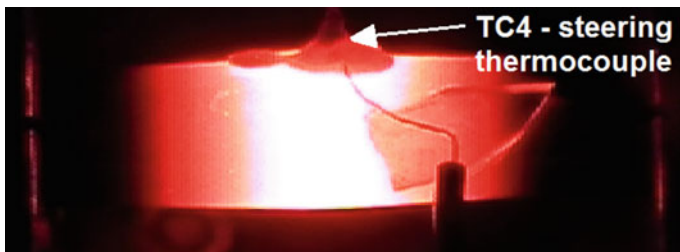


Fig. 7.10 A view of the sample during melting with the installed steering thermocouple

The maximum temperature achieved in the test was 1485 °C. The sample that was cooled to a temperature below 1400 °C failed. The obtained cooling rate within the temperature range 1483–1406 °C (thermoelement TC4) was about 91 °C/s. The maximum force achieved at the time of sample deformation was about –284 N. The sample was deformed at the moment of the cooling start. In the next third variant (Test no. 3) a third deformation was introduced, namely compression after cooling the sample to the set temperature. Deformation in the solidification phase was linearly increasing during the simultaneous injection of compressed air for 1.2 s. In addition, the nozzle direction was changed. The injection was directed at an angle of about 45°, not perpendicularly to the sample. This change stabilised the injection, by reducing the blowing of the liquid steel out of the sample. The sample cooling rate (thermocouple TC4) within the temperature range 1495–1385 °C was 76 °C/s. Cooling and compressing in the solidification phase was performed in the same manner as in the previous test. The maximum values of forces corresponding to the deformation in the melting phase and during accelerated cooling were –363 and –981 N respectively. Tensioning was planned immediately after achieving a temperature of 1200 °C in the sample. The maximum tensile stress was 2.53 kN. In the next stage, the load direction changed from tensile to compressive after cooling the sample to the set temperature. The results of these tests were conditional to achieving the main goal of the project, i.e. answering the question: “Is it possible to simulate the process of Integrated Casting and Rolling?” There had been concerns that further compression of a sample with a free length of about 35 mm and a diameter of 10 mm might cause buckling. Finally, a programme of further experiments was set. It is presented in Table 7.2 (Integrated Strip Casting and Rolling).

Table 7.2 Schedule of the pilot simulations of the integrated strip casting and rolling process

Soaking temperature (°C)		Holding time (s)	Heating velocity (°C/s)
1	1440	0	25
2	1450 + manual control	30	1
<i>Deformation parameters in the melting stage</i>			
Stroke (mm)		Stroke rate (mm/s)	Cooling velocity to the deformation temperature (°C/s)
–1.2		0.04	0
<i>Deformation parameters in the solidification stage</i>			
Stroke (mm)		Stroke rate (mm/s)	Cooling velocity to the deformation temperature (°C/s)
–1.5		–0.25	maximum
<i>Deformation parameters in the stage of preliminary rolling</i>			
Test number	T_d (°C)	Stroke (mm)	Stroke rate (mm/s)
Test no. 4	1200	–4	1.25
Test no. 5	1100	–4	1.25
Test no. 6	1000	–4	1.25

Table 7.3 The values of the selected parameters obtained in the tests

Test number	$TC4_{max}$ (°C)	T_d (°C)	V_{ch} (°C)	Melting F_{max} (N)	Solidification F_{max} (N)	Rolling F_{max} (kN)
Test no. 4	1480	1197	53	373	824	3.84
Test no. 5	1466	1130	44	500	1020	5.57
Test no. 6	1471	1015	57.5	304	637	7.87

Table 7.3 presents the most important selected parameters obtained during the conducted experiments.

In the conducted Integrated Strip Casting and Rolling Process simulation, the process was performed in three phases: melting, crystallization and preliminary rolling [3–6]. The task of deformation in the two first phases was to ensure the filling of the full volume of the melted sample and to eliminate shrinkage effects, including the formation of a shrink hole. The simulation of preliminary rolling was conducted in the solid state. It arises from the deformation parameters provided in Table 7.2 that the stroke of the simulator jaw towards the sample (compression) within the first two phases was maximum 1.5 mm, and 1.2 mm of this was performed in the melting phase. The maximum jaw stroke in the crystallisation phase was 2 mm, however there was a concern regarding breaking the quartz shield and the leakage of non-solidified steel. In both phases the compression of liquid improves the heating conditions and causes an increase in the temperature, hence the values of the maximum stresses obtained in the performed tests fluctuate (Table 7.3). The final position of the mobile jaw was 4 mm after the completion of the initial deformation simulation. In relation to the crystallisation phase, it corresponds to the sample length change of 2.5 mm. Therefore, assuming that the measurement length is the same as the melting zone length (about 5 mm), the average logarithmic strain will be -0.69 (50 % engineering). For a melting zone length of 15 mm, the average logarithmic strain will be -0.18 (17 % engineering).

7.2.1 The Dependence of Steel Microstructure Parameters on the Cooling Rate During Solidification

Connecting the cast strand microstructure parameters, such as the distance between dendrite branches or the austenite grain size, to the cooling rate of steel from the liquid state is crucial for the control of the continuous steel casting process [3–6]. Information concerning the influence of casting parameters on the cast strand microstructure parameters is difficult to obtain by experiments performed in industrial conditions. Also, results of measurements performed in laboratory conditions on small cast strands are of little credibility. In this respect the physical

simulation methods provide the most credible data, which based upon a very simple mathematical formalism can be transferred into industrial conditions. The basic parameter, which can be very accurately related to the cooling rate, is the average distance between the dendrite branches. The cooling rate at the solidus temperature $\left(-\frac{dT}{d\tau}\right)_{T_{\text{solidus}}}$ was used in the paper [11] to evaluate the crystallisation rate. In places where the cooling rate was unknown, the interdendritic distances were used to evaluate the crystallisation rate. These distances were calculated on the basis of a dependence obtained as a result of laboratory test result processing:

$$L = 168 \left(-\frac{dT}{d\tau} \right)_{T_{\text{solidus}}}^{-0.43} \quad (7.2)$$

Kurtz and Fisher [12] proposed a simplified criterion to determine the conditions in which a continuous cellular growth of crystals during solidification turns into a dendritic growth. This criterion was as follows:

1. The dendritic growth occurs when $V > \frac{V_c}{k}$
2. The cellular growth occurs when $V < \frac{V_c}{k}$.

In the above criteria, the critical crystallisation front speed V_c is given by the relationship $V_c = \frac{GD}{\Delta T_0}$ where:

- G the temperature gradient before the crystallisation front,
 D the diffusion coefficient of admixture atoms,
 ΔT_0 the difference between the solidus and liquidus temperatures,
 k distribution coefficient.

The distances between the primary and secondary dendrite branches $\aleph_1, \aleph_2$ are expressed by the following formulas [13]:

$$\aleph_1 = KG^{-m_1} V^{-m_2} \quad (7.3)$$

$$\aleph_2 = B \left(\frac{dT}{d\tau} \right)^{-n} \quad (7.4)$$

where K, m_1, m_2, n, B are constants which depend on the alloy chemical composition, V is the growth rate, T is the temperature and τ is the time. Shiang and Wray provided an identical relationship [14], where B and n coefficients in Eq. (7.4) for secondary dendrites were 156 and 0.36 respectively. Table 7.4 shows the measurement results of distances between secondary dendrites for the tested steel S355 [3–6].

The hardness obtained in tests without the last deformation phase was fairly uniform and was about 170 HV98 (for Test no. 1 and Test no. 2). The hardness of the Test no. 3 sample significantly differed (HV98 = 351 ± 52). For other tests (Test no. 4, Test no. 5 and Test no. 6) the average hardness value was around HV98 = 270 ± 32 . The pictures of sample structures magnified 20 times (Figs. 7.11, 7.12 and 7.13) show a diversification of the share of areas with a clear

Table 7.4 Results of measurements and calculations of distances between dendrites

Test no.	V_{ch} (T_{max} –1385 °C) (°C/s)	DAS (μm)	V_{SDAS}^a (°C/s)	V_{SDAS}^b (°C/s)	V_{SDAS}^c (°C/s)
Test no. 1	50	50–38	17.4–35.8	16.8–31.7	23.6–50.6
Test no. 2	90	38–25	35.8–107.8	31.7–84	50.6–161.8
Test no. 3	90	25	107.8	84	161.8
Test no. 4	53	37 ^c	–	–	–
Test no. 5	44	40 ^c	–	–	–
Test no. 6	57.5	38	35.8	31.7	50.6

V_{SDAS} is the crystallisation rate determined from the distance between secondary dendrites, from the formula: $DAS = B(V_{SDAS})^{-n}$

where:

$B = 148$; $n = -0.38^a$ [13]

$B = 168$; $n = -0.43^b$ [11]

$B = 156$; $n = -0.36^c$ [14]

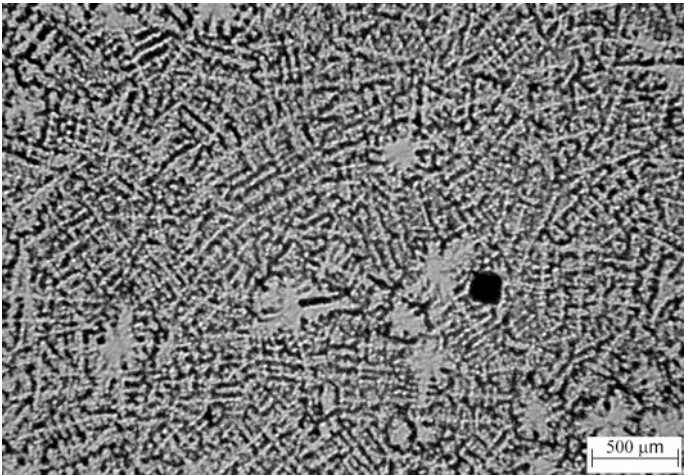


Fig. 7.11 The microstructure of sample (Test no. 1, magnification 20×)

dendritic structure. All samples have reached a temperature of 1481–5 °C before cooling started. The Test no. 1 sample was cooled within a crystallisation range at a rate of 50 °C/s, the other two about 90 °C/s. Within the temperature range of about 1000–650 °C, the cooling rates were within 26–30 °C/s. However, the method of sample deformation in the melting and crystallisation phases was different [2–6]:

Test no. 1: deformation only in the melting phase—stroke = 1.5 mm.

Test no. 2: deformation only in the solidification phase—stroke = 1.5 mm.

Test no. 3: deformation in the melting phase—stroke = 1.0 mm, and in the solidification phase—stroke = 2 mm.

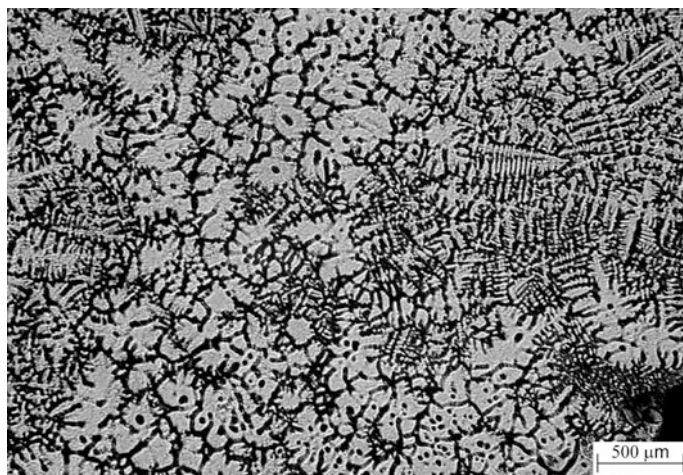


Fig. 7.12 The microstructure of sample (Test no. 2, magnification 20×)



Fig. 7.13 The microstructure of sample (Test no. 3, magnification 20×)

On the basis of measurements of distances between secondary dendrites (Table 7.4), we can find that the estimated crystallisation rate calculated according to the relationship given in paper [14] is the closest to the cooling rate measured in the experiments carried out. On the basis of the conducted literature analysis [15], one can find that the distances between secondary dendrites determined in this study (25–50 μm , Table 7.4) are smaller than for the conventional continuous casting process, but bigger for thin strip casting, where these distances do not exceed

10 μm [2–6]. The samples subjected to the Integrated Plate Casting and Rolling simulation had a similar average hardness level of about $270 \pm 30\text{HV}_{98}$.

The structure of samples after the simulation shown in Figs. 7.14, 7.15 and 7.16 reveals a much lower share of areas with clearly marked dendrites. The other areas resemble a structure with column grains (cross-section). The different image of the structure may result from the heat discharge conditions. A significant part of heat is discharged along the sample axis as a result of conduction. Copper grips of the sample are water cooled. The sample in the melting zone is surrounded by a quartz

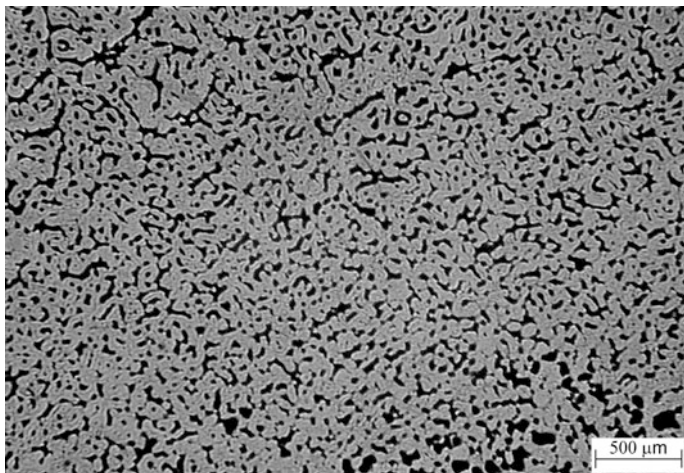


Fig. 7.14 The microstructure of sample (Test no. 4, magnification 20 $\times$)

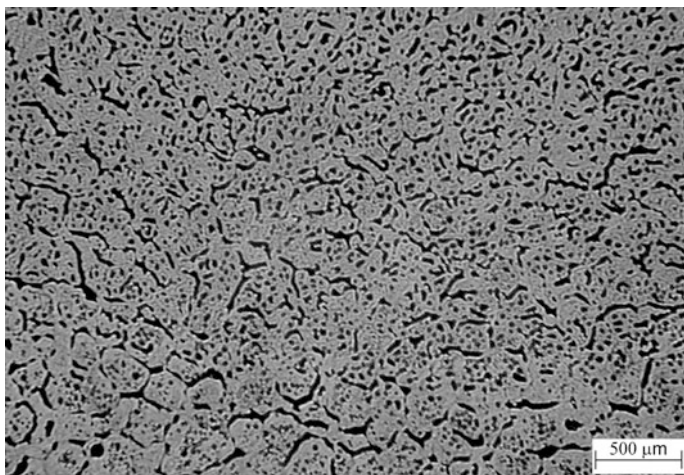


Fig. 7.15 The microstructure of sample (Test no. 5, magnification 20 $\times$)

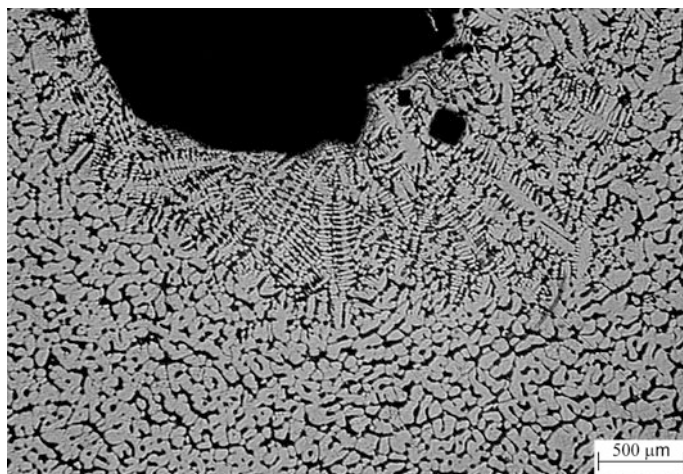


Fig. 7.16 The microstructure of sample (Test no. 6, magnification 20×)

shield, with a gap about 3 mm wide in its top part. The compressed air stream impacts directly this area only. The other interpretation of the structure observed is due to an insufficient melting zone and a bigger strain concentration [2–6].

7.2.2 *Steel Ductility Tests*

At the next stage of tests the strain-stress relationships for steel S355 were determined on the basis of the tensile test [2, 9, 10]. In the experiment the sample was heated to a temperature of 1420 °C at a rate of 20 °C/s. Further heating after reaching 1420 °C was carried out at a rate of 1 °C/s–1460 °C. The next step was holding samples at the set temperature for 60 s. The samples were cooled to the deformation temperature at a rate of 10 °C/s, and then were held at this temperature for 10 s. The purpose of the holding operation was to equalize the temperature in the sample cross-section. During the experiments, the force, temperature and simulator tool stroke were recorded. The fundamental problem related to the determination of the steel stress-strain curves at the final stage of the transformation of the state of aggregation is the enormous non-uniformity of the strain. It occurs due to the fact that in these conditions even a small temperature change causes significant differences in the yield stress values. Not only is the actual length of the deformation zone difficult to determine but so is its shape. An accurate determination of the average strain using the tensile test is not possible with the traditional methods. Therefore, we can assume approximately, that the initial length of the deformed zone of the sample equals the length of the free zone, understood as the distance between the holders. For 125 mm long samples it is about 30.5 mm for

grips with a long contact zone and 40 mm for short contact zone grips. The applied quartz shield length is about 30 mm.

The average value of the nil ductility temperature NDT of steel S355 was 1420 °C. On the basis of this result and the liquidus and solidus temperatures of the steel tested, tests of determination of the stress-strain relationship were carried out within the temperature range 1200–1450 °C for three various strokes of the tools V_n : 1, 20 and 100 mm/s. Figure 7.17 presents an example of the stress-strain relationship for a temperature of 1450 °C and the tool stroke 1 mm/s. The measurement points were obtained by translating the forces and physical simulator tool strokes into corresponding stresses and strains, assuming the uniaxial strain state and the uniformity of the strain field in the whole sample volume. However, there is a question: Are the curves obtained with this method adequate? If not, how far do they diverge from the actual curves? The analysis of Fig. 7.17 reveals a significant dispersion of the experimental data values. It is caused by small values of yield stress in the temperature range investigated. A similar dispersion of the experimental data values was obtained in other cases.

In order to practically utilize the obtained dependences in the simulation programs, the obtained courses were subjected to a data smoothing and filtering procedure (data entered in a table to the simulation programme). Figures 7.18, 7.19 and 7.20 present the obtained stress-strain relationships for the selected temperatures and tool strokes.

The obtained results were also approximated with the function [2]:

$$\sigma_p = m\epsilon^n \exp(A\epsilon) \quad (7.5)$$

where m, n, A are coefficients determined by approximation. For individual temperature values and tool strokes they are gathered in Table 7.5.

The obtained stress-strain change curves may constitute the basis for formulating a rheological model of steel S355 deformation within the temperature range of the

Fig. 7.17 The stress-strain change curve for $T_d = 1450$ °C and $V_n = 1$ mm/s

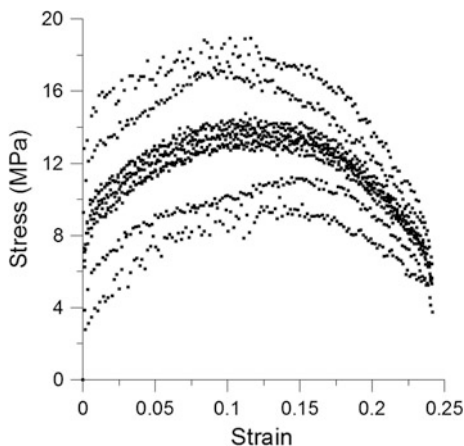


Fig. 7.18 Stress-strain curves obtained from the experiment ($V_n = 1 \text{ mm/s}$)

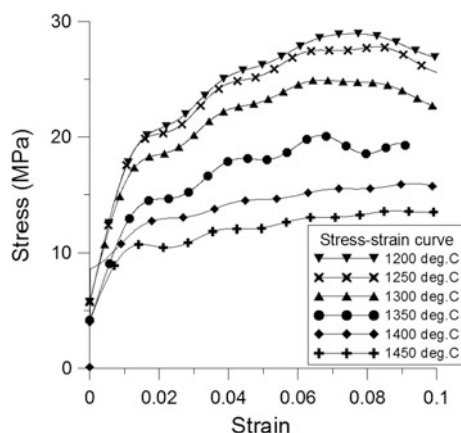
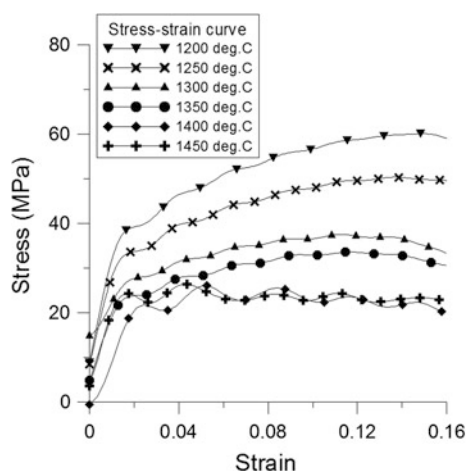


Fig. 7.19 Stress-strain curves obtained from the experiment ($V_n = 20 \text{ mm/s}$)



state of aggregation transformation. The methodology of construction of a rheological model of the steel deformation Simple Interval Methodology (SintM) that was first developed was based upon determined curves directly from the Gleeble 3800 simulator for individual tool rates and temperatures. Assuming a linear function allowed us to determine the stress value for intermediate temperatures. A modification of the SintM methodology applied in further work introduced a division of the temperature range into intervals, most often at every 100 °C, and approximated the curves obtained by the experiment with a specially selected function. Detailed results of research on the rheological model formulation (Simple Interval Methodology) for steel S355 are presented in the monograph [2] and publications [9, 10].

Fig. 7.20 Stress-strain curves obtained from the experiment ($V_n = 100 \text{ mm/s}$)

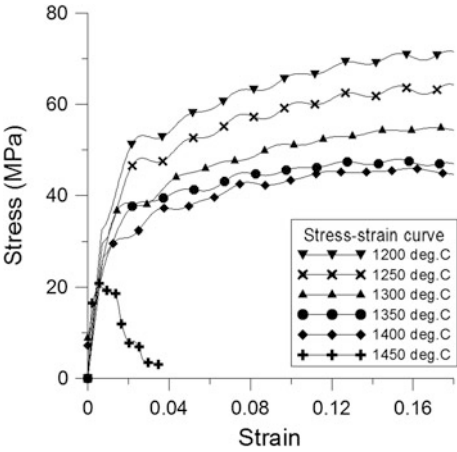


Table 7.5 Stress-strain curve coefficients for steel S355 at various temperatures and tool strokes

T_d (°C/s)	V_n (mm/s)	m	n	A
1200	1	117.0697489	0.418312167	-4.566957758
1250	1	107.7407648	0.4017957716	-4.516832285
1300	1	94.01052615	0.3868843913	-4.702148187
1350	1	75.35049	0.3965823529	-4.499293312
1400	1	23.32964971	0.1564999966	-0.09247129463
1450	1	25.52376015	0.2186685587	-1.275659582
1200	20	149.1443714	0.3427901273	-1.737736503
1250	20	123.2847737	0.3315518377	-1.79304434
1300	20	92.57466847	0.3021174602	-2.445758996
1350	20	111.777176	0.3914686819	-3.315423623
1400	20	295.9442278	0.6861286873	-9.187552751
1450	20	69.08856093	0.2763965104	-4.160013304
1200	100	137.5499673	0.2726421263	-1.060918466
1250	100	129.3482081	0.281996086	-1.253850315
1300	100	117.2058201	0.2976986252	-1.403660817
1350	100	89.3594977	0.23352588	-1.31201958
1400	100	108.8981602	0.3136666932	-1.879150985
1450	100	1904.562357	0.7391409234	-119.263809

Figure 7.21 presents the impact of the deformation temperature on the value of the maximum force measured during the tensile test. As expected, when the deformation temperature increases, the maximum force decreases.

Figure 7.22 presents changes in the ductility of steel S355 as a function of the deformation temperature determined on samples cooled from the liquid state to the deformation temperature at a rate of 10 °C/s. Because of the scope of work, the

Fig. 7.21 Changes of the maximum measured force as a function of the deformation temperature determined in the tensile test for three grip strokes

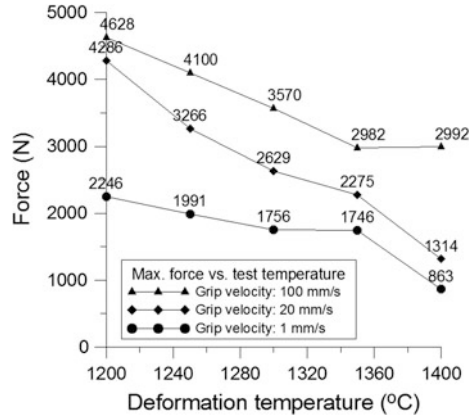
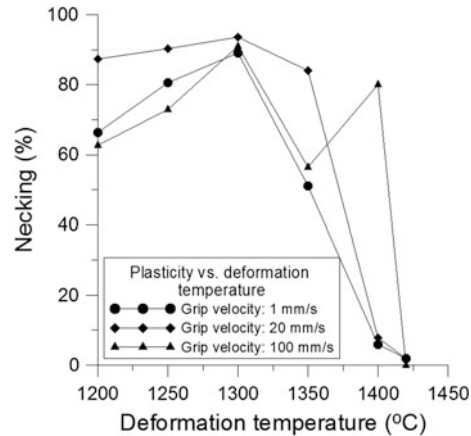


Fig. 7.22 Changes in the ductility of steel S355 as a function of the deformation temperature determined on samples cooled from the liquid state to the deformation temperature at a rate of 10 °C/s



changes in ductility of the steel tested were only determined within the temperature range 1200–1460 °C. Preparing the complete characteristic of ductility changes in a broader temperature range (and for various cooling rates and strain rates) allows one to determine ranges with a reduced ductility. As a result, the evaluation of mechanical properties of samples subjected to various simulation variants provides the basis for developing the so-called “process map” (or casting map), which enables the optimal parameters of continuous casting installation operation when casting the tested steel grade to be determined. In practice, time-temperature-reduction (TTR) diagrams similar to TTT diagrams are constructed. These diagrams show areas with a limited ductility, and thorough knowledge of those areas allows us to adjust the casting process parameters (e.g. the casting speed, the cooling intensity in the primary and secondary zone), so as to avoid the potential threat of breaks in the strand. It is assumed that breaking will occur when the reduction of area at fracture will be lower than 60 % [2].

Fig. 7.23 Changes in the ductility of steel S355 as a function of the deformation temperature determined on samples cooled from the liquid state to the deformation temperature at a rate of 20 °C/s

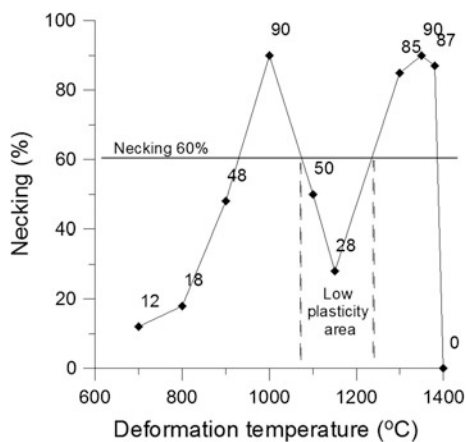


Figure 7.23 presents changes in the ductility of steel S355 as a function of the deformation temperature determined on samples cooled from the liquid state to the deformation temperature at a rate of 20 °C/s [2]. For instance, within the temperature range between 1250 and 1080 °C, cast strand shell breaks will be initiated [2–6].

The last stage of pilot tests involved conducting compression tests to evaluate the possibilities of deformation of the steel tested under the *NDT* temperature. The course of the experiments was based upon previous research. On the basis of the determined characteristic temperatures, the temperature range of experiments was set from the *NDT* temperature to 1460 °C.

The next step was a series of compression tests at a constant tool stroke of 1, 20 and 100 mm/s. The samples were compressed with a constant absolute reduction of 10 mm. In the experiment, the sample was heated to a temperature of 1420 °C at a rate of 20 °C/s. Subsequent heating after reaching 1420 °C was carried out at a rate of 1 °C/s. The next step was holding samples at the set temperature for 60 s. The samples were cooled to the deformation temperature at a rate of 10 °C/s, and then they were held at this temperature for 10 s. The holding operation had the purpose of equalising the temperature in the sample cross-section. During the experiments, the force, temperature and simulator tool stroke were recorded. All tests were carried out using holders with a short contact zone.

Figures 7.24, 7.25 and 7.26 present the selected stages (beginning-centre-end) of the sample deformation for the analysed deformation temperatures and tool strokes. During the physical simulation, the quartz shield, which protects the simulator inside against a potential leak of liquid metal, is destroyed. During the process the central part of the sample, where the biggest strain accumulation occurs, is deformed. During the process the flash effect for tests carried out at a temperature of 1425 °C was not observed, regardless of the applied tool stroke (Figs. 7.24, 7.25 and 7.26). When analysing the force parameters of the test carried out at a temperature of 1425 °C, an increase in the maximum measured force was observed

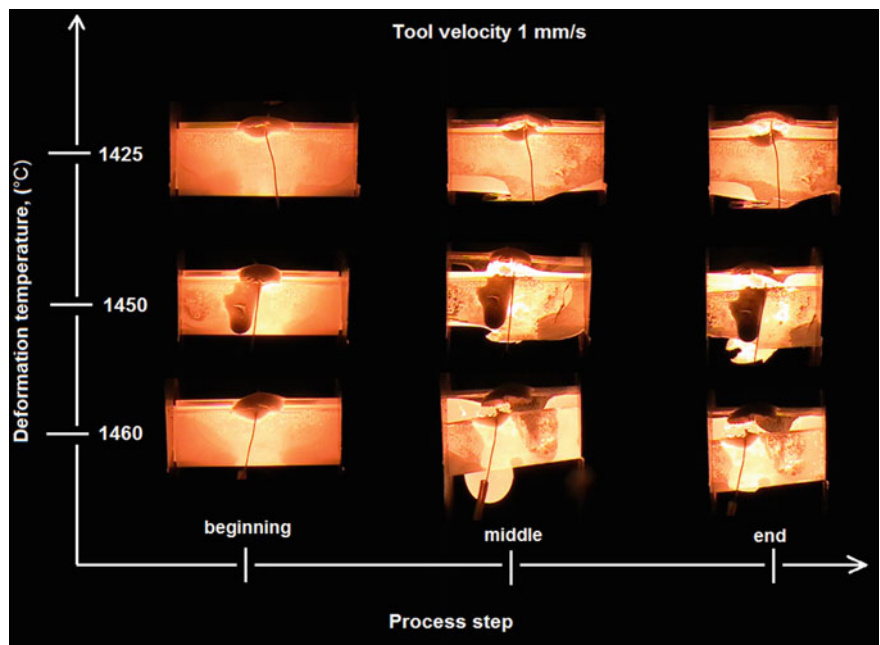


Fig. 7.24 Sample deformation stages for three temperatures and $V_n = 1$ mm/s

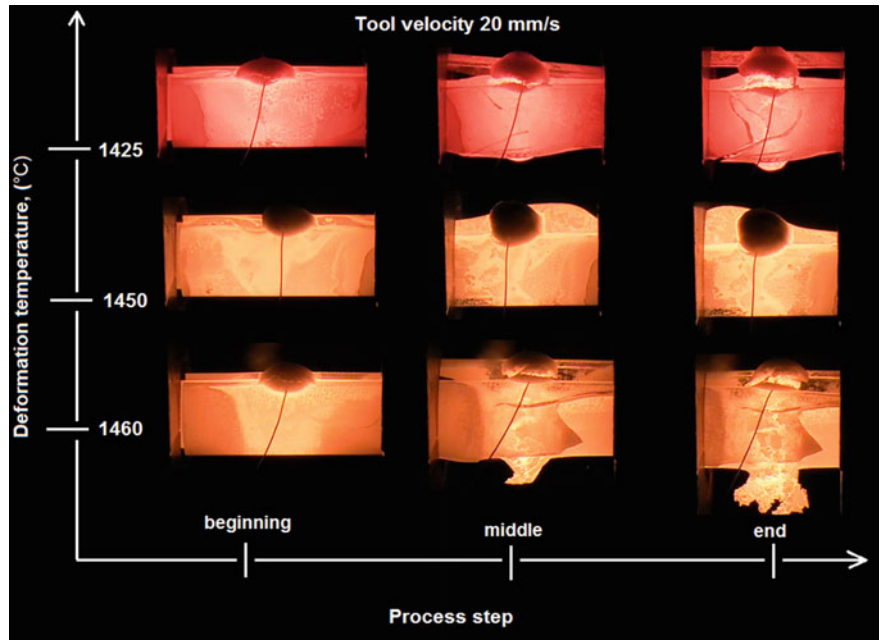


Fig. 7.25 Sample deformation stages for three temperatures and $V_n = 20$ mm/s

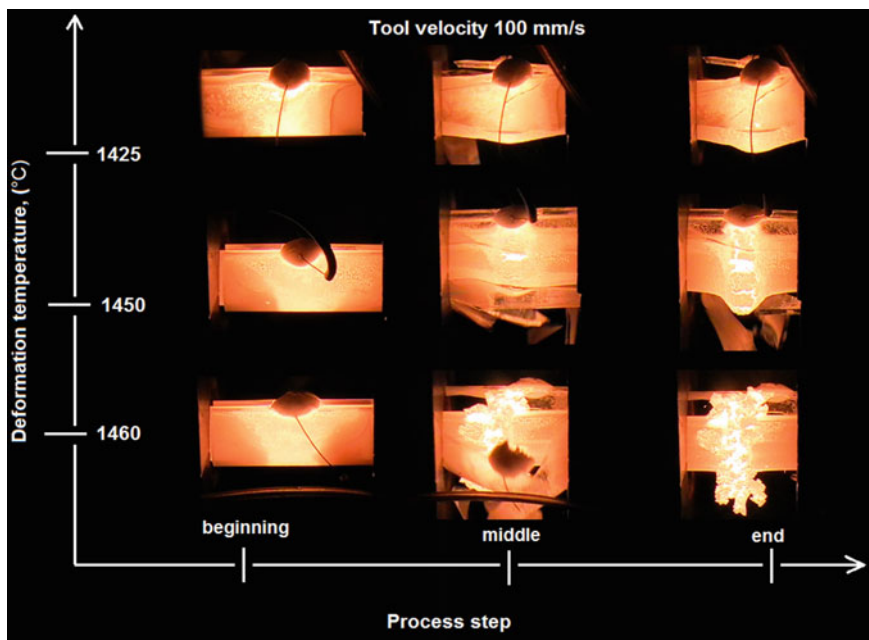


Fig. 7.26 Sample deformation stages for three temperatures and $V_n = 100$ mm/s

along with the tool stroke, which achieved the maximum value of the compression force for $V_n = 1$, $V_n = 20$ and $V_n = 100$ mm/s of -1960 , -2467 and -3534 N respectively [9, 10].

For deformation at temperatures of 1450 and 1460 °C, i.e. above the NST temperature, which for the grade analysed is 1448 °C, the process nature is rapid and unstable [9, 10]. During the deformation process, liquid steel flows out to the simulator inside, or a flash forms, which undergoes rapid crystallization. For deformation at temperatures of 1450 and 1460 °C, for $V_n = 1$, $V_n = 20$ mm/s similar values of the measured compression force were obtained, varying on average from 700 to 400 N. The obtained force values only result from the resistance of the quartz tube and the solidified surface layer of the sample, obtained as a result of cooling to the deformation temperature. In the subsequent deformation steps, the force value remained at a constant level of 400 N. In this case the force was only the resistance of the compressed liquid resulting from the loss of coherence of the solid phase skeleton ($NST = 1448$ °C). The exception was a test performed at 1450 °C for the tool stroke of $V_n = 100$ mm/s. Due to high process dynamics, no flash forming or liquid steel leakage was observed (Fig. 7.26). On the basis of the conducted observations, the deformation processes in conditions of the coexistence of the liquid and solid phase were classified into two categories:

- low dynamic processes (LDP),
- high dynamic processes (HDP).

For the low dynamic processes (LDP), the strain rate is selected so as to enable the deformation test to be conducted at a temperature slightly higher than the *NDT*. On the other hand, for the high dynamic processes (HDP), the strain rate is selected so as to enable the deformation test to be conducted within temperature ranges reaching *NST*.

7.2.3 *Macrostructure and Microstructure*

As part of additional tests a cycle of physical simulations was conducted. The effect of various cooling rates and strain parameters was examined to analyse the sample remelting zone and the forming porous zone. These simulations were performed with “cold” and “hot” grips, and they included tests without deformation and experiments with deformation at the sample remelting stage, during solidification, and a combination of these two variants at the same time. The schedule of physical simulations included the following tests, which in the first phase were performed according to the same temperature programme, i.e. heating to a temperature of 1400 °C at a rate of 20 °C/s, and then to 1485 °C at a rate of 1 °C/s. After heating to a temperature of 1485 °C there was a process of 30-s holding at this temperature. The subsequent stage was performed on the basis of the following programmes:

- Test no. 1 Deformation during remelting only. At the last stage the deformation was only performed in the remelting phase at a stroke of 1.2 mm and a stroke rate of 0.04 mm/s.
- Test no. 2 Deformation in the solidification phase (the beginning of cooling). At the last stage the cooling was performed at the maximum attainable cooling rate and the deformation was performed at the solidification stage (the beginning of cooling) at a stroke of 1.5 mm and a stroke rate of 0.25 mm/s.
- Test no. 3 Deformation in the remelting and solidification phases (the beginning of cooling). Test no. 3 combines the first and second tests. The deformation was performed in the remelting phase at a stroke of 1.2 mm and a stroke rate of 0.04 mm/s, and next at the solidification stage (the beginning of cooling) at a stroke of 1.5 mm and a stroke rate of 0.25 mm/s.
- Test no. 4 Test performed without deformation. Cooling with the set maximum cooling rate of 30 °C/s for the “cold” grips and 10 °C/s for the “hot” grips.
- Test no. 5 Test performed without deformation. Cooling with the set minimum cooling rate of 1 °C/s.
- Test no. 6 Test performed without deformation. Cooling with the set medium cooling rate of 15 °C/s for the “cold” grips and 5 °C/s for the “hot” grips.

Figures 7.27, 7.28, 7.29, 7.30, 7.31 and 7.32 present macrostructures of samples for individual tests. Their nature differs depending on the applied tool variant. After the process of sample etching, the occurrence of a column crystal zone was found in

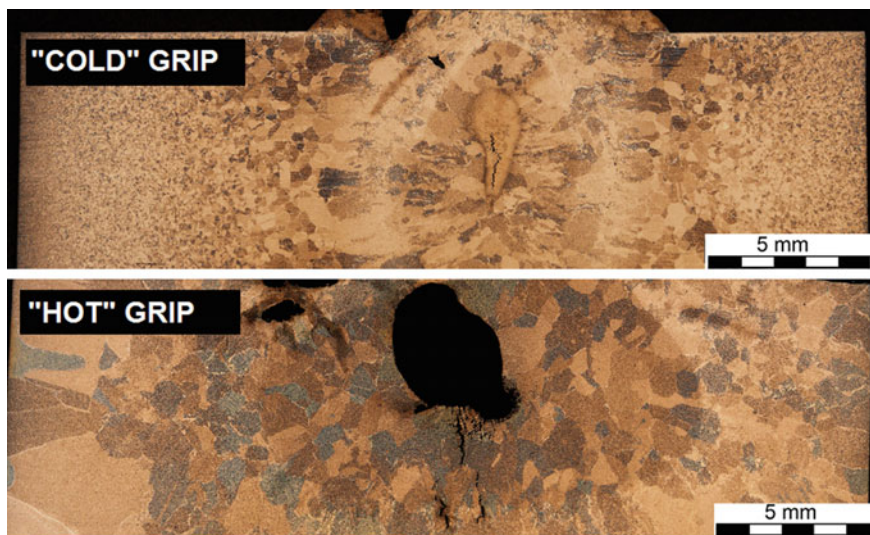


Fig. 7.27 Macrostructure of samples for the variant with deformation in the remelting phase only

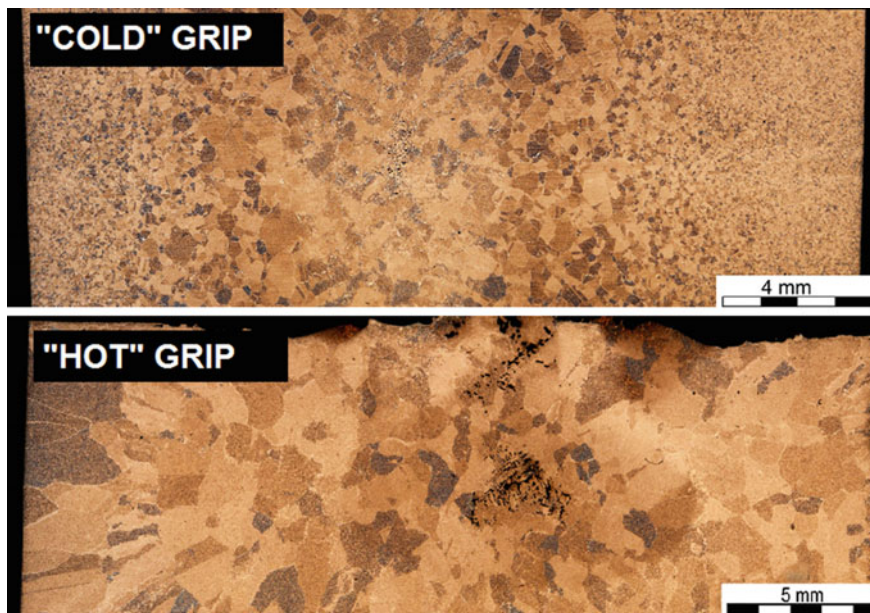


Fig. 7.28 Macrostructure of samples for the variant with deformation in the solidification phase only

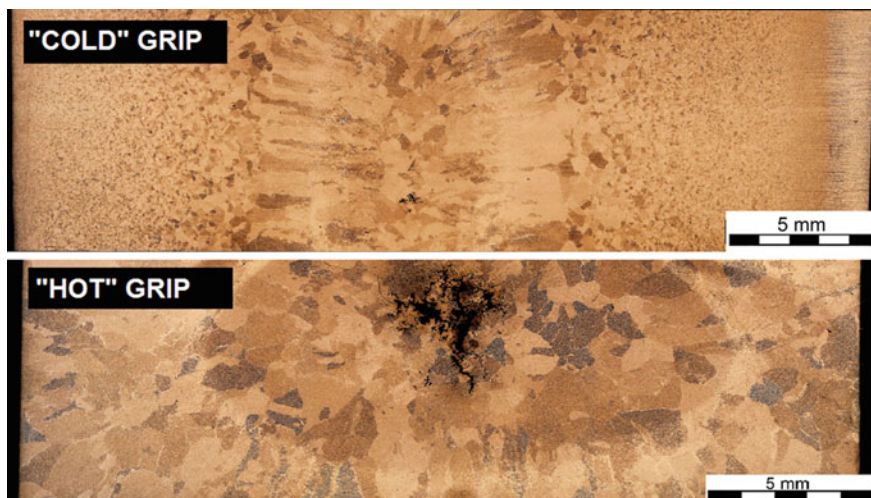


Fig. 7.29 Macrostructure of samples for the variant with deformation in the remelting and solidification phases

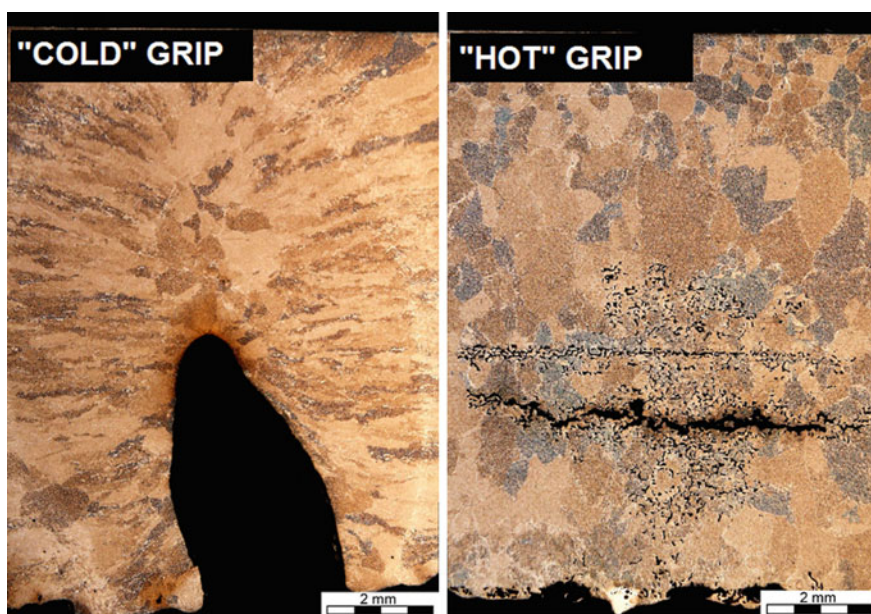


Fig. 7.30 Macrostructure of samples cooled at the maximum rate

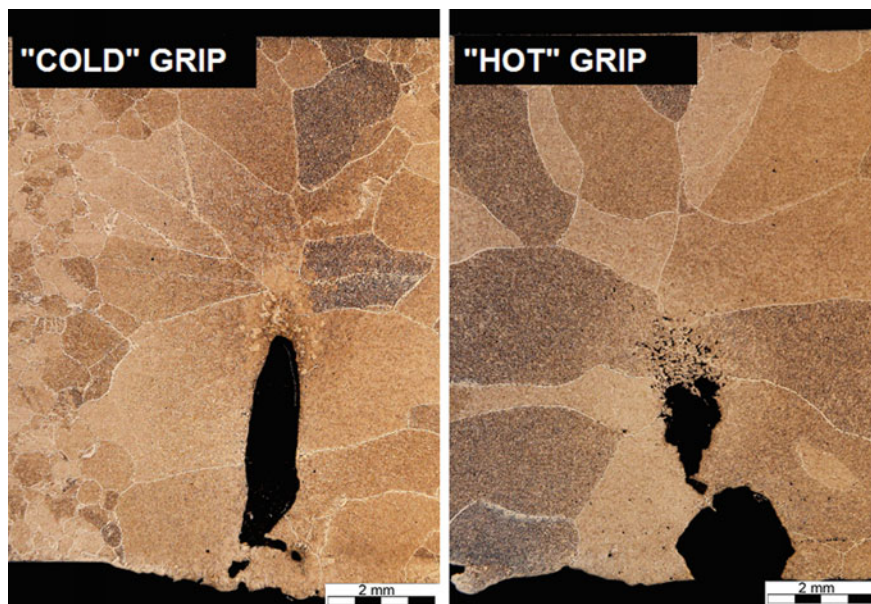


Fig. 7.31 Macrostructure of samples cooled at the minimum rate

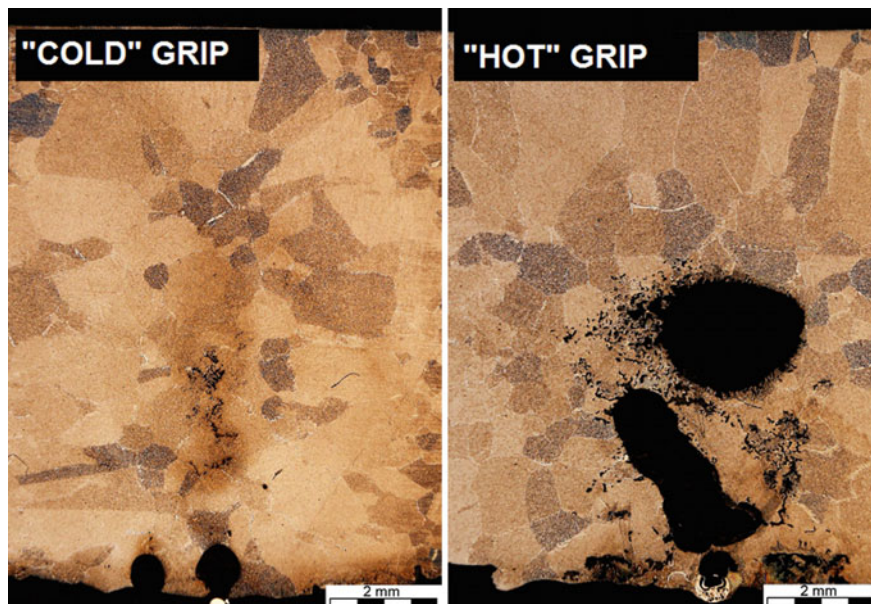


Fig. 7.32 Macrostructure of samples cooled at the average rate

the remelting zone. The crystals were growing in the heat discharge direction (Figs. 7.27, 7.28 and 7.29). In some samples in the middle of the remelting zone a central porosity was found (Figs. 7.27 and 7.29) and in the samples that had not been deformed (Figs. 7.30, 7.31 and 7.32) or had been deformed in the remelting phase only (Fig. 7.27) a shrink hole was found near the place of the control thermocouple installation. Deformation in the solidification phase eliminates the shrink hole, although the occurrence of central porosity was noticed in the samples, which may indicate that insufficient strain was applied.

The nature of the macrostructure of the remelting zone of samples cooled at various rates (Figs. 7.30, 7.31 and 7.32) for both types of grips is characterised by a variable structure. The crystal grain size decreases gradually as the cooling rate increases. The applied grips insignificantly impact the grain size. Apart from a shortened remelting zone (Fig. 7.31) when the “cold” grips are applied, the grain size is slightly smaller compared to grains formed as a result of the “hot” grip application.

Figures 7.33, 7.34, 7.35, 7.36, 7.37 and 7.38 present examples of microstructures for samples cooled using “cold” grips. The simulation variants covered cooling samples with three extremely different cooling rates (Test no. 4, Test no. 5 and Test no. 6). Microstructural tests were performed for two areas of a sample. The sample was first heated and then cooled. The first area covered the core of the

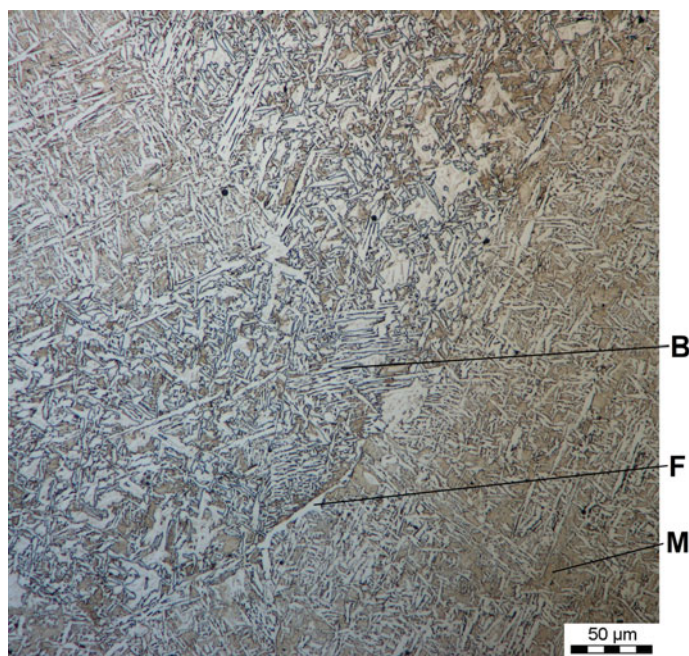


Fig. 7.33 Microstructure of samples cooled at the maximum rate (core of the sample, “cold” grips)

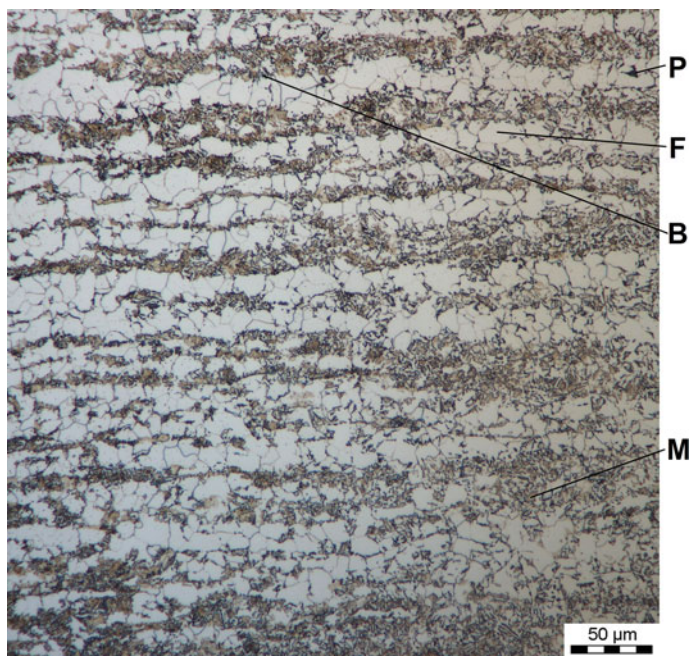


Fig. 7.34 Microstructure of samples cooled at the maximum rate (transition zone, “cold” grips)

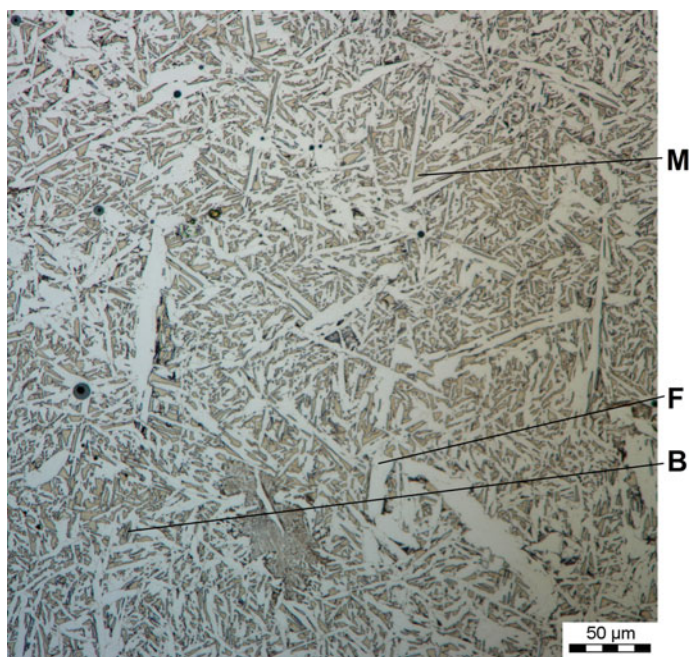


Fig. 7.35 Microstructure of samples cooled at the minimum rate (core of the sample, “cold” grips)

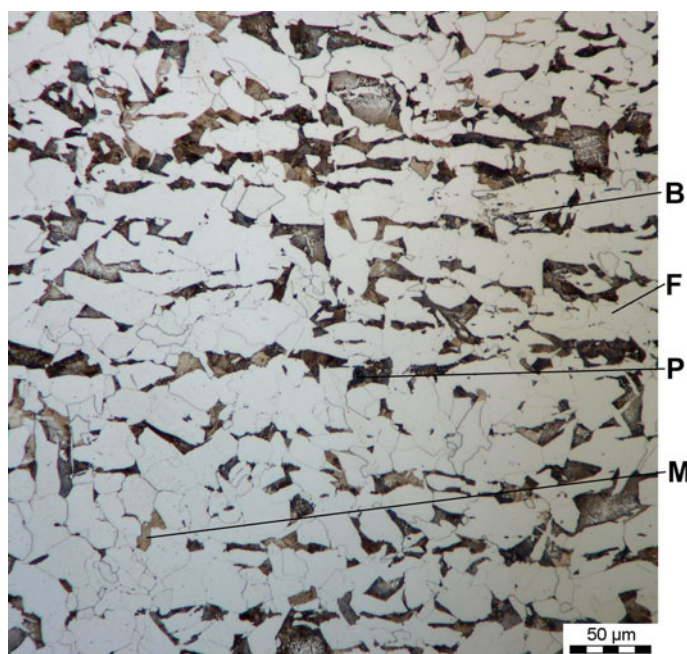


Fig. 7.36 Microstructure of samples cooled at the minimum rate (transition zone, “cold” grips)

sample, whereas the second area included the transition zone. The sample core comprises a mixture of three phases—martensite, bainite, and ferrite. Bainite is a prevailing phase. Ferrite decorates grain boundaries of the former austenite, which are rather large due to a very high temperature (below the solidus temperature) obtained in this sample area. The former austenite is primarily bainite and martensite formed after quenching to the ambient temperature. The martensite share declines in favour of bainite and ferrite when moving towards the transition zone. The ferrite morphology changes from acicular to grainy—and more precisely the ferrite grains have a polygonal (equiaxed) shape. Their size depends on the achieved cooling rate. In the sample zone where the temperature probably has not exceeded A_{c3} we have a banded ferritic-perlitic structure with a certain amount of bainite and/or martensite. The perlite colour depends on the etching degree and may change from dark brown to black. It can be unambiguously shown with e.g. scanning electron microscopy (SEM). In presented Figs. 7.33, 7.34, 7.35, 7.36, 7.37 and 7.38 the individual phases are identified with individual letters: F (ferrite), M (martensite), P (perlite), B (bainite).

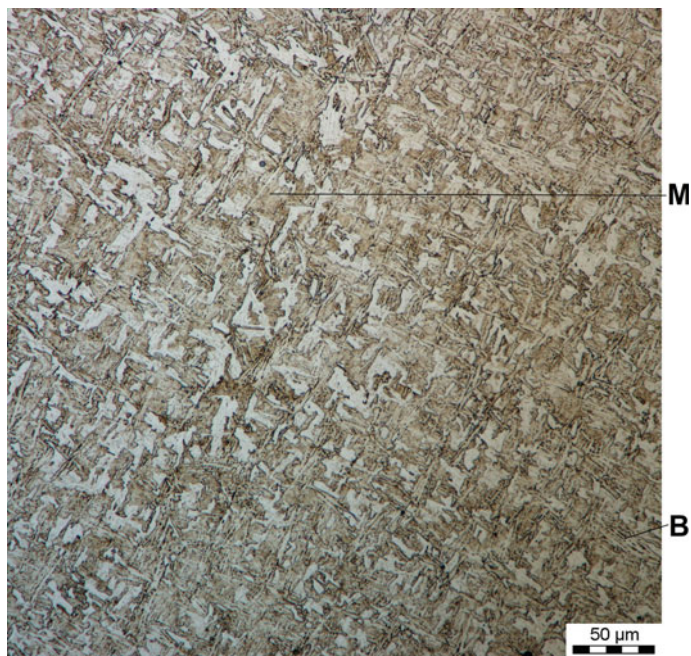


Fig. 7.37 Microstructure of samples cooled at the average rate (core of the sample, “cold” grips)

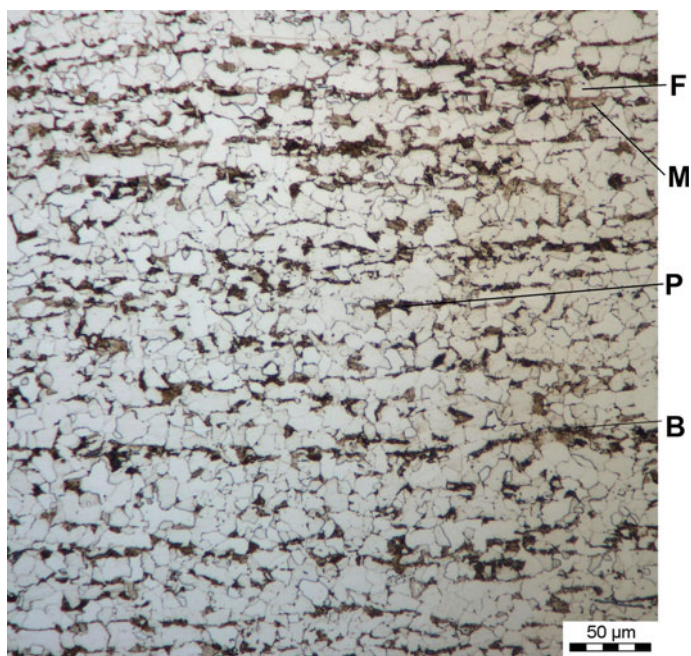


Fig. 7.38 Microstructure of samples cooled at the average rate (transition zone, “cold” grips)

7.3 Summary

This chapter presents the preliminary results of the steel deformation physical simulation in conditions of liquid and solid phase coexistence conducted with a modern thermo-mechanical Gleeble 3800 simulator. Tests were carried out so as to ascertain the possibilities of determining the material characteristics for physical simulations of industrial processes of integrated plate casting and rolling where the essential aim of the simulation was to reconstruct (on a small sample) the changes in temperature and stress in a material which was subjected to both deformation and solidification. Preliminary tests allowed the preliminary concept of a structural model and the research methodology applied in subsequent research to be determined. The structural model will be restricted to the two-phase state, i.e. the mushy zone. The physical simulation will start with melting a sample on a specific section, and next cooling it to the specific deformation temperature T_d . The variables are: temperature T , melting time $\tau_{melting}$ and the rate of cooling V_{ch} to the deformation temperature T_d . The next experiment phase covers the determination of the mechanical properties for a specific state. The variables in this phase are: deformation temperature T_d , strain rate $\dot{\epsilon}$, strain value ϵ and the solid phase fraction f_s . It is essential for the structural model that the stress may be transferred through the solid phase only, the share in the load transfer through the non-solidified liquid may only be related to the resistance dependent on the liquid viscosity. If the liquid can move freely, then we will have a situation similar to real conditions, i.e. reverse liquid flow. Generally, one may assume that probably the share of this component is small, which can be determined on the basis of the parameters of the force recorded during the compression of the liquid in the melting phase. The characteristics necessary to be determined at this stage are the flow curves obtained during tensioning (including the determination of the reduction of area at fracture) and compressing. The obtained stress-strain change curves may constitute the basis for formulating a rheological model of steel deformation within the temperature range of the state of aggregation change. It is important here to stabilise the length of the melted zone. During the execution of the experiment at this stage, cooling at various rates should be planned from the solid state temperature, and then to the ambient temperature in order to determine the influence of this parameter on the structure parameters such as distances between the primary $\aleph_1$ and secondary $\aleph_2$ dendrites. In experiments conducted with deformation performed by compressing a sample, the share of the area with a clearly dendritic structure A_{dend} should be determined and the dependence of this parameter on thermal and mechanical parameters should be determined. It will allow us to assess at which plastic working parameter values the dendritic structure disappears. The samples after deformation should also be cooled quickly enough to determine the grain size of the former austenite and the interdendritic distance. From the perspective of the structural model, one may expect that dependences allowing one to relate the structure parameters to process parameters are obtained. The interdendritic distances $\aleph_1$ and $\aleph_2$ may be determined according to the relationship (Eqs. 7.3 and 7.4), and calculations may be verified by

measurements, which may lead to the determination of new coefficients of Eqs. (7.3) and (7.4) for the steel grade tested. The share of solid phase after precise deformation of the liquidus T_l and solidus T_s temperatures, or the share of dendritic areas may be related to the strain parameters $f(T_d, \varepsilon, \dot{\varepsilon})$. However, to describe the dependence of the yield stress on the temperature and strain rate, Voce's equation may be applied [9, 10].

The conducted experimental research also leads to the following supplementary conclusions:

1. Accurate determination of characteristic temperatures of solidifying steel is necessary to determine the temperature range for which the material cannot be processed plastically.
2. The determined characteristic temperatures allow the steel's susceptibility to fracture to be determined.
3. The Gleeble 3800 simulator may be used to carry out simulation of the soft-reduction and integrated strip casting and rolling processes and to carry out tests to determine the material characteristics.
4. The crystallization rate determined from the relationship provided in the paper [14], on the basis of measurements of distances between secondary dendrites is the best to reflect the measured cooling rate in the conducted experiments.
5. Implementation of the strain in the crystallisation phase causes the dendritic structure to disappear.

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Chapter 8

Modelling Concept Based upon Axially Symmetrical Models

The present chapter presents identification strategies of yield stress investigation of steels based on tensile and compression tests at very high temperatures as well as in the semi-solid state. The methodologies of stress-strain curves investigation combine the possibility of direct simulation using the Gleeble 3800 thermo-mechanical simulator with the developed dedicated DEFFEM system with implemented axial-symmetrical solutions. The constitutive parameters identified by these procedures have been successfully applied in additional three-dimensional tests (see Chap. 9). Due to very high sensitivity of the material rheology to temperature changes, the testing procedure requires as uniformly distributed temperature as possible. As part of the research aimed at the development of the foundation of the methodology for determining the mentioned stress-strain relationships, comprehensive tests were performed covering the influence of the applied grips on the temperature distribution along the heating zone and in the sample cross-section, as well as macro- and microstructural tests, and comprehensive tomographic tests. The findings of the conducted tests allowed the obtained computer simulation results to be verified. The computer simulations were performed using the modelling concept based upon axially symmetrical models.

8.1 Direct Simulation Using the Gleeble Thermo-Mechanical Simulator

Deformation processes of steels in the semi-solid state and their resistance heating close to the solidus line are effectively supported by the use of physical simulations [1]. Resistance heating is the first stage of the testing procedure. Steel grade C45 was selected as the test material. Cylindrical specimens with a diameter of 10 mm and a length of 125 mm were tested with the Gleeble 3800 thermo-mechanical simulator. The specimen was heated by resistance heating, with an automatically controlled

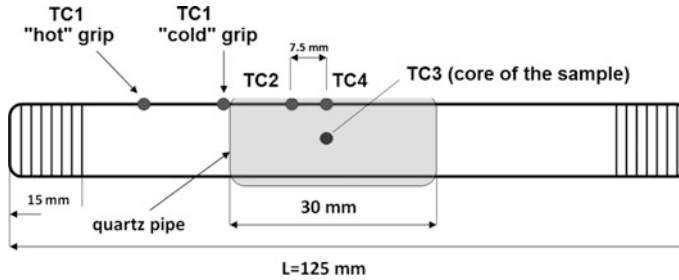


Fig. 8.1 Samples with thermocouples locations used for the experiments: TC1, TC2, TC3 and TC4 thermocouples

alternating current being introduced into the specimen through cooper grips. At the first stage, the specimen was rapidly heated up to $1350\text{ }^{\circ}\text{C}$ at a heating rate of $20\text{ }^{\circ}\text{C/s}$. At the second stage, the specimen was slowly heated up to $1430\text{ }^{\circ}\text{C}$ at a heating rate of $1\text{ }^{\circ}\text{C/s}$ and held at this temperature for 30 s . Finally, the specimen was cooled down to the nominal test temperature (T_{nom}) at a cooling rate of $10\text{ }^{\circ}\text{C/s}$ and held at this temperature for either one minute or 10 s depending on the kind of test. Material testing of semi-solid steel should be carried out under isothermal conditions (as isothermal as possible) due to the very high sensitivity of the steel rheology to temperature changes. This is why the temperature distribution inside the tested specimens should be analysed. The basic reason for non-uniform temperature distribution inside specimens on the Gleeble 3800 simulator is their contact with the cooper grips during resistance heating. During the whole testing period, the current intensity is automatically controlled in response to the difference between the prescribed temperature and the actual temperature measured by a thermocouple welded to the surface of the samples at half of their heights (Fig. 8.1). To prevent oxidation, the specimen is located in a vacuum chamber. A transparent quartz sleeve was used to protect against a potential leakage of the metal during remelting. In order to find out the temperature distribution along the heating zone within the specimen, temperatures are continuously measured at several locations (Fig. 8.1)—along the heating zone of the specimen, at three locations: mid-length (TC4), 7.5 mm from the centre (TC2) and near the contact interface sample-die (TC1). This provides information on the axial temperature gradient. Additionally, a TC4 thermocouple is used for the monitoring of the electrical input. The last thermocouple (TC3) was mounted in the core of the specimen by drilling a hole at an angle of 45° . In comparison with TC4, this gives access to the radial temperature gradient.

8.1.1 Testing the Temperature Distribution

As mentioned above, due to the very high sensitivity of the material rheology to temperature changes, the testing procedure requires as uniform temperature

Fig. 8.2 Changing the temperature during the heating and melting process (variant with the “cold” grips)

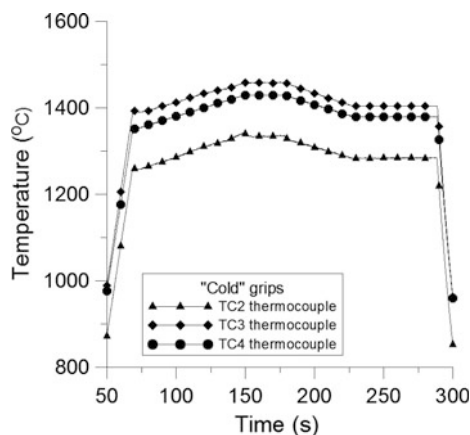
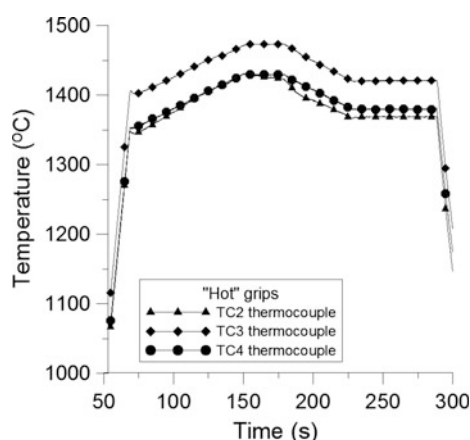


Fig. 8.3 Changing the temperature during the heating and melting process (variant with the “hot” grips)



distribution as possible [1]. In the case of direct modelling with the Gleeble 3800 simulator, the temperature gradient always exists at high temperatures. Because the mechanical properties of steel are temperature dependent, such thermal gradients are the main sources of deformation heterogeneity in the test samples.

Figures 8.2 and 8.3 present the courses of temperature changes measured by thermocouples (TC2, TC3, TC4) for a test conducted at a temperature of 1380 °C using both “cold” and “hot” grips. The analysis of the obtained courses clearly indicates that a significant temperature gradient exists between the temperature measured by the control thermocouple (TC4) and by the thermocouple installed inside the sample (TC3). The conducted additional experiments showed that the effect of holding time in the final remelting phase (60 s) did not influence the temperature gradient. Therefore, in the subsequent tests this time was shortened to 10 s, and some tests were repeated twice [1].

Table 8.1 Temperature measurement results for the test with the “cold” grips (thermocouples TC3 and TC4)

“Cold” grips	Test no. 1		Test no. 2	
	TC4 (°C)	TC3 (°C)	TC4 (°C)	TC3 (°C)
Stage just before deformation	1380	1411	1380	1412
Difference between TC4 and TC3	+31	–	+32	–

Table 8.2 Temperature measurement results for the test with the “cold” grips (thermocouples TC1, TC2 and TC4)

“Cold” grips	Test no. 1			Test no. 2		
	TC4 (°C)	TC1 (°C)	TC2 (°C)	TC4 (°C)	TC1 (°C)	TC2 (°C)
Stage just before deformation	1380	637	1291	1380	631	1284
Difference between TC1 and TC4	–	+743	–	–	+749	–

Table 8.3 Temperature measurement results for the test with the “hot” grips (thermocouples TC3 and TC4)

“Hot” grips	Test no. 1		Test no. 2	
	TC4 (°C)	TC3 (°C)	TC4 (°C)	TC3 (°C)
Stage just before deformation	1380	1419	1380	1421
Difference between TC4 and TC3	+39	–	+41	–

Table 8.4 Temperature measurement results for the test with the “hot” grips (thermocouples TC1, TC2 and TC4)

“Hot” grips	Test no. 1			Test no. 2		
	TC4 (°C)	TC1 (°C)	TC2 (°C)	TC4 (°C)	TC1 (°C)	TC2 (°C)
Stage just before deformation	1380	341	1368	1380	343	1369
Difference between TC1 and TC4	–	+1039	–	–	+1037	–

The measurements for individual readings of thermocouples for the recorded stage just before the sample deformation process with the “cold” grips are compared in Tables 8.1 and 8.2. For experiments with the “hot” grips the temperature measurements for individual thermocouples are shown in Tables 8.3 and 8.4. The obtained difference between the control thermocouple (TC4) and the thermocouple

measuring the temperature at the sample core (TC3) for tests with the “cold” grips was on average about +31.5 °C (Table 8.1). For the measurement along the sample heating zone length between thermocouples TC1 and TC4, installed near the place of contact of the tool with the sample, it was on average about +746 °C (Table 8.2).

For the tests carried out with the “hot” grips, the obtained difference between the control thermocouple (TC4) and the thermocouple measuring the temperature at the sample core (TC3) was on average about +40 °C (Table 8.3), whereas for the measurement along the sample heating zone length between thermocouples TC1 and TC4, installed near the place of contact of the tool with the sample, it was on average about +1038 °C (Table 8.3).

In both tool variants the obtained sample core temperature was higher than the reading of the control thermocouple (TC4). The analysis of the obtained findings on the basis of the determined characteristic temperatures (for steel C45 the liquidus T_l and solidus T_s temperatures were 1495 and 1410 °C, respectively) indicated the existence of the semi-solid phase within the sample core. For the tests carried out at higher temperatures the temperature gradient in the sample cross-section increased (readings between thermocouples TC3 and TC4).

8.1.2 Macrostructure and Microstructure

The analysis of temperature distribution along the sample heating zone (readings between thermocouples TC1 and TC4, see Tables 8.2 and 8.4) indicate a significant influence of the applied grip type on the temperature distribution along the heating zone. When analysing the sample macrostructure (Fig. 8.4) one can specify four visible zones: the zone of applied grip direct impact (1), the area of heat impact only (2), the transient zone (3) and the total remelting zone (4).

Figure 8.5 presents the macrostructures obtained for the test performed at a nominal temperature of 1425 °C for both tool variants. Metallographic specimens were made for two areas: the sample core and the area near the direct contact of the sample with the tool. The macrostructure of the sample core and the nominal test temperature (above the solidus temperature) in both variants indicates the formation of a distinct porous zone. The porous zone was caused by remelting of the central

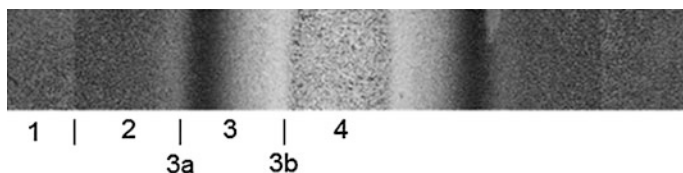


Fig. 8.4 A photo of the sample macrostructure with marked zones: (1) the impact area of “cold” grips, (2) the heat impact area, (3a) the beginning of the transition zone, (3b) the end of the transition zone, (4) the total remelting

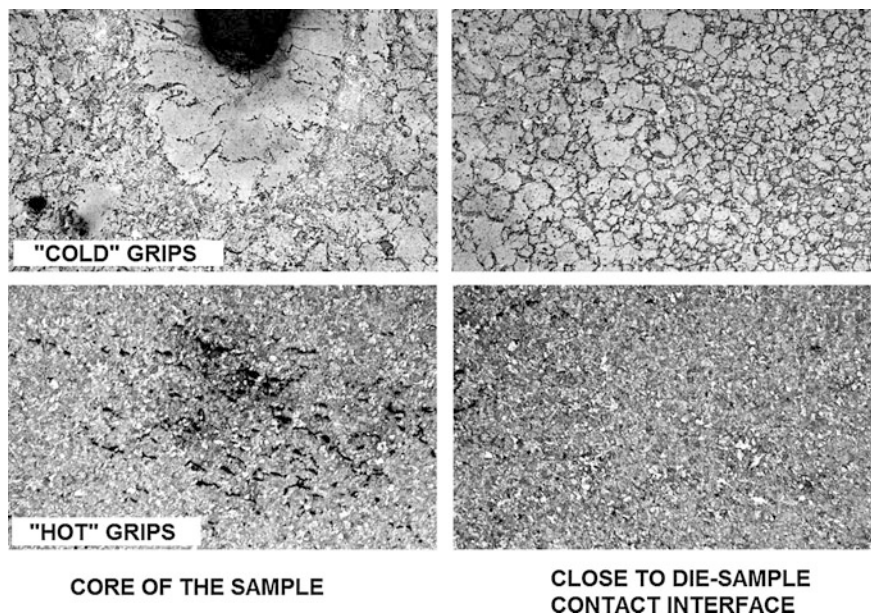


Fig. 8.5 The macrostructure of samples for two specific regions of the sample ("hot" and "cold" grips, TC4 = 1425 °C)

part of the sample during the experiment. The macrostructure of the areas of direct contact of the sample with the tool is entirely different. The application of the "hot" grips variant in the experiments leads to the obtaining of a fine structure. For the "cold" grips variant the obtained structure is coarse.

The macrostructures presented in Fig. 8.6 were made for the same areas of the sample. For the "cold" grips a clear transient zone is visible, while for the "hot" grips variant the sample remelting zone effect can also be seen (a porous zone area can be observed).

As may be concluded, the type of applied grips directly influences the size of the attainable sample remelting zone, which for the "hot" grips is bigger than for the "cold" grips (Fig. 8.7).

Metallographic specimens (longitudinal sections) of samples deformed at various temperatures with "cold" grips are presented in Fig. 8.8. Photos of macrostructures were presented in two forms: a standard flat view and a stereoscopic view (anaglyph). To analyse the obtained macrostructure in a 3D view, one needs to use red-cyan type spectacles, which are commonly available. The applied anaglyph technology is amongst the oldest technologies of stereoscopic imaging. It is about superimposing coloured pictures of a stereo-pair, slightly shifted horizontally. The component images of the stereo-pair are very similar but they slightly differ in the angles of view of the objects and details of mutual obstruction of objects in the scene. These slight differences convey the information about the third

Fig. 8.6 The macrostructure of the samples for the same regions of a sample (the “hot” and “cold” grips, TC4 = 1425 °C)

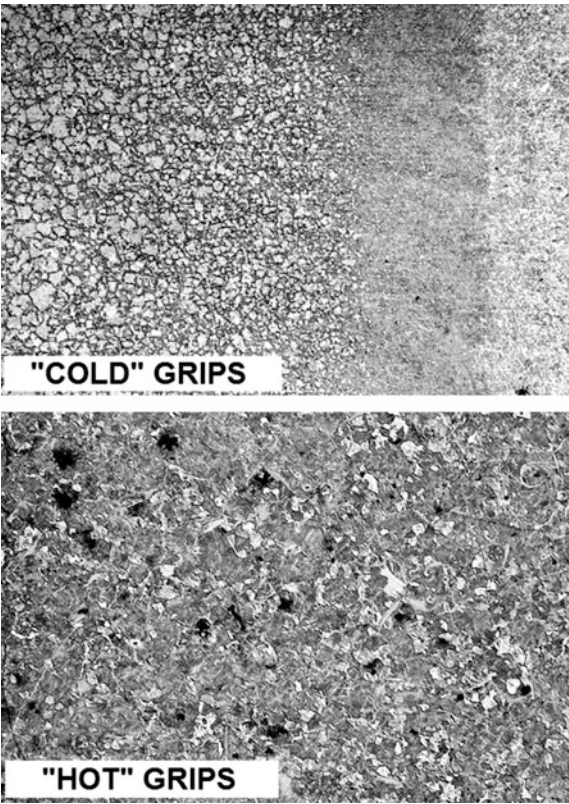
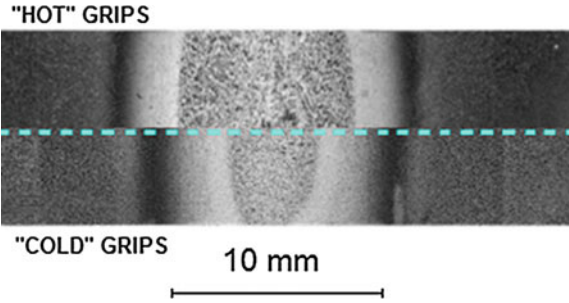


Fig. 8.7 Comparison of remelting zone sizes for both variants of the applied tools



dimension. The macrostructure of samples deformed with the “hot” grips is presented in Fig. 8.9. Bearing in mind the existing temperature gradient on the cross-section of the sample (regardless of the applied grips), areas of the mushy zone occurrence can be seen in the sample core. The size of this zone is determined by the type of the applied grips, where for the “hot” grips (Fig. 8.9) this zone is bigger than for the “cold” grips (Fig. 8.8).

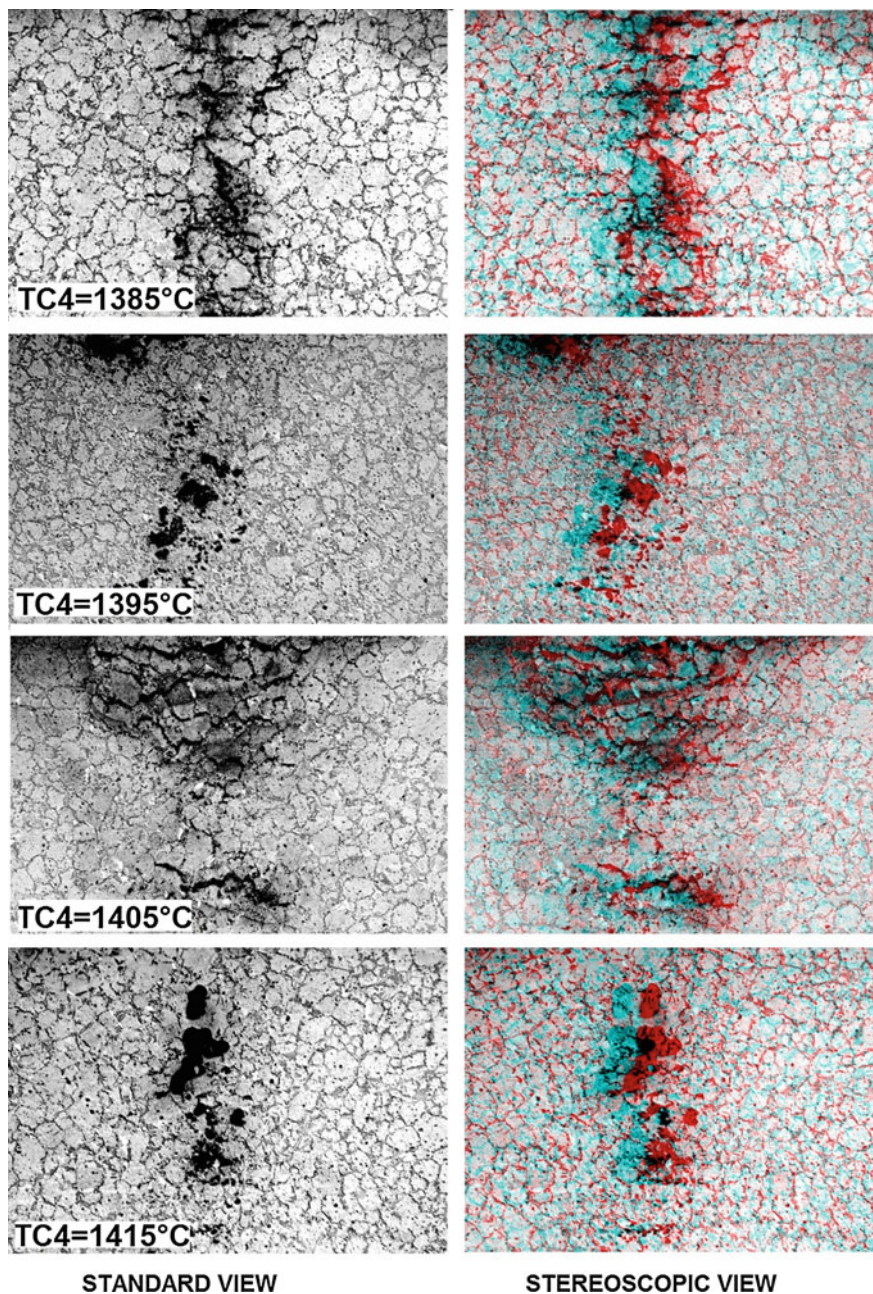


Fig. 8.8 Macrostructure of the samples deformed at various temperatures (the variant with the “cold” grips, magnification 10×, standard and stereoscopic view)

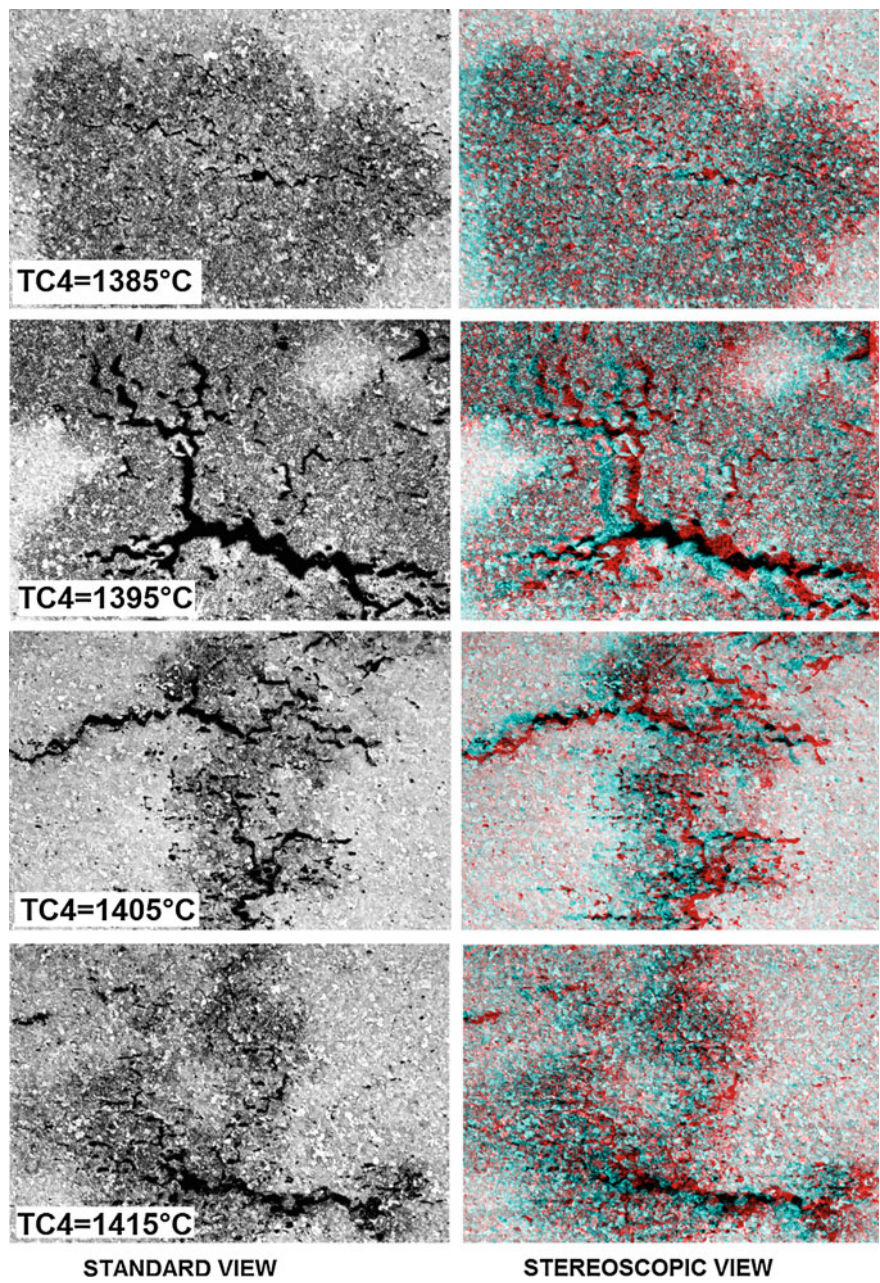


Fig. 8.9 Macrostructure of the samples deformed at different temperatures (the variant with the “hot” grips, magnification 10×, standard and stereoscopic view)

Table 8.5 The average cooling rate within the range of 800–500 °C for the samples heated in the “cold” grips

Nominal test temperature (°C)	Average cooling rate within the range of 800–500°C (°C/s)
1385	16.75
1395	14.82
1405	16.97
1415	16.98
1425	16.98

Table 8.6 The average cooling rate within the range of 800–680 °C for the samples heated in the “hot” grips

Nominal test temperature (°C)	Average cooling rate within the range of 800 °C–ca. 680 °C (°C/s)
1385	7.74
1395	7.93
1405	7.69
1415	8.05
1425	8.11

The next stage of the basic tests was the determination (estimate) of the average cooling rate of samples heated in the “cold” and “hot” grips. The temperature range in which the cooling rate was analysed was 500–800 °C. Results obtained for the “cold” grips are presented in Table 8.5 and for the “hot” grips in Table 8.6.

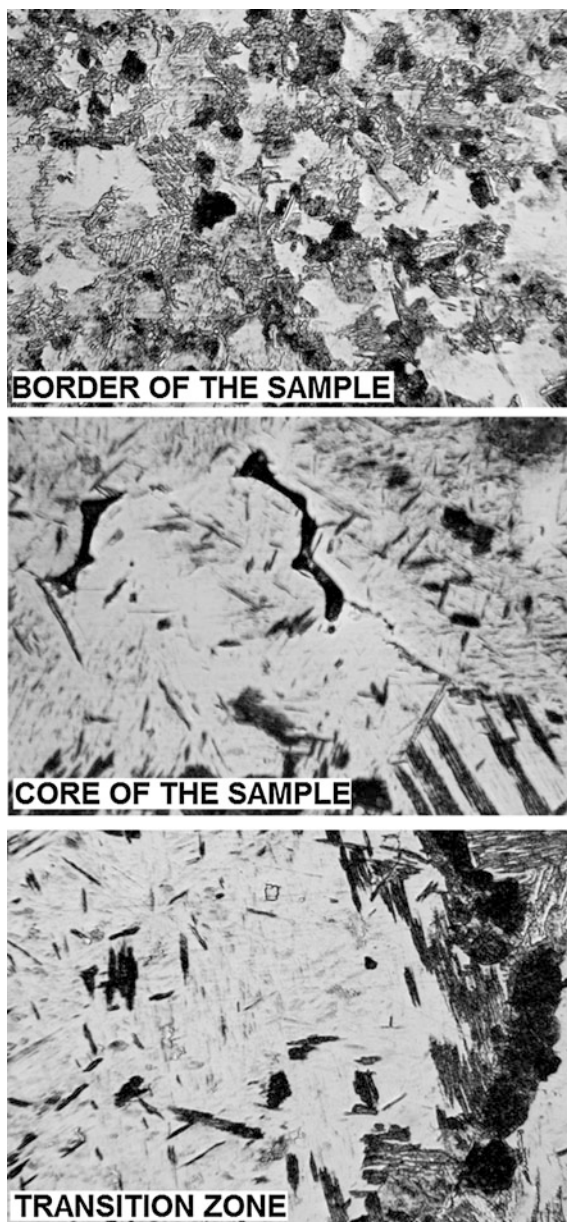
As mentioned above, regardless of the applied method of temperature measurement one can notice a substantial temperature difference between the centre and the surface of a sample, and the temperature measured in the centre of the sample is higher. This difference may exceed 40 °C for the “hot” grips, while for the “cold” grips it reaches about 32 °C.

Also, a decrease in the cooling rate by almost half was found. The cooling rate within the temperature range 800–680 °C was about 8 °C/s for the “hot” grips. For the “cold” grips the average cooling rate within the temperature range 800–500 °C was about 17 °C/s.

Figures 8.10, 8.11, 8.12 and 8.13 present the microstructure of the samples heated in the “cold” and “hot” grips. For the samples cooled in the “cold” grips (Figs. 8.10 and 8.11) the microstructure consists of perlite (the black phase, pie-shaped areas), bainite (the grey phase), bright ferrite (mainly at the edge of the sample), and martensite (in the middle and in the transient zone). The martensitic areas differ from ferrite by a clear needle-like surface relief.

The microstructure of samples cooled in the “hot” grips (Figs. 8.12 and 8.13) clearly differs from the ones previously discussed and consists mainly of perlite (the darkest phase), bainite (the grey phase mainly near the grain boundaries) and bright

Fig. 8.10 The microstructure of the samples for three specific regions of the sample (“cold” grips, TC4 = 1425 °C, magnification 400×)



ferrite. Phase composition like this results in a broad remelting zone and the cooling rate for the samples heated in the “hot” grips is lower by almost half. In the central part of the samples, holes of various shapes are observed. Apart from the porosity (oval-shaped holes), there are cracks on grain boundaries, which result from shrinkage during the solidification of the re-melted part of the material.

Fig. 8.11 Microstructure for the border of the sample (“cold” grips, TC4 = 1385 °C, magnification 400×)



Fig. 8.12 The microstructure for the border of the sample (“hot” grips, TC4 = 1425 °C, magnification 400×)

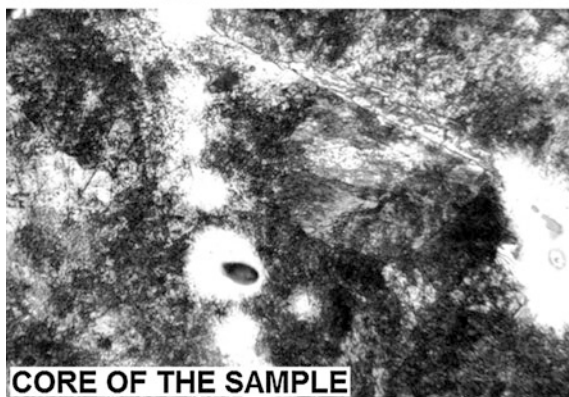
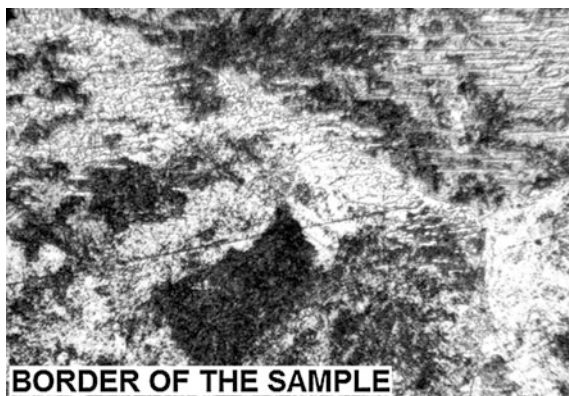
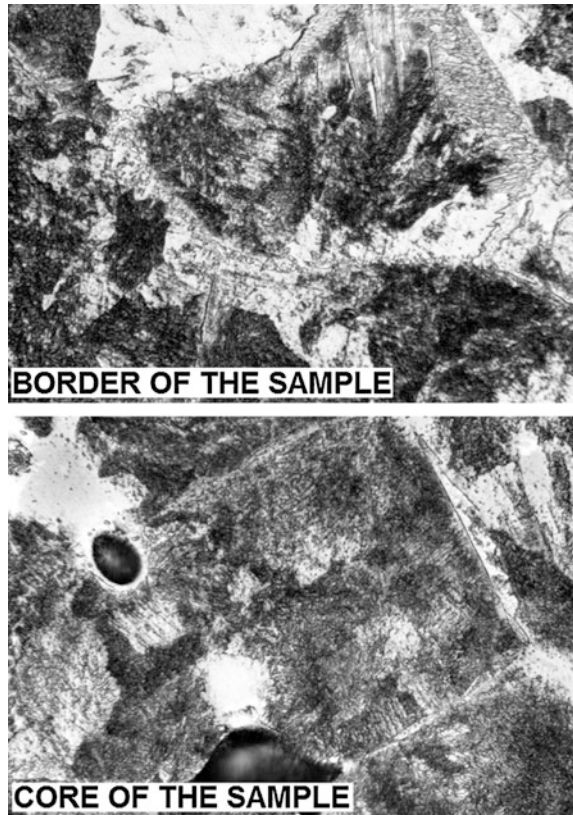


Fig. 8.13 The microstructure for the border of the sample (“hot” grips, TC4 = 1385 °C, magnification 400×)



8.2 Application of Tomography to the Spatial Analysis of the Melting Zone

The micro-tomography measurements were performed using a NANOTOM 180 N device [2]. The machine is equipped with a nanofocus X-ray tube with a maximum voltage of 180 kV. The tomograms were recorded on a Hamamatsu 2300×2300 pixel detector. The reconstruction of the measured objects was performed with the aid of proprietary GE software datosX ver. 2.1.0 with the use of the Feldkamp algorithm for cone beam X-ray CT [3]. The post-reconstruction data treatment was performed using VGStudio Max 2.1 [4] and free Fiji software [5] with plugin BoneJ [6] and Voxler 3 Golden Software [7]. All examined specimens were scanned at 160 kV of source voltage and 60 μA , with a rotation of the specimen by 360° in 1600 steps. An aluminium filter of 0.5 mm was applied between the source and the sample. The exposure time was 500 ms and a frame averaging of 6 and image skip of 1 were applied, resulting in a scanning time of 93 min. The reconstructed images had a voxel size of 6.2 μm .

Both samples denoted as C1 (the variant with the “cold” grips) and H1 (the variant with the “hot” grips) underwent the same initial preparations before the final analysis. The reconstructions were denoised using a 3D median filter with a kernel size of $3 \times 3 \times 3$, followed by the edge smoothing procedure with a 2D median filter with a 3×3 kernel. Next, both samples were reoriented in the way that the origin of the reference system was located in the middle of the vertical axis (Z axis) of the sample. The Y axis has a radial direction and coincides with the porous changes in the sample. The X axis is perpendicular to Y and Z with its direction fulfilling the clockwise reference system orientation (Fig. 8.14). Figure 8.14 shows the reconstructed surface of the samples with a visible melting zone produced during the experimental process. The surface topography shows significant differences between samples. Substantial changes on the sample C1 surface were observed, the structure formed in the melting zone resembles a porous material. For the second sample (H1) similar changes were observed, although they were smaller, and the surface in this area was rougher. Changes on the surface had an impact on the defected area inside the samples.

In Fig. 8.15 both samples were presented with a transparent surface, enabling to observe not only the outer surfaces of the sample but also its inside.

The nature of the obtained pores for both samples was different. In both cases, behind the melted area, visible on the surface, a considerable defected area occurred. Despite the C1 sample having a much more complex surface structure of the melt, the porous area formed behind that area was much smaller in terms of the total volume than in the H1 sample. Specific defects, visible as bright spots on the material surface at the bottom of the sample, were observable. These were the areas of the material stratification. In the H1 sample, despite a much more extensive area with visible pores and some observable regularities in their spatial arrangement, no defects close to the surface were observed. In both cases, the porous area ends near the sample symmetry axis.

In the next step, a threshold value within the tomography images was selected, to differentiate between the areas filled with the material and the voids (empty areas). For this purpose, signal intensity changes on the reconstruction images were analysed. Figure 8.16 presents these changes for voids spaced apart from each other

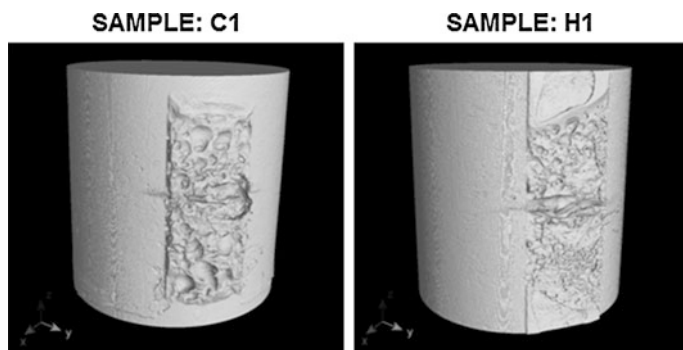


Fig. 8.14 Reconstructed surface of the sample C1 (“cold” grips) and H1 (“hot” grips)

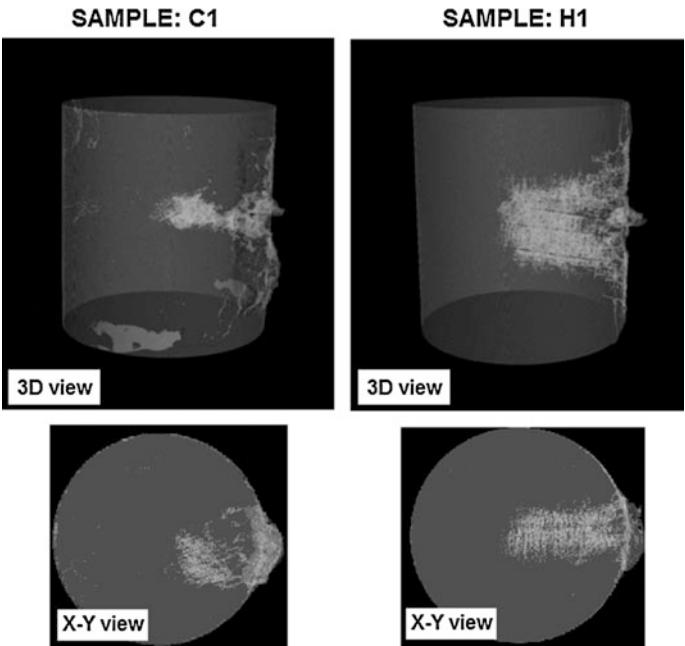


Fig. 8.15 Visualization of samples with transparency

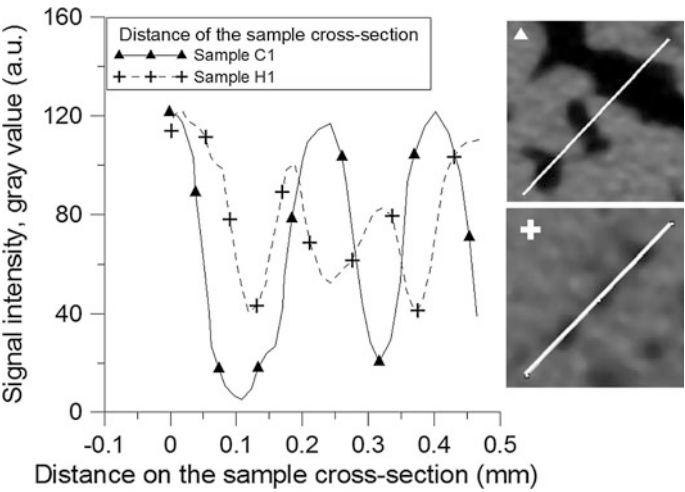


Fig. 8.16 Signal intensity on sample reconstruction cross-section measured along *lines* marked in *triangles* and *crosses*. *Dark* parts of the images correspond to the *holes*, *light* parts to the *metal*

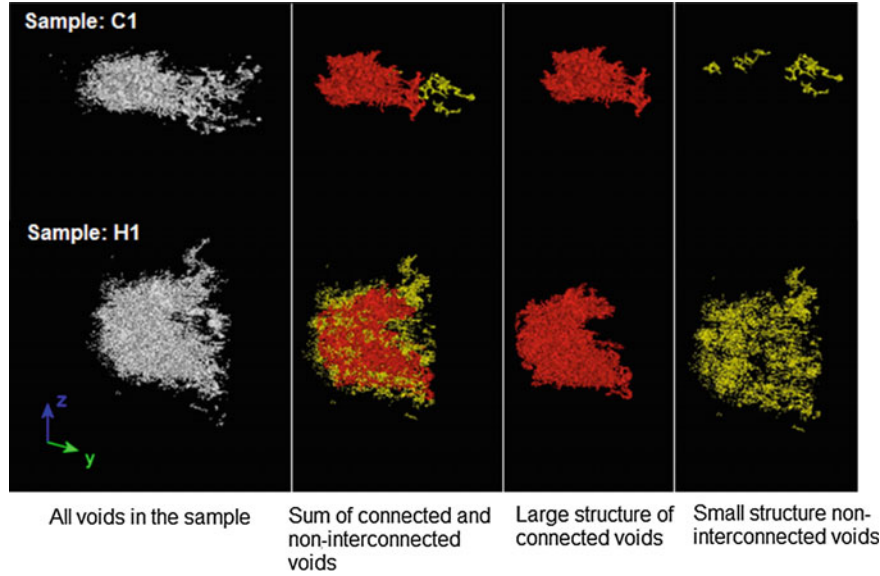


Fig. 8.17 The spatial structure of all voids in samples C1 and H1

(solid line with triangles) and closely located (broken line with crosses). On the basis of the curve analysis, it was decided to assume the threshold value of 70. The reconstructed object areas with values below the threshold will be treated as voids, the areas above the threshold as solid metal.

After binarisation a complex internal structure of the voids in both samples was obtained (Fig. 8.17). Further analysis was based on the description of the voids within the material. For this purpose, fragments belonging to the surface were removed from the data analysed. The analysis of the voids' continuity shows that in each sample there are only one large structure of interconnected voids and numerous small separated voids. Figure 8.17 presents the spatial structure of all voids—a large structure of connected voids and small separated voids.

To evaluate the structure topology in both samples several parameters were calculated (detailed definitions of all parameters are given in [6, 7]). Short descriptions of the calculated parameters are listed below. All parameters were calculated using ImageJ with Plugin BoneJ. The results are presented in Table 8.7:

- (a) Volume: the total volume in the selected volume of interest.
- (b) Surface: the surface area of the structure. An iso-surface forms a triangular surface mesh by marching cubes algorithm and the surface area is calculated as the sum of the areas of the triangles making up the mesh. The triangulation uses smoothing algorithms, so the sum of the area calculated for the structure and for the holes does not have to be equal to the area calculated together for the structure and the holes.

Table 8.7 Morphological parameters calculated for examined samples

Parameter	Units	Sample: C1			Sample: H1		
		Total	Structure	Holes	Total	Structure	Holes
Volume	(mm ³)	1.27	1.10	0.05	4.69	3.76	0.93
Surface	(mm ²)	77	58	4	300	304	80
Roughness	–	60.8	53.0	75.5	64.0	80.9	0.20
Mean diameter	(mm)	0.069	0.075	0.053	0.053	0.057	0.040
St. dev. of mean diameter	(mm)	0.034	0.033	0.022	0.019	0.019	0.016
Maximal diameter	(mm)	0.181	0.181	0.107	0.149	0.149	0.120
Degree of anisotropy	–	0.09	0.10	1.0	0.45	0.49	0.42

- (c) Roughness: the area of the particle divided by the volume of the particle. A low value of roughness means a smoother surface. A high value of this ratio means a more rugged surface.
- (d) Mean diameter: the average diameter.
- (e) St. dev. of mean diameter: the standard deviation of the mean diameter of a particle.
- (f) Maximal diameter: the diameter of the largest particle.
- (g) DA: the degree of anisotropy, DA is 0 for isotropy and 1 for extremal anisotropy.

Distributions of the void diameters are presented in Fig. 8.18. In both samples a large number of unconnected voids was found. In the C1 sample, there were more than 1500 and in the H1 sample over 4500 holes. The void size (volume) distribution for both samples is shown in Fig. 8.19. For both samples, the volume of the voids in each 6.25 μm-thick layer, perpendicular to the sample symmetry axis, was determined. The centre of the coordinate system was arbitrarily located in the position of the sample higher porosity (close to the centre). The void volume distribution along the sample symmetry axis

Fig. 8.18 Distribution of the void diameters in both samples

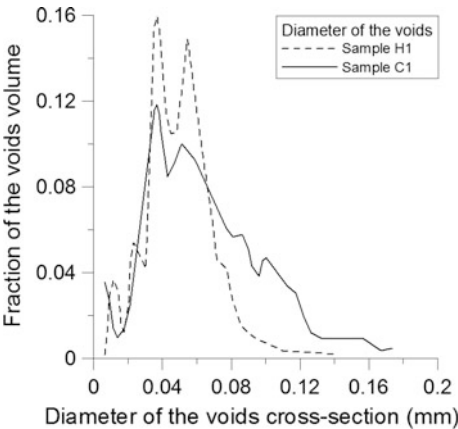


Fig. 8.19 Distribution of hole volumes in both samples

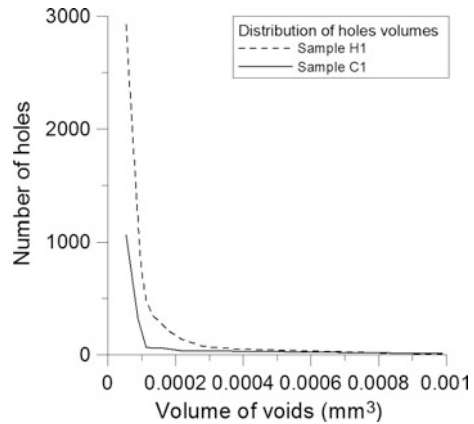
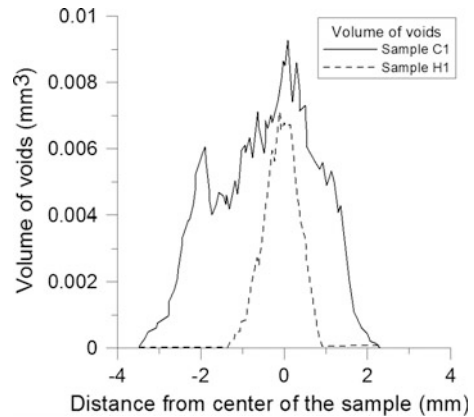


Fig. 8.20 Volume of the voids in the 6.25 μm layer perpendicular to the symmetry axis of the samples



is presented in Fig. 8.20. Both samples have a comparable maximum porosity near the centre, but the porous zone is much wider in the C1 than in the H1 sample.

In order to present the spatial distribution of coherent structures inside each sample, the projections in XY, YZ and XZ planes were calculated. The results are presented in Figs. 8.21 and 8.22. From these projections, it appears that the porous areas within the samples have a regular structure. This is especially evident for sample H1. The structure of the projections on the plane shows some preferred directions, which are the bar axis and the direction along the radius. It is not so clear for sample C1, but some preferred directions of slits were also observed.

In both samples, one coherent area of a high volume joining the majority of the voids inside is observed. Furthermore, in each sample, there is a large number of considerably smaller, irregularly shaped voids not connected with the main structure. The elongation of the voids in both samples is similar. In each of them, about 65 % of the voids have a spherical or slightly elongated shape. As well, approximately 8 % of the voids are very or extremely elongated. The main difference

Fig. 8.21 The spatial distribution of coherent structures for sample C1 with the projections of these structures on the XY, YZ and XZ planes

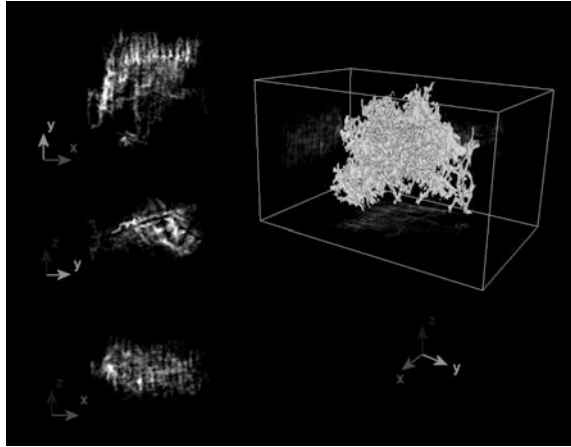
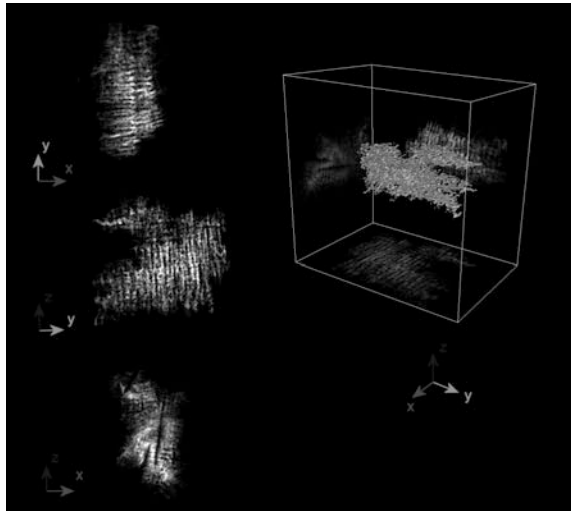


Fig. 8.22 The spatial distribution of coherent structures for sample H1 with the projections of these structures on the XY, YZ and XZ planes



between the two examined samples is the size of the voids. In sample C1 they occupy only 1.27 mm^3 , and in sample H1 up to 4.69 mm^3 . In both samples, the uniform structure is rougher than individual holes, which is probably due to its complex shape. The main structure of sample C1, while being smaller in terms of volume, is much larger in a mean diameter (average $75 \text{ }\mu\text{m}$ compared to $53 \text{ }\mu\text{m}$ in sample H1). This means that there are fewer slits in sample C1, but they are larger than in the H1 sample. On the other hand, the voids within sample C1 are more condensed than in H1.

8.3 Numerical Modelling with the DEFFEM Simulation System

The process of numerical modelling of steel deformation under conditions in which the solid and liquid phases coexist may be divided into two consecutive main stages. The first stage is the heating process, with the main purpose of obtaining the desired sample remelting zone (the assumed temperature field distribution within the sample volume). The temperature distribution obtained from the first stage should be as close to the actual distribution as possible, as the known temperature field constitutes the initial condition for the second stage, which is the deformation process. The quality of the obtained results from the heating process simulation, due to high sensitivity of rheological properties of the material tested to temperature changes, directly influences the flow pattern or the values of yield stress within the deformation zone. Extensive experimental research presented partially in this chapter, and also in Chap. 7, constitutes a large knowledge base which will be used to verify the developed numerical algorithms, and first of all the assumed model assumptions.

8.3.1 *Modelling of the Resistance Heating Process*

The accuracy of determination of the temperature field within the sample volume, depends primarily on the correct determination of the boundary conditions necessary to solve the heat flow problem. As part of the model tests, analogous to in the experimental tests, two types of grips were applied (“hot” and “cold”).

Figures 8.23 and 8.24 present detailed diagrams of the cylindrical sample heating process model, using “cold” and “hot” grips respectively. The two models differ primarily in the length of the free zone, which for the “cold” grips is about 30 mm (Fig. 8.23), and for the “hot” grips about 67 mm (Fig. 8.24). This in turn determines the area of contact of the sample with the copper grips. In the variant with the “cold” grips nine heat transfer zones were defined, which were denoted from Γ_0 to Γ_8 respectively. Different boundary conditions must be defined for each zone. Zones identified as Γ_0 , Γ_1 , Γ_2 , Γ_6 , Γ_7 , and Γ_8 define the contact zones of the sample with steel bolts. Zones Γ_3 and Γ_5 define the contact area of the sample with the copper grips. From the perspective of the numerical model it is one of the key zones, where heat is intensively discharged to the tool. The last zone is Γ_4 , which defines the free area of the sample surrounded by the quartz shield.

In the variant with “hot” grips eleven heat transfer zones were defined, which were denoted from Γ_0 to Γ_{10} respectively. Zones identified as Γ_0 , Γ_1 , Γ_2 , Γ_8 , Γ_9 and Γ_{10} define the contact zones of the sample with steel bolts. Zones Γ_3 and Γ_7 define the contact area of the sample with the copper grips. Zone Γ_5 defines the free area of the sample surrounded by the quartz shield. The last zones, Γ_4 and Γ_6 define the free area of the sample, which is not surrounded by the quartz shield.

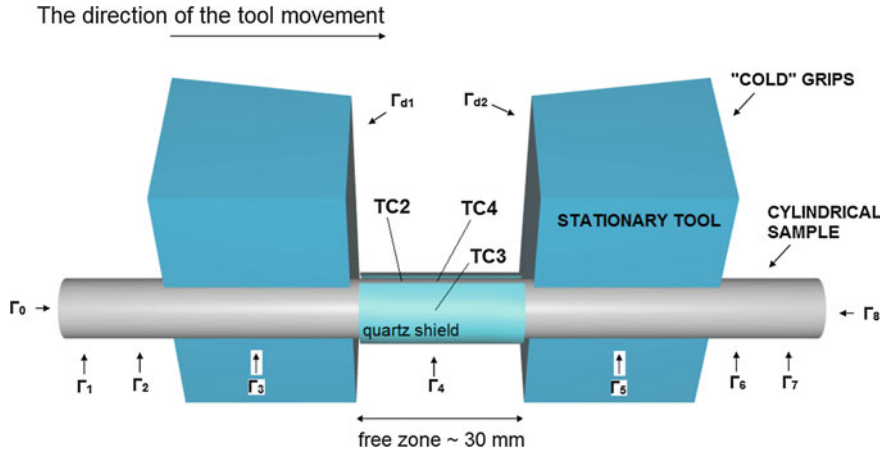


Fig. 8.23 The numerical model divided into heat transfer zones, along with the location of numerical sensors (TC4, TC3, TC2) for the “cold” grips

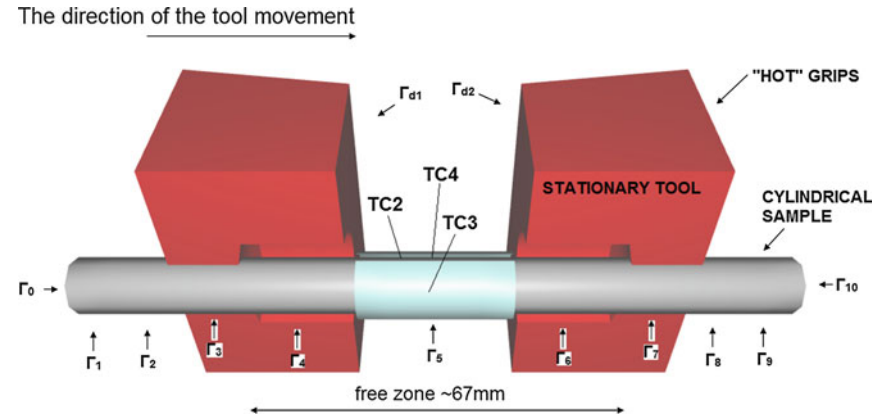


Fig. 8.24 The numerical model divided into heat transfer zones, along with the location of numerical sensors (TC4, TC3, TC2) for the “hot” grips

On both numerical model diagrams the location of numerical sensors (TC4, TC3, TC2) was also indicated. These sensors are the equivalents of actual thermocouples installed in experiments. In addition, only for orientation purposes, the geometry of both types of grips was considered, along with the defined heat transfer zones Γ_{d1} and Γ_{d2} . Currently, taking the full 3D geometry of the grips into account, as well as the related algorithm of thermal contact, are the subject of additional implementation work related to complete 3D solutions. As mentioned above, the correct selection of the boundary conditions in the model simulating resistance heating has an essential effect on the final strain pattern in the sample, as the

obtained temperature field is an input field in the mechanical model. In the presented model the boundary conditions were defined in each zone in the form:

$$q_i = \alpha_i(t - t_i) \quad (8.1)$$

where: α_i is the effective heat transfer coefficient for a given zone, t_i is the temperature of the medium being in contact with the zone area. The initial condition was assumed in the form of a known temperature distribution:

$$t(r) = t_0(r) \quad (8.2)$$

In most papers related to the issue of heat transfer [8, 9] contact effects are modelled with the heat transfer coefficient α . The biggest problem is related to the proper selection of this coefficient. The values given in numerous publications differ considerably from each other, even by an order of magnitude. In most of the papers the coefficient values α were determined by matching the temperature calculation results obtained with various methods to the results of measurements carried out during the process. For the purposes of the presented numerical model the coefficient value α for zones in contact with the steel bolts was assumed as 2000 W/m²K. For the zone with the most intensive heat discharge to the copper grips, which during the experiments are cooled with water, the heat transfer coefficient is 5000 W/m²K. The last zone is the area surrounded by the quartz shield. The quartz shield, as a very good insulator, prohibits free heat transfer between the sample surface and the environment. For the purposes of the simulation it could be assumed that the heat losses in this zone are modelled with using small effective heat transfer coefficient. The foregoing approach would be fully correct if the quartz shield surrounded the sample on its full circumference. The quartz shields applied in the tests, with the main function of protecting the simulator inside against accidental leakage of liquid metal during a remelting test, have a gap of about 3 mm, which enables the control thermocouple TC4 and additional auxiliary thermocouples to be installed. As shown by tomographic and macrostructural tests, the said gap is a source of disturbances in the heat transfer on the sample circumference, regardless of the applied holders. Figures 8.25 and 8.26 present the selected radial sections, along the remelting zone, for the tests performed with the “cold” and “hot” grips respectively. The samples were cooled at the final stage to a nominal temperature of 1400 °C. As shown by previous tomographic tests, in this case as well the obtained porous zone is bigger than for the application of “hot” grips. The shape of the porous zone itself changes depending on the adopted section plane for both tool variants. When analysing the obtained sections in the context of application of the modelling concept using axi-symmetrical models, one should aim at obtaining an identical temperature field in each of the sections (the ideal variant) or minimizing the effect of the temperature field asymmetry (the real variant).

The next component of the resistance heating model is the method of taking into account the liberated heat resulting from the current flow. The current flow through

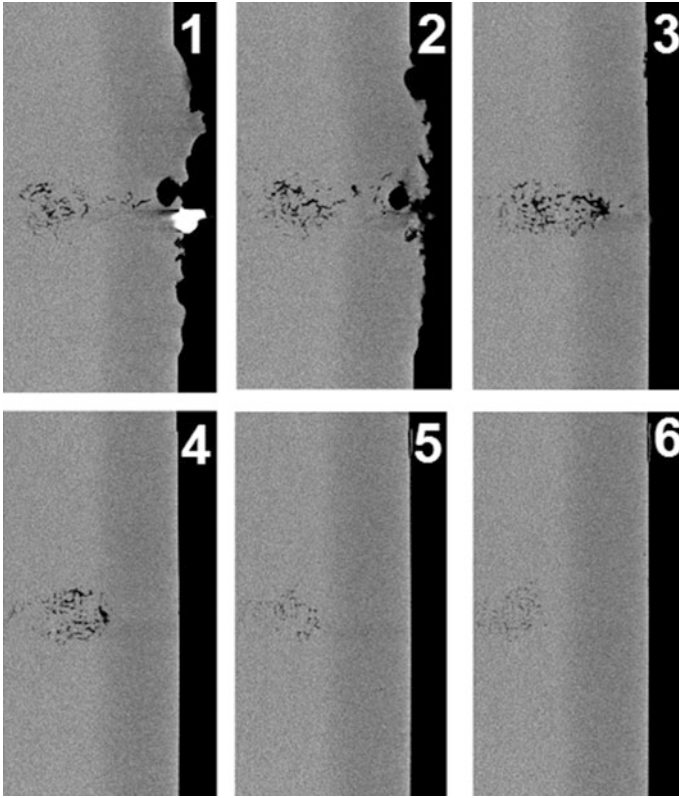


Fig. 8.25 Selected radial sections along the remelting zone, “cold” grips, TC4 = 1400 °C

a conductor (resistor) is always accompanied by heat release. It means that in components with a certain resistance, electrical energy changes into thermal energy. The Joule-Lenz law dictates the amount of released heat: The amount of heat Q released in a conductor with the resistance of R during the flow of current with the intensity of I is proportional to the current intensity squared, resistance and time of the current flow. During the modelling of the resistance heating simulation, the heat accompanying the current flow was included in the integer:

$$\int_V rQndV \quad (8.3)$$

The heat source efficiency Q in the model discussed is a function of resistance R , which in turn depends on temperature T and function A which represents intensify of heating:

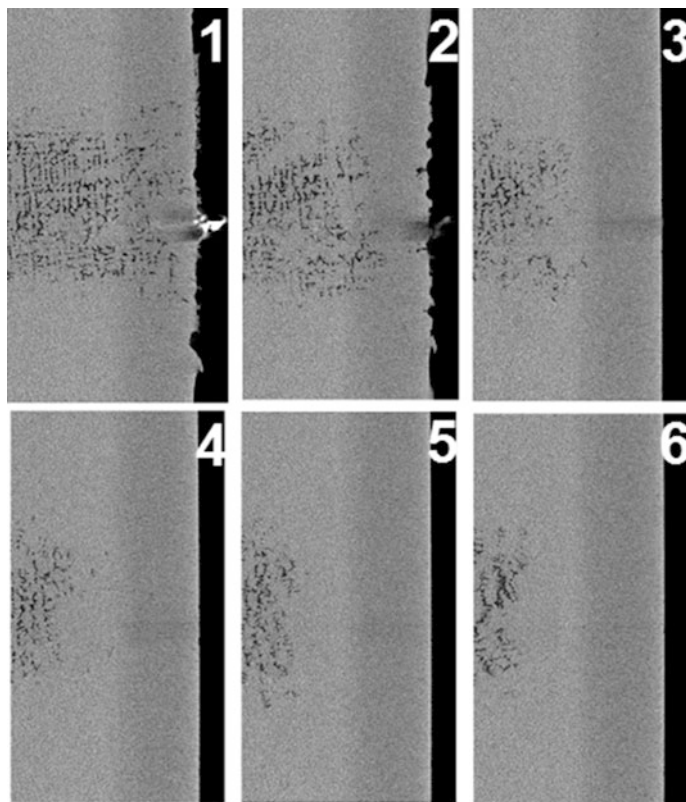


Fig. 8.26 Selected radial sections along the remelting zone, “hot” grips, TC4 = 1400 °C

$$Q = f(A(\tau)I^2(\tau)R(T)) \quad (8.4)$$

It corresponds to resistance changing in the actual model, and the internal heat source efficiency changes together with the resistance. When modelling the Joule heat generation, it was assumed that its equivalent in the numerical model will be the voluminal heat source with its power realated to the resistance and the square of electric current I during simulation time τ . The characteristics of the current intensity change as a function of heating time can be directly recorded during physical tests with the Gleeble 3800 simulator. For samples heated with the use of the “cold” grips maximum current intensity values close to 1400 A were achieved, whereas for samples heated with the “hot” grips s it was close to 1200 A. The differences in the current intensity measurement depending on the adopted type of grips arise primarily from the thermal conditions in the Gleeble 3800 simulator system. For “cold” grips, with the shortest sample heating/remelting zone, the heat discharge from the heated sample to the intensively cooled copper grips is the most intensive. In order to maintain the assumed experiment schedule (the heating

schedule) more energy should be supplied to the system. On the basis of the temperature reading from the control thermocouple and the assumed heating schedule, the simulator automation adjusts the current intensity automatically. The last important factor necessary to solve the heat flow problem is the correct selection of dependences taking into account the changes in the basic thermo-physical properties as a function of temperature. The necessary characteristics were determined for the needs of the simulation on the basis of the chemical composition using the commercial software JMatPro v.8. The calculated thermo-physical properties of the steels analysed were attached as an annex to this monograph (Appendix B).

8.3.1.1 Example Results of Resistance Heating

During the steel sample heating and remelting process, the electric current flows through a sample between the grips. As the copper grips in the simulator system are intensively cooled with water—compared to other simulator system components conducting electricity—during the electrical current flow, the heat liberation within the sample is the most intensive. The temperature programme of the numerical simulation of the heating process for a steel C45 sample is the same as in the conducted experiments (see Sect. 8.1). Figures 8.27, 8.28, 8.29, 8.30, 8.31 and 8.32 present the temperature distributions on the longitudinal section of the samples heated to nominal temperatures of 1400, 1380, 1350, 1300, 1250 and 1200 °C, respectively. The simulations were carried out with “cold” grips (long sample-tool contact zone). The analysis of the obtained results indicates that a wide temperature gradient exists on the sample section. The difference between the sample surface temperature (the reading of numerical sensor TC4 for the nominal test temperature of 1400 °C) and the temperature calculated at the sample core (the reading of numerical sensor TC3) is 40 °C (Fig. 8.27). This value decreases as the nominal test temperature declines, achieving a difference of 16 °C between the readings of both numerical sensors (TC4-TC3) for a test carried out at a temperature of 1200 °C (Fig. 8.32).

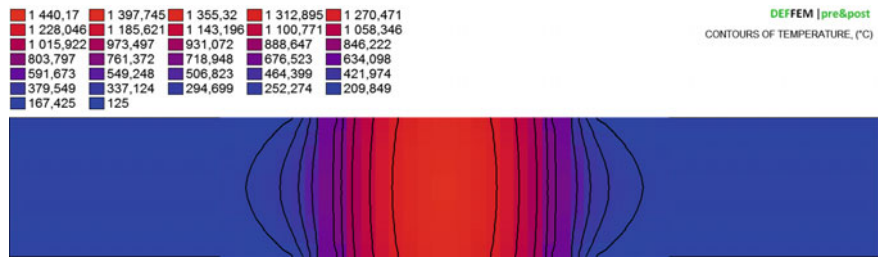


Fig. 8.27 The temperature distribution of the sample heated to a nominal temperature of 1400 °C (the variant with the “cold” grips)

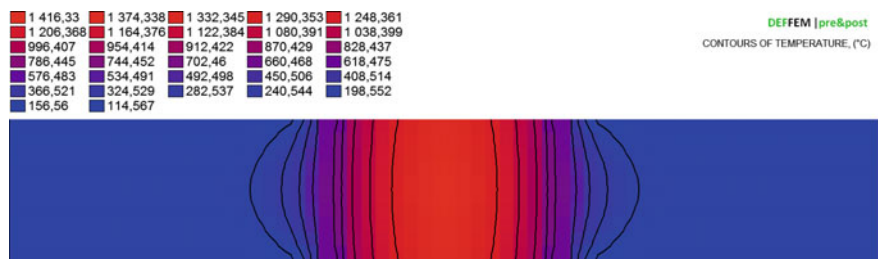


Fig. 8.28 The temperature distribution of the sample heated to the nominal temperature of 1380 ° C (the variant with the “cold” grips)

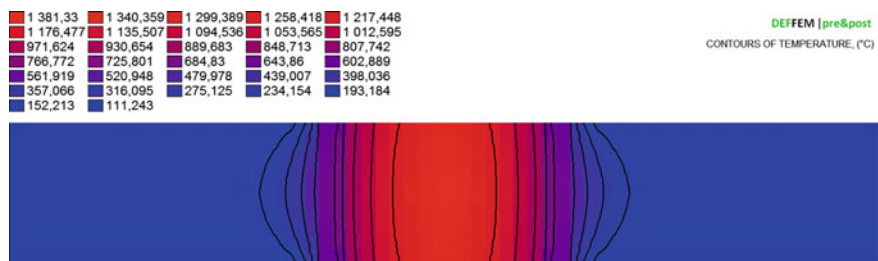


Fig. 8.29 The temperature distribution of the sample heated to the nominal temperature of 1350 ° C (the variant with the “cold” grips)

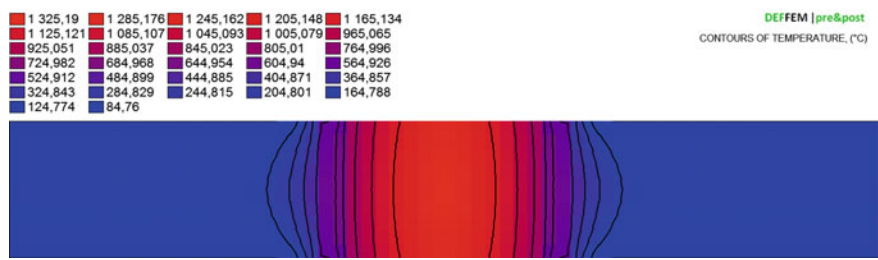


Fig. 8.30 The temperature distribution of the sample heated to the nominal temperature of 1300 ° C (the variant with the “cold” grips)

In order to verify the obtained results, tests with an additional thermocouple (TC3) were carried out. This thermocouple measured the temperature at the sample core. Thermocouple TC2 measured the temperature at a distance of 7.5 mm from the control thermocouple TC4 for the nominal test temperature of 1380 °C. The obtained temperature measurements of 1411, 1291 and 637 °C for thermocouples TC3 (core), TC2 and TC1 are close to the results of the simulations 1416, 1295 and 650 °C for the respective numerical sensors (Fig. 8.28). The difference between the calculated and experimentally determined core temperature is 5 °C. For

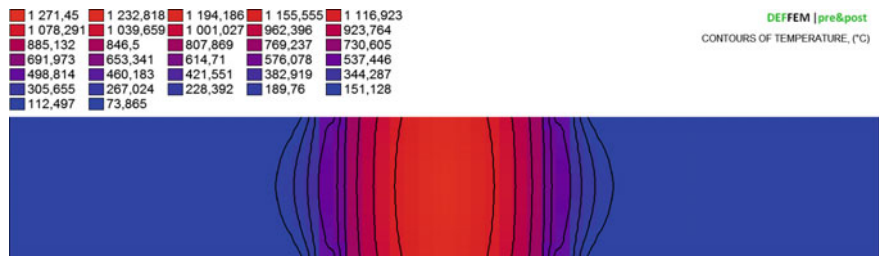


Fig. 8.31 The temperature distribution of the sample heated to the nominal temperature of 1250 °C (the variant with the “cold” grips)

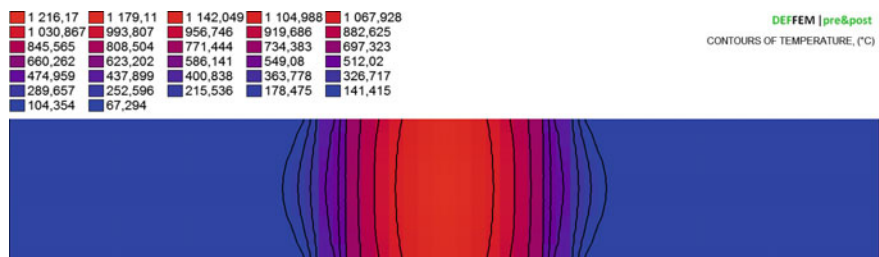


Fig. 8.32 The temperature distribution of the sample heated to the nominal temperature of 1200 °C (the variant with the “cold” grips)

Table 8.8 The comparison of temperatures determined by the experiment and calculated (the variant with the “cold” grips)

Nominal test temperature (°C)	Thermocouple TC1 (°C)		Thermocouple TC2 (°C)		Thermocouple TC3 (°C)	
	Gleeble	FEM	Gleeble	FEM	Gleeble	FEM
1400	674	662	–	1314	–	1440
1380	650	637	1295	1291	1411	1416
1350	611	600	–	1259	–	1381
1300	561	555	–	1206	–	1325
1250	524	529	–	1156	–	1271
1200	502	508	–	1105	–	1216

thermocouple TC2 the difference in the readings was 4 °C. When analysing the readings of the thermocouple and the numerical sensor TC1, the difference in the readings was 12 °C for a test at a temperature of 1400 °C, achieving lower values for tests carried out at lower temperatures. Table 8.8 presents the results of experimental measurements and of calculations. The maximum relative errors for thermocouples TC1, TC2 and TC3 were 2, 0.3 and 0.35 %, respectively.

The analysis of the obtained results for the tests performed with the short contact zone holders (the “hot” grips) leads to the same conclusions as for the simulation with the long contact zone grips. Figures 8.33, 8.34, 8.35, 8.36, 8.37 and 8.38 present the temperature distributions on the longitudinal section of the samples heated to nominal temperatures of 1400, 1380, 1350, 1300, 1250 and 1200 °C, respectively. The analysis of the obtained results indicates that a slightly steeper temperature gradient exists on the sample section compared to the variant with the

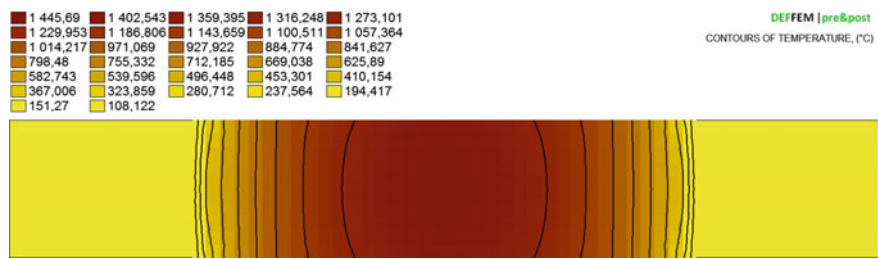


Fig. 8.33 The temperature distribution of the sample heated to a nominal temperature of 1400 °C (the variant with the “hot” grips)

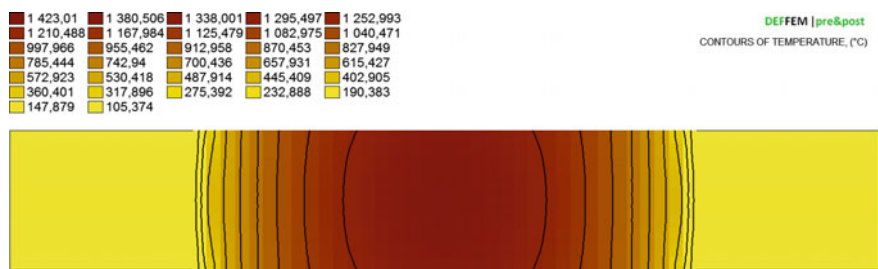


Fig. 8.34 The temperature distribution of the sample heated to a nominal temperature of 1380 °C (the variant with the “hot” grips)

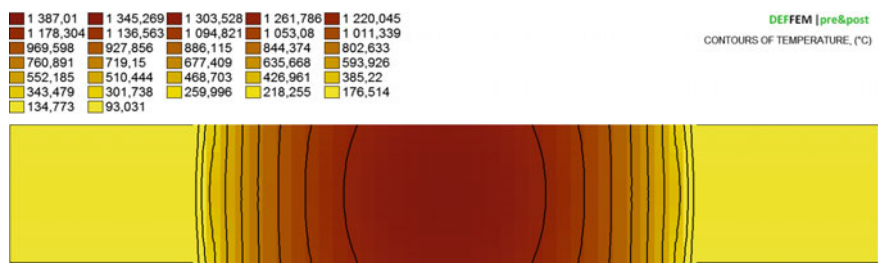


Fig. 8.35 The temperature distribution of the sample heated to a nominal temperature of 1350 °C (the variant with the “hot” grips)

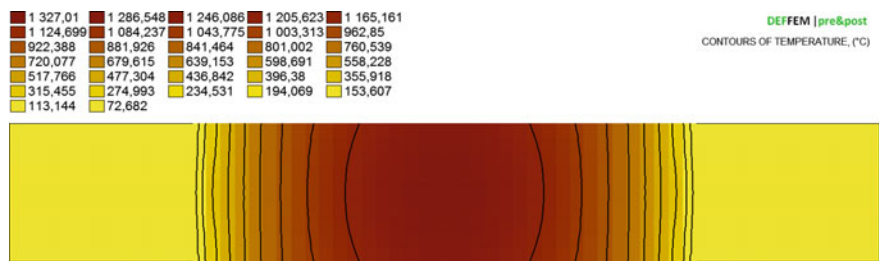


Fig. 8.36 The temperature distribution of the sample heated to a nominal temperature of 1300 °C (the variant with the “hot” grips)

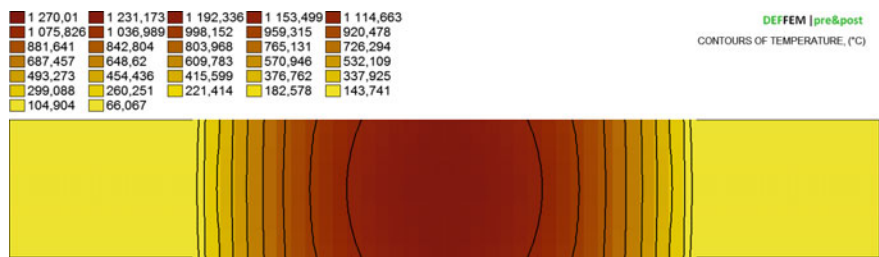


Fig. 8.37 The temperature distribution of the sample heated to a nominal temperature of 1250 °C (the variant with the “hot” grips)

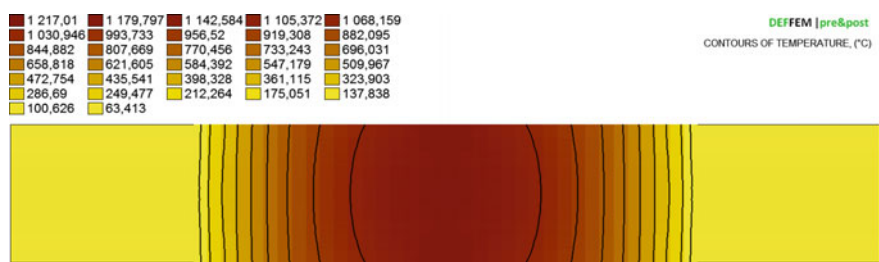


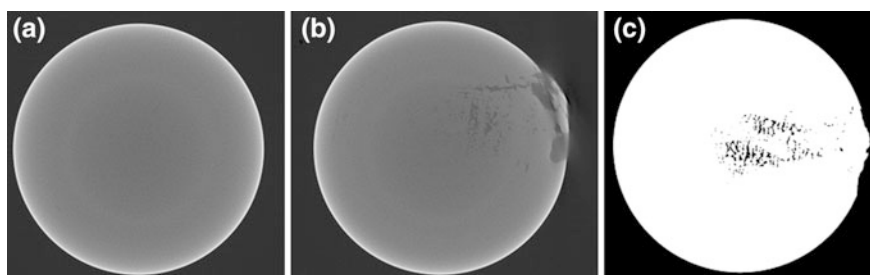
Fig. 8.38 The temperature distribution of the sample heated to a nominal temperature of 1200 °C (the variant with the “hot” grips)

“cold” grips. The difference between the sample surface temperature (the reading of numerical sensor TC4 for the nominal test temperature of 1400 °C) and the temperature calculated at the sample core (the reading of numerical sensor TC3) is 45 °C (Fig. 8.33). This value decreases as the nominal test temperature declines, achieving a difference of 17 °C between the readings of both numerical sensors (TC4-TC3) for a test carried out at a temperature of 1200 °C (Fig. 8.38).

Analogous to in the previous variant, in order to verify the obtained results, tests with additional thermocouples (TC3, TC2 and TC1) were performed. The obtained

Table 8.9 The comparison of temperatures determined experimentally and calculated (the variant with the “hot” grips)

Nominal temperature of the test (°C)	Thermocouple TC1 (°C)		Thermocouple TC2 (°C)		Thermocouple TC3 (°C)	
	Gleeble	FEM	Gleeble	FEM	Gleeble	FEM
1400	350	367	–	1392	–	1445
1380	341	344	1368	1371	1419	1423
1350	333	328	–	1336	–	1387
1300	313	308	–	1275	–	1327
1250	295	292	–	1221	–	1270
1200	291	285	–	1168	–	1217

**Fig. 8.39** The tomography of samples heated directly to a nominal temperature of **a** 1350 °C, **b** 1380 °C, **c** 1400 °C (the variants with the “hot” grips)

temperature measurements of 1419, 1368 and 341 °C for thermocouples TC3 (core), TC2 and TC1, respectively, are similar to the results of the simulations at 1423, 1371 and 344 °C for the respective numerical sensors (Fig. 8.34). The difference between the calculated core temperature and the temperature determined experimentally was 4 °C. For thermocouple TC2 the difference of the readings was 3 °C. The other temperature measurements are compared in Table 8.9. The maximum relative errors for thermocouples TC1, TC2 and TC3 were 4.85, 0.21 and 0.28 %, respectively.

With respect to the temperature range between the solidus T_s and liquidus T_l , which for the tested steel C45 are 1410 and 1495 °C, respectively, and the maximum calculated temperatures at the core sample, one may find out that a mushy zone exists in the samples heated to the nominal temperatures of 1380 °C (Figs. 8.28 and 8.34) and 1400 °C (Figs. 8.27 and 8.33). The foregoing conclusion was also confirmed during macrostructural/tomography tests. Modifying heating programmes, for instance by heating directly to the nominal test temperature, does not eliminate the effect of formation of a temperature gradient on the sample section. The shape of the porous zone slightly differs. Figure 8.39 presents examples of sections obtained from tomographic tests of the samples heated to the nominal test

temperatures of 1350, 1380, and 1400 °C, respectively, with the “hot” grips. In the variant of heating to 1350 °C, no clear occurrence of a porous zone—which would indicate local remelting of the sample—was found (Fig. 8.39a). A small contour of the porous zone manifested on the section of the sample heated to the temperature of 1380 °C (Fig. 8.39b), which indicated a local occurrence of the semi-solid phase. A distinct contour of the porous zone was formed as a result of heating the sample to a temperature of 1400 °C, slightly lower than the determined solidus temperature T_s of 1410 °C (Fig. 8.39c).

The results obtained by a simulation for both tool variants feature good compatibility with the results obtained experimentally. When assessing the differences occurring between the measured and computed temperature values one should bear in mind that they were determined with a few simplifying assumptions. In the numerical model, couplings of the temperature field and the electrical field were not included directly. It was modelled by an internal voluminal heat source. Therefore, the influence of the changing electrical properties of the heated sample on the electrical charge density and local voluminal heat source power could not be analysed. At the present stage of implementation work, it is difficult to state that taking the thermo-electrical impact into account would constitute significant progress and would allow more precise results to be obtained. If formulating such a conclusion is possible, it would be a fundamental argument to focus the software development work on a thermo-electrical impact module. The experimental test results indicating a similar dispersion of temperature measurements for tests that were doubled (see results in Tables 8.1, 8.2, 8.3 and 8.4) are an additional fact supporting the above statement.

8.3.2 *Modelling the Deformation Process*

During the numerical modelling of the steel deformation process under the conditions of the liquid and solid phase coexistence, one should notice the occurrence of substantial differences in the yield stress for individual sub-areas of the deformation zone. In the temperature range discussed, these differences are caused even by small temperature fluctuations. The mere modelling of effects occurring in steel during deformation within the range including the coexistence of the liquid and solid phases is very complex. As the properties related to the occurrence of the mushy zone in the central part of the deformed sample are not uniform, the effects occurring both in the skeleton layer (the solidified part) and in the semi-solid core need to be analysed. Rapid changes in the plastic and mechanical properties undergoing temperature changes require applying special methods in mathematical modelling of the deformation process at temperatures over the hot working range. Therefore, the model of function of the stress change versus strain for the defined areas of the deformation zone is an inherent part of the mathematical models presented in this monograph. Knowledge of the stress-strain relationships is extremely important for modelling effects occurring in steel during deformation within the temperature range of a

change in the state of aggregation. However, determining these relationships for a semi-solid material is much more difficult than when this material is deformed at lower temperatures. A large number of effects accompanying the solidification creates substantial difficulties in precise determination of the stress-strain curves. For such high temperatures, the traditional methods of determining stress-strain curves, based only on the experimental results, are insufficient. In these experiments a number of disturbances occur (strain non-uniformities, heat generated as a result of deformation work), which significantly influence the obtained results. Therefore, in order to eliminate these disturbances, a combination of the solution of the so-called direct problem based upon the finite element method with the inverse calculation method, based on the proposed methodologies, was adopted. The basic objective of the inverse analysis is the determination of parameters of the rheological model of the material deformed on the basis of the conducted experiments. The inverse calculation model consists of three parts:

1. An experiment, which provides information on the measured values, which are the foundation for the construction and optimisation of the objective function of the inverse analysis module.
2. Solutions to the direct problem, that is a simulation of compression or a tensile test on the basis of the finite element method.
3. Optimization algorithms, allowing one to identify the searched parameters by minimization of the defined objective function.

The direct solution module of any physical process may be presented as a system of equations in the following form [10]:

$$\mathbf{d} = (\mathbf{x}, \mathbf{p}) \quad (8.5)$$

where: $\mathbf{d} = (d_1, \dots, d_n)$ is the vector of the output process values,

$\mathbf{x} = (x_1, \dots, x_n)$ is the vector of the searched process parameters,

$\mathbf{p} = (p_1, \dots, p_n)$ is the vector of the input values.

The objective of the inverse analysis is to determine the optimal values of the process vector $\mathbf{x}$.

8.3.2.1 Rheological Model

The general form of the rheological model was proposed in the following form:

$$\emptyset = \begin{cases} L(\varepsilon, \dot{\varepsilon}, T); & T < 700^\circ\text{C} \\ M(\varepsilon, \dot{\varepsilon}, T); & 700^\circ\text{C} \leq T \leq 1200^\circ\text{C} \\ N(\varepsilon, \dot{\varepsilon}, T); & 1200^\circ\text{C} \leq T \leq T_{critical} \\ 0; & T \geq T_{critical} \end{cases} \quad (8.6)$$

where: $\emptyset$ is a parameter characterising a specific material, $T_{critical}$ is the critical temperature, which for heating may be tantamount to the nil strength temperature

(*NST*) or the nil ductility temperature (*NDT*), while for cooling it may be tantamount to the ductility recovery temperature (*DRT*). Introduction of a differentiation like this is relevant as we relate the mentioned temperatures to the time of solid constraint loss (it means dendrites forming joints), capable of load transfer. The forces recorded, which occur in the simulator system, are related to overcoming the friction resistance in the mechanical system, overcoming the friction resistance related to the material viscosity in the fully liquid state or with a solid phase share. The solid phase does not form permanent bindings, but they are capable of transferring the set load.

The research aimed at the determination of function $L(\varepsilon, \dot{\varepsilon}, T)$ parameters may be performed with common instruments, with traditional methods or with inverse calculation methodology [10]. For a temperature range under 700 °C (this is a zone which is practically not subject to deformation) one may adopt commonly used equations for carbon steels, taking into account the strain rate, strain degree and temperature to describe changes in stress as a function of strain. As part of this project, the modern testing machine was used to determine parameters of the adopted function L on the basis of the proposed methodology presented in the following section.

For the function $M(\varepsilon, \dot{\varepsilon}, T)$ within the temperature range from 700 to 1200 °C (a zone also practically not deformed), the empirical Shida equation was adopted, in the following form [9]:

$$\sigma = \sigma_f f \left(\frac{\dot{\varepsilon}}{10} \right)^n \quad (8.7)$$

where for

$$\underline{t} \geq 0.95 \frac{C + 0.41}{C + 0.32} \quad (8.8)$$

$$\sigma_f = 0.28 \exp \left(\frac{5}{\underline{t}} - \frac{0.01}{C + 0.05} \right) \quad (8.9)$$

$$m = (-0.019C + 0.126)\underline{t} + (0.075C - 0.05) \quad (8.10)$$

whereas for

$$\underline{t} \leq 0.95 \frac{C + 0.41}{C + 0.32} \quad (8.11)$$

$$\sigma_f = 0.28q(C, \underline{t}) \exp \left[\frac{C + 0.32}{0.19(C + 0.41)} - \frac{0.01}{C + 0.05} \right] \quad (8.12)$$

$$q(C, \underline{t}) = 30(C + 0.9) \left(\underline{t} - 0.95 \frac{C + 0.49}{C + 0.42} \right)^2 + \frac{C + 0.06}{C + 0.09} \quad (8.13)$$

$$m = (0.081C - 0.154)\underline{t} - 0.019C + 0.207 + \frac{0.027}{C + 0.32} \quad (8.14)$$

The other parameters were defined as:

$$f = 1.3(5\varepsilon)^n - 1.5\varepsilon \quad (8.15)$$

$$n = 0.41 - 0.07C \quad (8.16)$$

$$\underline{t} = (t + 273)/1000 \quad (8.17)$$

For the function $N(\varepsilon, \dot{\varepsilon}, T)$ within the temperature range $1200^\circ\text{C} - T_{critical}$ (a zone with the biggest plastic deformations), the following equation was adopted [11]:

$$\sigma = \frac{\varepsilon^n}{\alpha} ASINH \left[\left(\frac{\dot{\varepsilon}}{A} \right)^m \exp \left(\frac{mQ}{RT} \right) \right] \quad (8.18)$$

where α, A, m, n are parameters of the yield stress function, T is the temperature, R is a gas constant (8.314 J/molK).

8.3.2.2 The Numerical Identification Methodology (NIM) for the Low Temperature Range

The methodology of determination of parameters of the yield stress function for the temperature range under 700°C using the inverse calculation method has been the subject of many papers and reports. The conclusion and possibilities of the practical application in the parameter identification was presented in detail in papers [10]. As part of research work aimed at the identification of the yield stress function parameters for the steel analysed, the modern Zwick Z250 testing machine was used. A great advantage of this testing unit is the capability to carry out compression tests in isothermal conditions up to a temperature of 750°C . The proposed research methodology covers the following stages:

- I. Preparation of cylindrical samples with a diameter of 5 mm and a height of 6 mm.
- II. Calibration of the measuring systems and performing test heating-cooling cycles for the tool set with a steel sample within a temperature range from 20 to 750°C , and then cooling to a temperature of 400°C . The measurement system consists of a three-zone furnace with three control Pt-Rd-Pt thermocouples (furnace, controller and driver by MAYTEC), an eight-channel

recorder by CRAPHTEC MidiLogger GL90 to acquire measurement data, and three additional Ni-Cr-Ni K-type thermocouples (two in the tools T1, T2; and one in the sample T3). Thermocouple T3 was placed in the core of the cylindrical sample. A hole with a diameter of 1 mm and a depth of 2.5 mm was made in the sample at half of its height, so that a thermocouple with a diameter of 0.5 mm was placed centrally in the middle of the sample (Fig. 8.40).

Figure 8.41 presents the obtained courses of temperature changes for the lower and upper tools and the sample core. The differences between readings of all thermocouples before starting the cooling process were small, and were

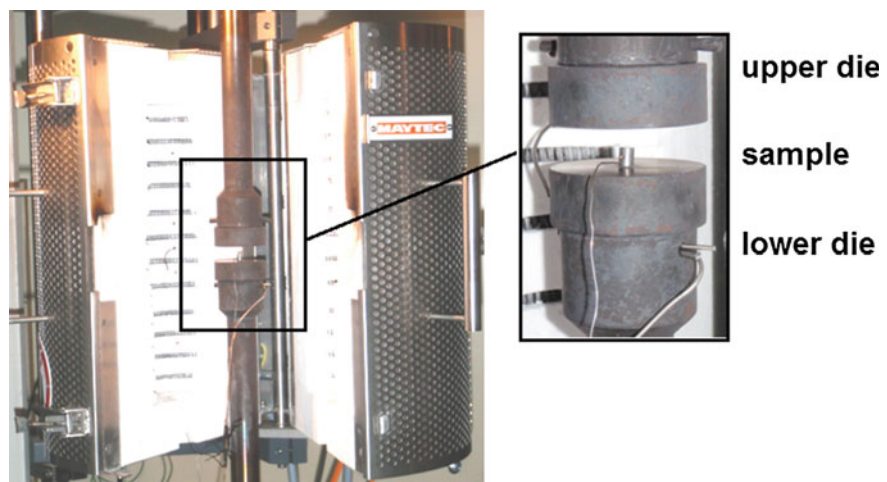
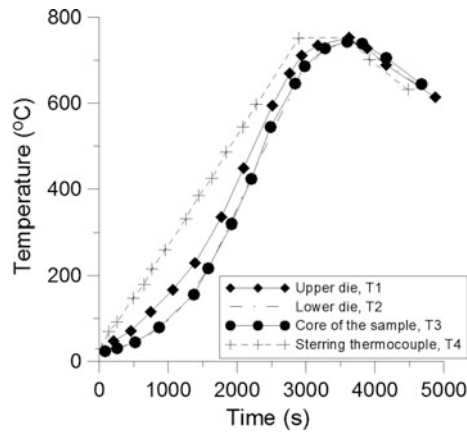


Fig. 8.40 A view of the Zwick Z250 machine system, along with the sample prepared for tests

Fig. 8.41 The course of temperature changes for the heating and cooling processes of the tool set and the steel sample



accommodated within the limits from 1 to 3 °C. The obtained results allow us to assume isothermal conditions in the direct solution of the compression test.

- III. In the third stage a series of compression tests within a temperature range from 20 to 700 °C was conducted at two strain rates, of 0.01 and 1 s⁻¹. During the tests, the displacement of the tool and the compression force were recorded. The obtained courses of force changes constituted the foundation for construction of the objective function, which was defined as follows:

$$\varphi(\mathbf{x}) = \sum_{i=1}^n \left[\frac{F_i^c(\mathbf{x}, \mathbf{p}) - F_i^m}{F_i^m} \right]^2 \quad (8.19)$$

So defined objective function (8.19) is the error norm between the measured values of the compression force F^m and the values calculated by the finite element method F^c .

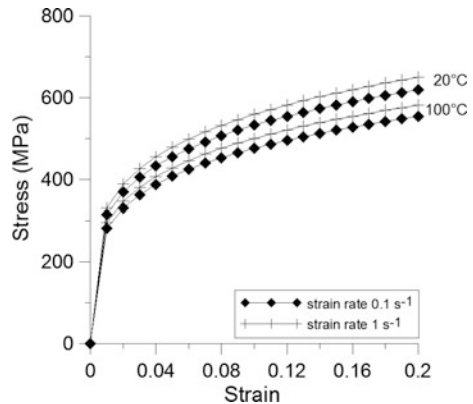
- IV. At the last stage, using the optimization platform of the DEFFEM package, parameters for the selected yield stress function were identified:

$$\sigma = A\epsilon^m \exp(Bt)\dot{\epsilon}^n \exp(C\epsilon) \quad (8.20)$$

The following five parameters are the searched parameters of the yield stress function: A, m, B, n, C . As a result of inverse calculations the following values of the searched coefficients were obtained: respectively, 989.12, 0.231346, -0.001398, 0.021111 and -0.091119.

Figure 8.42 presents examples of yield stress curves for temperatures of 20 and 100°C and two strain rates of 0.01 and 1 s⁻¹.

Fig. 8.42 Yield stress curves determined from the inverse solution



In order to check the determined actual curves for correctness they were applied in the compression test model. The force courses as a function of the tool stroke obtained from the simulation were practically comparable (average relative error within 1.35–3.43 %). The application of traditional methods to determine the yield stress (assuming a constant sample temperature) will lead to underrating of the yield stress. The occurring differences are caused by the plastic deformation heat, causing a reduction of the yield stress as a result of the sample temperature increase. The above mentioned effect is taken into account in the methodology based upon the inverse solution, which results in obtaining actual yield stress curves.

8.3.2.3 The Direct Identification Methodology (DIM) for the Extra-High Temperature Range

The determination of the yield stress function parameters for the needs of computer simulations for the temperature range above 1200 °C is a complex issue. In studies aimed at developing the methodology for determination of the searched function parameters one should use computer aided experimental comprehensive tests. As part of the studies, the capabilities of the thermo-mechanical Gleeble 3800 simulator and the developed simulation system DEFFEM were utilized. Two methodologies were proposed. The first one is based upon measurements directly from the Gleeble 3800 simulator (Direct Identification Methodology), while the other uses the inverse calculation methodology to identify the searched parameters (Numerical Identification Methodology).

The DIM (Direct Identification Methodology) covers the following stages:

- I. The preparation of samples for testing with the simulator. Cylindrical samples with a length of 125 mm and a diameter of 10 mm. A quartz shield and copper grips with a long contact zone (so-called “cold” grips) were applied. During the tests one thermocouple TC4 was applied, placed in the middle of the sample heating zone. At the same time, this thermocouple was the control thermocouple.
- II. The proposed experiment programme included heating to a temperature of 1350 °C at a rate of 20 °C/s, and then further heating to a temperature of 1430 °C at a rate of 1 °C/s. Cooling to the nominal deformation temperature was performed at a rate of 10 °C/s, and after holding for 10 s at the set temperature the tensioning process was performed (stroke 0.5–2 mm) at a tool stroke rate of 1–10 mm/s. The basic test cycle covered the temperature range from 1200 to 1380 °C. This range is defined on the basis of the nominal test temperatures. One should remember, as showed by previous tests, that during the resistance heating process the temperature achieved in the sample core is higher than the temperature measured at the surface.
- III. Carrying out preliminary simulations in order to estimate the length of the deformable zone. On the basis of the preliminary test results and the analysis of the temperature fields the length L_0 of the effective working zone can be

estimated at 10 mm. Within this zone, the strain rate and the stress are supposed as uniaxial. The nominal strain $\varepsilon_{nominal}$ and the nominal strain rate $\dot{\varepsilon}_{nominal}$ are defined as follows:

$$\varepsilon_{nominal} = \frac{\Delta L}{L_0} \quad (8.21)$$

where ΔL is the grip stroke (the elongation of the effective working zone at time τ) and L_0 effective working zone.

$$\dot{\varepsilon}_{nominal} = \frac{stroke_rate}{L_0} \quad (8.22)$$

The nominal stress is calculated with the following relationship:

$$\sigma_{nominal}^{exp} = \frac{F}{S_0} \quad (8.23)$$

where F is the tensile force measured by the Gleeble 3800 simulator and S_0 is the original cross-section area of the sample.

IV. The function form describing the dependence of the nominal stress on the nominal strain is analogous to the Eq. (8.18). After application of designations in accordance with the methodology assumptions, the function assumes the following form:

$$\sigma_{nominal}^{exp} = \frac{\varepsilon_{nominal}^n}{\alpha} ASINH \left[\left(\frac{\dot{\varepsilon}_{nominal}}{A} \right)^m \exp \left(\frac{mQ}{RT_{nominal}} \right) \right] \quad (8.24)$$

The last parameter that should be defined in Eq. (8.24) is the value of the nominal temperature $T_{nominal}$. On the basis of direct measurements of thermocouple TC4 on the sample surface and thermocouple TC3 installed in the sample core, three methods for determining the nominal temperature were proposed. The nominal temperature will be assigned to the relevant experiment. In the first method the nominal test temperature is equal to the sample surface temperature:

$$T_{nominal}^{(1)} = T_{surface}^{exp} \quad (8.25)$$

In the second method the nominal test temperature is equal to the sample core temperature:

$$T_{nominal}^{(2)} = T_{core}^{exp} \quad (8.26)$$

The last, third method assumes the nominal test temperature, which is the averaged value between the surface temperature $T_{surface}^{exp}$ and the core temperature T_{core}^{exp} :

$$T_{nominal}^{(3)} = \frac{(T_{core}^{exp} + T_{surface}^{exp})}{2} \quad (8.27)$$

In this study, the first method was assumed for calculations, and the nominal temperature was defined as the sample surface temperature.

- V. The last stage of the proposed methodology is defining the objective function for the purpose of identification of the searched parameter vector $\mathbf{x} = (\alpha, n, A, m, Q)$ of the function (8.24). On the basis of the paper [10] a modified form of the objective function was proposed:

$$\varphi(\mathbf{x}) = \frac{1}{N_t} \frac{1}{N_{pr}} \sum_{i=1}^{N_t} \sum_{j=1}^{N_{pr}} \left[\frac{\sigma_{nominal,ij}^{calc}(\mathbf{x}) - \sigma_{nominal,ij}^{exp}}{\sigma_{nominal,ij}^{exp}} \right]^2 \quad (8.28)$$

where:

- N_t —the number of experiments (tensile tests),
 N_{pr} —the number of measurement points,
 $\sigma_{nominal}^{calc}$ —the nominal stress from calculations,
 $\sigma_{nominal}^{exp}$ —the nominal stress from experiments.

The searched parameter vector $\mathbf{x}$ can be identified by minimization of the objective function φ when applying the DEFFEM package optimisation platform. The proposed DIM methodology, which does not take the direct solution of the tensile test with the finite element method into account, is the faster and more effective methodology. Gradient-free optimisation techniques by Hooke-Jaevs, Rosenbrock and Nelder-Mead were utilized to minimize the objective function (8.28). The identified parameters of vector $\mathbf{x}$, based on the Direct Identification Methodology, are collected in Table 8.10.

The calculated and deducted nominal stress-strain curves are shown in Figs. 8.43, 8.44, 8.45 and 8.46. All measurement points obtained from the experiment are included in the graphs, in order to present the scatter of the experimental data. Before using them in the optimisation procedures, such data were previously

Table 8.10 Identified parameters by the Direct Identification Methodology (DIM)

α (MPa ⁻¹)	n	A (s ⁻¹)	m	Q (J/mol)
0.06072	0.14888	1.45E+17	0.16264	529964.1

Fig. 8.43 Comparison between the directly predicted (*symbols*) and calculated (*lines*) strain-stress relationships at the nominal temperatures of 1200–1300 °C and the nominal strain rate 0.1 s⁻¹

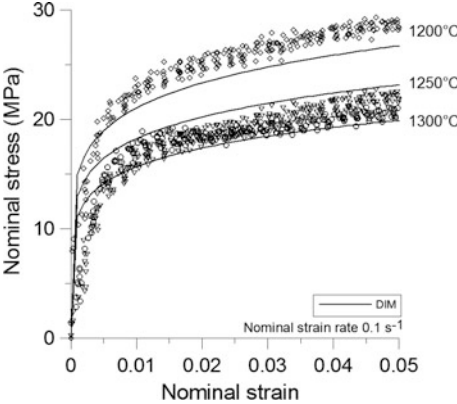


Fig. 8.44 Comparison between the directly predicted (*symbols*) and calculated (*lines*) strain-stress relationships at the nominal temperatures of 1350–1380 °C and the nominal strain rate 0.1 s⁻¹

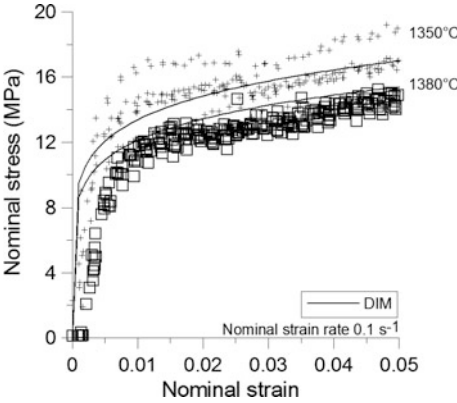


Fig. 8.45 Comparison between the directly predicted (*symbols*) and calculated (*lines*) strain-stress relationships at the nominal temperatures of 1200–1300 °C and the nominal strain rate 1 s⁻¹

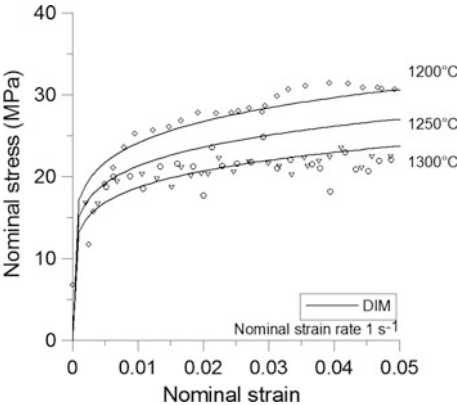
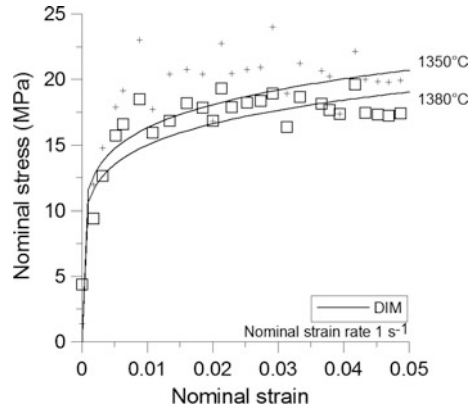


Fig. 8.46 Comparison between the directly predicted (symbols) and calculated (lines) strain-stress relationships at the nominal temperatures of 1350–1380 °C and the nominal strain rate 1 s^{-1}



subjected to a smoothing procedure. A reasonable agreement can be observed between the calculated and the directly predicted nominal stress-strain curves. The maximum relative errors for temperatures 1200, 1250 and 1300 °C and strain rate 0.1 s^{-1} were 5.57, 0.78 and 4.39 %, respectively. For temperatures 1350, 1380 °C were 2.11, 9.7 %, respectively.

The maximum relative errors for temperatures 1200, 1250 and 1300 °C and strain rate 1 s^{-1} were 3.6, 12.11 and 0.66 %, respectively. For temperatures 1350, 1380 °C were 7, 6.4 %, respectively.

In order to assess the accuracy of the developed nominal stress-strain relationships, numerical simulations were performed with the DEFFEM package. The simulations were conducted while attempting to reflect the conditions of the conducted experiments as accurately as possible. The first simulation stage is the process of resistance heating. The heating issues are presented in details in Sect. 8.3.1. The deformation process simulation was carried out in two variants. In the first variant a small strain was applied (stroke = 0.5 mm). The samples were deformed at a nominal temperature of 1380 °C at a tool stroke rate of 1 mm/s and 10 mm. In the second variant a slightly higher strain was applied (stroke = 2 mm). The samples were deformed at nominal temperatures at a tool stroke rate of 1 mm/s. The simulation was repeated for the deformation variant at a temperature of 1380 °C. The other one was performed for a temperature of 1300 °C. The basic aim of the simulation was to evaluate the suitability of the developed function describing changes in stress versus strain for the defined temperature range, and to verify the capabilities of the simulation package in applications related to steel deformation in the conditions of the liquid and solid phase coexistence. Figures 8.47 and 8.48 present the radial v_r and axial v_z components of the stroke rate field, for a sample deformed at a nominal temperature of 1380 °C. The visualisation was performed on the section along the whole sample and symmetrically with respect to the Z axis. The plastic flow zone is located in the central part of the sample (Fig. 8.48). The radial v_r component of the stroke rate field reaches its maximum values at the sample surface, propagating radially towards the sample core (Fig. 8.47).

Fig. 8.47 The velocity field distribution (radial component v_r) on the longitudinal sample section, $T = 1380\text{ }^{\circ}\text{C}$, stroke = 0.5 mm, stroke rate = 1 mm/s

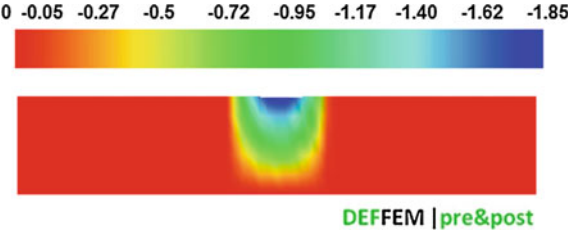


Fig. 8.48 The velocity field distribution (axial component v_z) on the longitudinal sample section, $T = 1380\text{ }^{\circ}\text{C}$, stroke = 0.5 mm, stroke rate = 1 mm/s

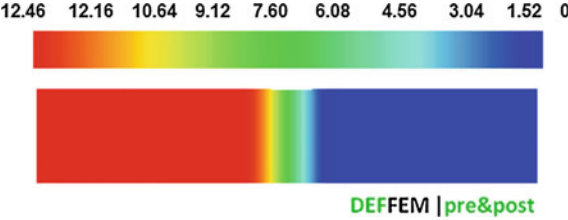
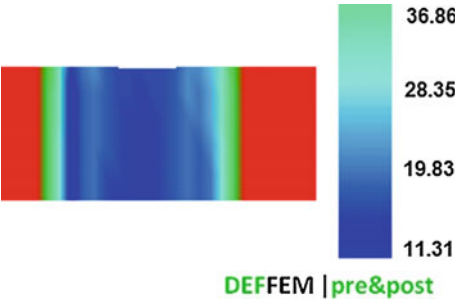


Fig. 8.49 The nominal stress distribution within the deformation zone on the longitudinal sample section, $T = 1380\text{ }^{\circ}\text{C}$, stroke = 0.5 mm, stroke rate = 1 mm/s



In the flow zone the lowest values of nominal stress occur, achieving the values within a range from 11 to 28 MPa (Fig. 8.49).

Figure 8.50 presents changes in the force as a function of the tool stroke, calculated and experimentally determined, for deformation test at a nominal temperature of $1380\text{ }^{\circ}\text{C}$ for two stroke rates of 1 and 10 mm/s. The obtained courses of force changes feature a fairly large discrepancy between the calculated and experimentally determined forces. The maximum force range reaches about 1600 N. In both simulation variants higher force values were obtained than in the experiments. One should bear in mind that in the calculations, the sample surface temperature was assumed as the nominal temperature. The core sample temperature was about $36\text{--}40\text{ }^{\circ}\text{C}$ higher.

In the second simulation variant a slightly higher strain was applied (stroke = 2 mm). Figure 8.51 presents changes in the force as a function of the tool stroke, calculated and experimentally determined, for the deformation test at a nominal temperature of 1300 and $1380\text{ }^{\circ}\text{C}$ and a stroke rate of 1 mm/s. In the first

Fig. 8.50 The comparison of the calculated and measured force-displacement curves at a nominal temperature of 1380 °C and two stroke rates of 1–10 mm/s

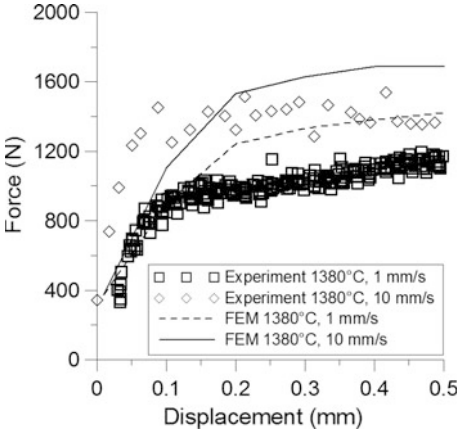
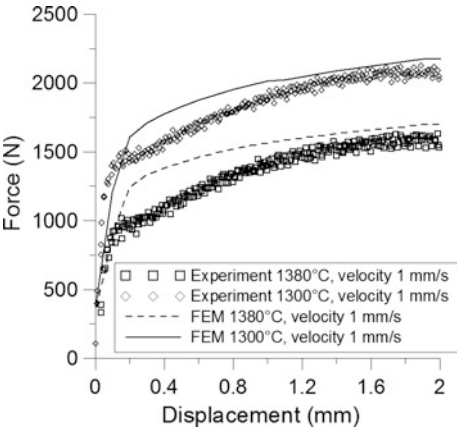


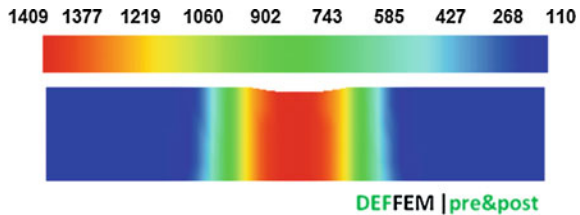
Fig. 8.51 The comparison of the calculated and measured force-displacement curves at a nominal temperature of 1300–1380 °C and a stroke rate of 1 mm/s



deformation phase the differences between the calculated and measured forces diverge. The tendency of the course changes in the second deformation phase, and the obtained forces begin to fall virtually within the same range of values.

On the basis of the obtained simulation results one can see that the application of the developed DIM methodology to determine parameters of the function describing changes leads to the final results. The average error value is at a level of 7.3 % for the test at a temperature of 1300 °C and 17.2 % for the test at a temperature of 1380 °C. However, the obtained results indicate a certain non-uniformity of the deformation zone itself, as well as rapid changes in the plastic and mechanical properties along with a temperature change. Figure 8.52 presents a temperature field on the longitudinal section of a sample deformed at a nominal temperature of 1380 °C (stroke rate 1 mm/s) after the end of the tensioning process (stroke = 2 mm). When analysing the temperature field after the resistance heating process (Fig. 8.28), which at the same time is the initial condition for the

Fig. 8.52 The temperature field distribution on the longitudinal sample section, $T = 1380\text{ }^{\circ}\text{C}$, stroke = 2 mm, stroke rate = 1 mm/s



mechanical solution, and the temperature field after the tensioning process (Fig. 8.52), one may observe a slight reduction of the maximum (from 1416 to 1409 $^{\circ}\text{C}$) and minimum temperatures (from 114 to 110 $^{\circ}\text{C}$). For the analysed temperature range even such small temperature changes within the deformation zone can cause rapid changes in the plastic and mechanical properties.

8.3.2.4 The Numerical Identification Methodology (NIM) for the Extra-High Temperature Range

As shown by the obtained results for such high temperatures, the methods of direct determination of stress-strain curves, based only on the experimental results, are insufficient. In these experiments a number of disturbances occur (deformation non-uniformities, heat generated as a result of deformation work, rapid heat discharge to the medium being in contact), which significantly influence the obtained results. Therefore, in order to eliminate these disturbances a combination of the direct solution based upon the finite element method with the inverse calculation method, based on the proposed NIM (Numerical Identification Methodology) methodology, was suggested.

The NIM (Numerical Identification Methodology) methodology covers the following stages:

- I. The preparation of samples for testing with the Gleeble 3800 simulator. Cylindrical samples with a length of 125 mm and a diameter of 10 mm. As in the tensile tests, a quartz shield and copper holders with a long contact zone were applied. During the tests one control thermocouple TC4 was applied.
- II. The proposed experiment programme included heating to a temperature of 1350 $^{\circ}\text{C}$ at a rate of 20 $^{\circ}\text{C/s}$, and then further heating to a temperature of 1430 $^{\circ}\text{C}$ at a rate of 1 $^{\circ}\text{C/s}$. Cooling to the nominal deformation temperature was performed at a rate of 10 $^{\circ}\text{C/s}$, and after holding for 10 s at the set temperature the compression process was performed with the reduction of 10 mm, and the tool stroke rate of 1 and 10 mm/s. The basic test cycle covered the deformation scope within a temperature range from 1200 to 1380 $^{\circ}\text{C}$. During the tests, the changes in the tool position and the compression force were recorded. The obtained courses of force changes as a function of the tool displacement constituted the vector of input parameters

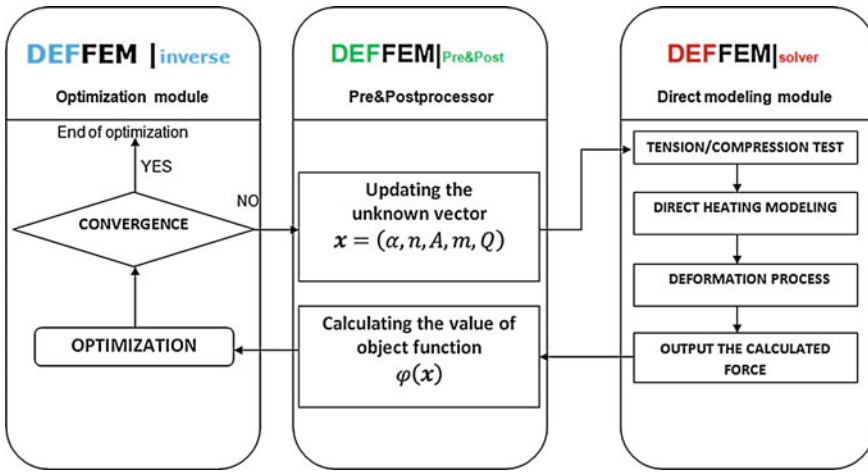


Fig. 8.53 DEFFEM package optimisation platform

to the direct calculation module, as part of the methodology based upon inverse solution.

- III. The following stage of the proposed methodology is the utilization of inverse calculations to identify the function parameters describing changes of stress versus strain. The general diagram of the inverse solution is presented in Fig. 8.53. As part of the modelling work, the optimisation platform being an integral part of the developed DEFFEM package was utilized. The optimisation platform allows the search parameters of the function describing changes of stress versus strain to be identified in an interactive and automatic manner and on the basis of experimental data.

As is shown in Fig. 8.53, the DEFFEM solver, responsible for the modelling of the Gleeble 3800 compression physical tests, is linked with DEFFEM inverse module by DEFFEM Pre and Post module, that is used to transfer the successively updated sets of parameters x from the DEFFEM inverse module to the DEFFEM solver and to calculate the values of the object function and then to transfer them to the DEFFEM inverse module. At the beginning of the inverse calculation initialisation, the vector x of the searched parameters constitutes the start parameters for the DEFFEM solver. The start parameters unambiguously defining the function describing changes of stress versus strain are included in the compression process numerical model. The curve of change of force as a function of tool displacement is an output parameter. This curve is then transferred to the Pre and Postprocessor module to calculate the objective function in accordance with following equation [10]:

$$\varphi(\mathbf{x}) = \frac{1}{N_t} \frac{1}{N_{pr}} \sum_{i=1}^{N_t} \sum_{j=1}^{N_{pr}} \left[\frac{F_{ij}^{calc}(\mathbf{x}) - F_{ij}^{exp}}{F_{ij}^{exp}} \right]^2 \quad (8.29)$$

where:

N_t —the number of experiments (compression tests),

N_{pr} —the number of measurement points,

F_{ij}^{calc} —the calculated compression force,

F_{ij}^{exp} —the measured compression force.

After calculating the objective function values, the DEFFEM inverse module corrects the parameters of the vector $\mathbf{x}$, which is then used to define the function describing changes of stress versus strain in the following iteration of the DEFFEM solver module. The iterative cycle is repeated until the obtained values of changes of the objective function are lower than the assumed stop criterion $eps < 0.00001$. When the actual search region becomes narrower than eps , at least for one of the parameters, the optimisation procedure stops. As in the DIM methodology, gradient-free optimisation techniques by Hooke-Jaevs, Rosenbrock and Nalder-Mead were utilized to minimize the objective function (8.29). The identified parameters of vector $\mathbf{x}$, based on the Numerical Identification Methodology (NIM), are collected in Table 8.11.

Figure 8.54 presents examples of stress-strain curves obtained as a result of inverse calculations for temperatures from the range from 1300 to 1410 °C and strain rates of 0.1 s⁻¹. The values of stresses for a temperature range close to 1400–1410 °C are from 10 to 12 MPa and increase to about 16 MPa for the temperature of 1300 °C.

An example of the strain intensity distribution for deformation tests at nominal temperatures of 1200, 1300, 1350 and 1380 °C and a tool stroke rate of 1 mm/s is presented in Figs. 8.55, 8.56, 8.57, and 8.58. Visualisations were made along the sample maintaining the symmetry with respect to the Z and R axes. When analysing the obtained results one may observe a concentration of the maximum strain intensity values in the middle sample part. As the nominal temperature of the compression test increases, the maximum values of the intensity increase from 0.92 for the deformation test at a temperature of 1200 °C (Fig. 8.55), to 1.36 for the deformation test at a temperature of 1380 °C (Fig. 8.58). An increase in the nominal test temperature also influenced the size and the range of formation of the deformation zone itself. As the temperature increased, an extension of the deformation zone in the radial direction (increase in the deformation zone radius), and an extension of the non-deformed zone (in the longitudinal direction) were observed.

Table 8.11 Identified parameters by the Numerical Identification Methodology (NIM)

α (MPa ⁻¹)	n	A (s ⁻¹)	m	Q (J/mol)
0.05879	0.06986	1.33E+17	0.15869	469964.1

Fig. 8.54 Examples of stress-strain curves obtained as a result of inverse calculations for temperatures from the range from 1300 to 1410 °C and strain rates of 0.1 s⁻¹

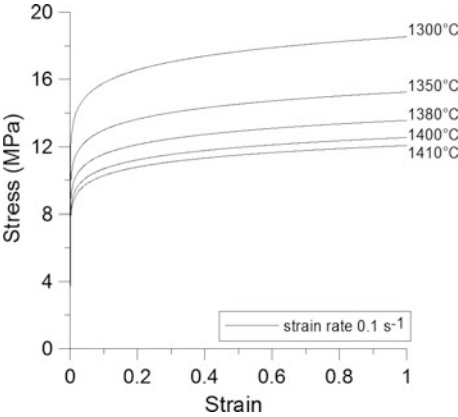


Fig. 8.55 The strain intensity distribution on the longitudinal sample section, T = 1200 °C, stroke rate = 1 mm/s, steel C45

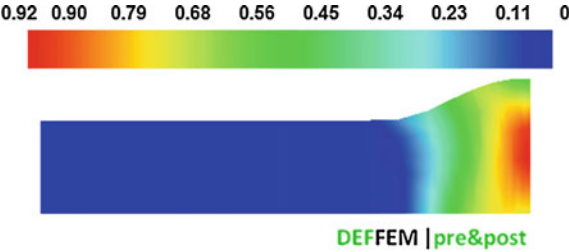


Fig. 8.56 The strain intensity distribution on the longitudinal sample section, T = 1300 °C, stroke rate = 1 mm/s, steel C45

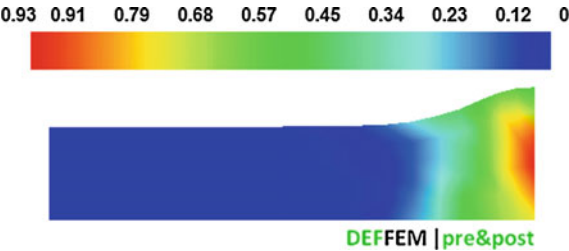


Fig. 8.57 The strain intensity distribution on the longitudinal sample section, T = 1350 °C, stroke rate = 1 mm/s, steel C45

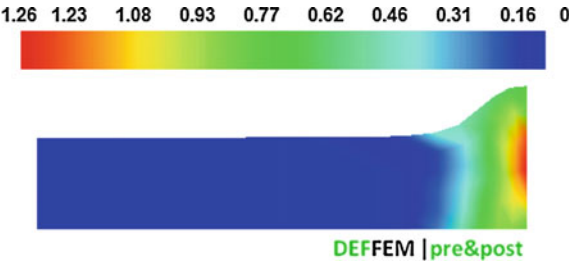


Fig. 8.58 The strain intensity distribution on the longitudinal sample section, $T = 1380\text{ }^{\circ}\text{C}$, stroke rate = 1 mm/s, steel C45

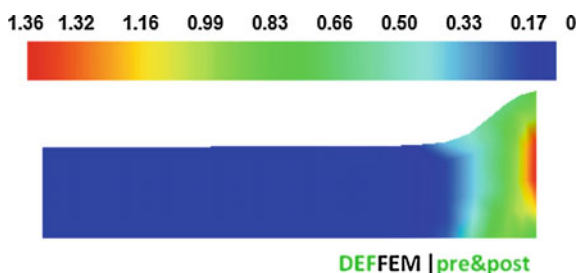
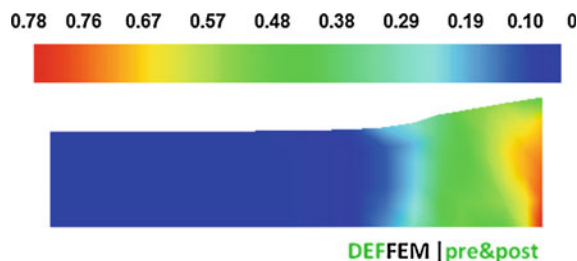


Fig. 8.59 The strain intensity distribution on the longitudinal sample section, $T = 1200\text{ }^{\circ}\text{C}$, stroke rate = 1 mm/s, steel S355



For deformation of C45 steel samples within a temperature range of 1200–1380 $^{\circ}\text{C}$ for two various tool stroke rates, the shape of the deformation zone for all tests was very similar. For steel S355, the deformation zone shape was different as the nominal temperature of deformation increased. As the temperature increased, a distinct deformation zone extension in the radial direction and a distinct extension of the non-deformed zone were observed. An example of the strain intensity distribution for deformation tests at a nominal temperature of 1200 $^{\circ}\text{C}$ and a tool stroke rate of 1 mm/s for steel S355 is presented in Fig. 8.59. When compared to the deformation of a C45 steel sample at the same temperature (Fig. 8.55), the deformation nature is different and features a smaller extension of the deformation zone in the radial direction, at a slight expense to the non-deformed zone.

IV. The obtained results were verified experimentally on the basis of the methodology, which included:

- a comparison of force courses of the process obtained from the simulations and experiments,
- measurements of the deformation zone and a comparison with the results obtained from computer simulations. Three comparative criteria were used for the verification:
- comparison between the measured and calculated shapes of the sample cross-section,
- comparison between the measured and calculated length of the zone which is not subjected to the deformation,
- comparison of the measured and calculated maximum sample radius.

Fig. 8.60 The comparison of the calculated and measured force-displacement curves at several temperatures and a stroke rate of 1 mm/s

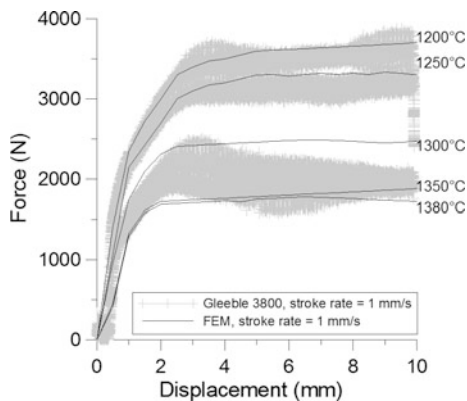


Figure 8.60 presents a comparison of calculated and experimentally determined courses of force changes in the function of tool stroke for samples deformed at a tool stroke rate of 1 mm/s. All measurement points obtained from the experiment are included in the graph, in order to present the scatter of the experimental data. The force courses (experimental) for the temperatures of 1300, 1350 and 1380 °C fall virtually within the identical force range of 2000 N. When analysing the obtained results one may find out that the nature of their course is very similar. The applied NIM methodology allowed the parameters of the function describing the changes of stress versus strain for the zone with the highest plastic strains to be correctly identified. It leads to the correct description of force parameters in the numerical model. The maximum relative errors for temperatures 1200, 1250 1300, 1350 and 1380 °C were: 2.5, 3.19, 19.24, 2.9 and 5.28 %, respectively.

The next stage of the verification of the obtained results was a comparison of parameters describing the obtained and calculated deformation zones. The samples were scanned with an ATOS Triple Scan scanner by GOM. It is a high resolution, industrial, optical 3D scanner. It very quickly and accurately provides 3D data of the measured model. It presents the object geometry by capturing its surface in a dense cloud of points or a polygon mesh. The operation of this scanner utilizes a narrow-band blue light, which enables precise measurements to be made regardless of the environmental lighting conditions. Its principle of operation is projecting light lines onto the scanned object surface. Their image is distorted on the surface of the object examined, accordingly to the shape of this surface. The location of the distorted light lines is recorded by two cameras set at appropriate angles. For each camera pixel, through optical transformation equations, the device software calculates its coordinates (x, y, z). These coordinates form a point set in the space (the so-called point cloud). The device records the object surfaces from each of its sides, which results in many images. Individual measurements are automatically processed into a single coordinate system with reference points, which are applied onto the scanned surface in order to enable the surface to be oriented in the space and to connect images to each other. The very process of sample dimensioning was carried

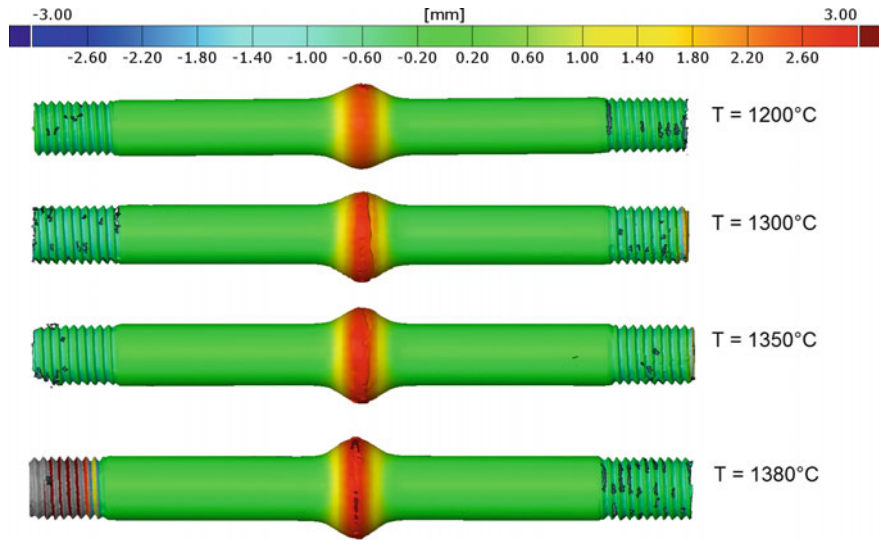


Fig. 8.61 Maps of measurements of samples deformed at a stroke rate of 1 mm/s

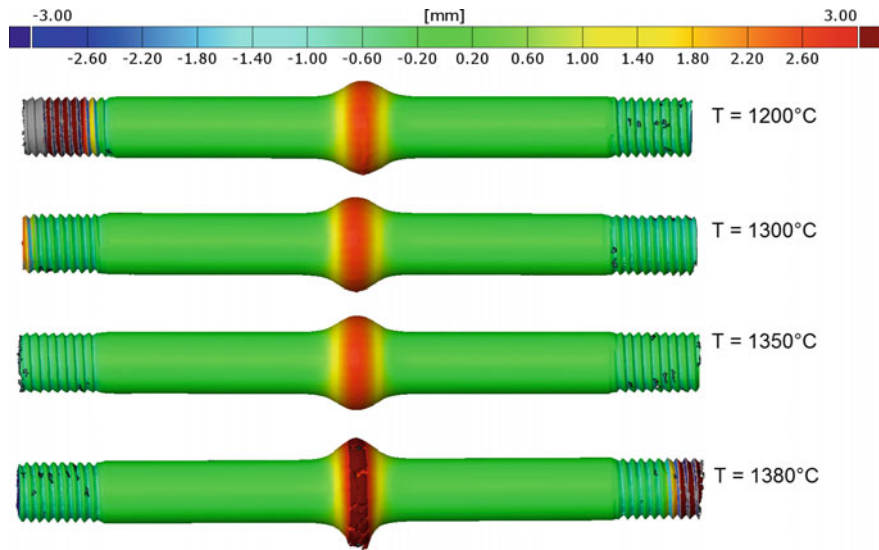


Fig. 8.62 Maps of measurements of samples deformed at a stroke rate of 10 mm/s

out in the GOM Inspect program. Figures 8.61 and 8.62 present the actual measurement maps for samples deformed at a stroke rate of 1 and 10 mm/s respectively, for the selected temperatures. The obtained results in the form of deviation maps were made on the basis of the reference shape of a non-deformed cylindrical sample.

Table 8.12 Comparison of calculated and measured lengths of non-deformed zones

Nominal test temperature (°C)	Stroke rate (mm/s)	Experiment (mm)	Simulation (mm)	Relative error (%)
1200	1	97.291	97.587	0.3042
1300	1	98.373	97.978	0.4
1350	1	99.175	98.689	0.49
1380	1	98.589	99.163	0.58
1200	10	98.494	98.101	0.39
1300	10	98.411	98.122	0.29
1350	10	98.173	98.732	0.56
1380	10	97.307	99.232	1.97

Table 8.13 The comparison of the calculated and measured radii of the deformation zone

Nominal test temperature (°C)	Stroke rate (mm/s)	Experiment (mm)	Simulation (mm)	Relative error (%)
1200	1	7.462	7.385	1.03
1300	1	7.451	7.298	2.05
1350	1	7.446	7.901	6.11
1380	1	7.575	8.107	7.02
1200	10	7.426	7.394	0.43
1300	10	7.461	7.387	0.99
1350	10	7.393	7.979	7.92
1380	10	8.378	8.314	0.76

The obtained results are compared in Tables 8.12 and 8.13. The calculated and measured lengths of non-deformed zones are compared in Table 8.12. The maximum relative error of 1.97 % was achieved for the deformation test at a temperature of 1380 °C (deformation within the range of the liquid and solid phase coexistence).

On the other hand, in Table 8.13 the calculated and measured values of the deformation zone radii are presented. The maximum relative error reached the value of 7.92 %.

The obtained results are characterized by good compatibility with the results obtained during experiments. Figure 8.63 presents the results of analysis by comparing the 3D shape of the deformation zone of the scanned sample and the shape of the sample obtained from the numerical calculations. The numerically calculated three-dimensional geometry of the sample deformation zone results from a rotation of the sample profile (obtained from the simulation) by 360° with respect to axis Z. The procedure of comparison of both shapes was performed with software by an American company—Engineering Technology Associates, eta/Dynaform. When analysing the obtained deviation map (Fig. 8.63), one can specify the areas where the deviation differences between the numerically calculated zone and the measured

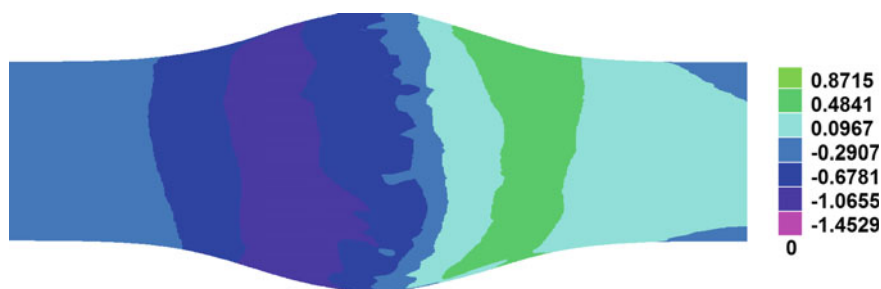


Fig. 8.63 The comparison of the calculated and measured shape of the sample deformed at 1380 °C at a stroke rate of 1 mm/s (eta/Dynaform)

zone (experiment) reach from +0.8715 mm to -1.4529 mm. The biggest differences form in the upper part of the sample deformation zone, achieving the value of the deviation field of -1.4529 mm. The lower part of the deformation zone is characterized by lower values of the deviation field, which achieve the value of +0.8715 mm. The obtained results are for orientation only, providing primarily information, among others, about obtaining the non-uniform sample deformation zone during the experiment. One should bear in mind that the geometry of the sample deformation zone obtained from the simulation was built on the basis of the obtained section, and then its rotation around the Z axis. An approach like this defines the 3D geometry, and maintains full symmetricalness of the deformation zone.

8.4 Summary

The conducted experimental research and computer simulations of the deformation process on the basis of the modelling concept using axially symmetrical models yielded a number of results concerning the behaviour of steel during deformation in the conditions of a change in the state of aggregation, which allowed drawing the following fundamental conclusions:

1. The hybrid thermo-mechanical model applied in the studies allows us to predict the metal flow and temperature fields in the zone deformed. It was confirmed by verification tests showing conformity of the obtained results with the experimental data.
2. The methodology for analysis of the deformation or the remelting zone developed in this project using computer tomography allows us to accurately estimate the porous zone shape, and to analyse qualitatively. The obtained results show large asymmetry of the remelting zone within the sample volume. The quartz shield is a key component disturbing the heat transfer on the sample circumference. To minimise this disturbance, one should aim at e.g. modifying the

methodology of test performance by giving up the shield and precisely controlling the heating and remelting process of the sample.

3. The Direct Identification Methodology (DIM) and Numerical Identification Methodology (NIM) developed as part of the project, allow the most important parameters of the equation describing changes of stress as a function of deformation to be correctly identified. This has had a decisive impact on the correctness of the obtained results.
4. The modelling of steel deformation at extra-high temperatures is related to the need to overcome a number of problems specific to this temperature range. Difficulties in the determination of material constants for this range are the primary problems. The DEFFEM simulation system that is developed, being an integral part of the developed methodologies for determining the stress-strain relationships, allows these difficulties to be overcome.
5. The prepared sample resistance heating model correctly predicts the initial temperature distribution on the sample section, which essentially influences the prediction of the final values of strains within the deformation zone.
6. Rapid changes in the plastic and mechanical properties, and in the quickly changing temperature require applying special methods of mathematical modelling of the deformation process at temperatures over the typical hot working range. The application of the controlled volume condition in the analytical form has led to the formulation of a correct mathematical model of the steel deformation process in the semi-solid state, taking into account the influence of steel density changes in all component models.

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Chapter 9

Modelling Concept Based upon Three-Dimensional Models

This chapter presents examples of results of numerical analyses of the deformation process in conditions of liquid and solid phase coexistence, conducted on the basis of a modelling concept using three-dimensional models. The analysis was carried out with simplifying assumptions arising from the limited capabilities of the computing environment designed. The analyses take into account the complete characteristic of the thermo-physical data in the whole temperature range concerned. The model reconstructs the most important main effects and is able to analyse qualitatively the resistance heating process course, and next the deformation process. The chapter is supplemented with results of physical simulations, along with macro- and microstructural test results obtained on the basis of the modified research methodology.

9.1 Modified Experimental Research Methodology

Physical simulations of resistance heating and steel deformation processes in the semi-solid state were carried out with a Gleeble 3800 thermo-mechanical simulator [1]. The fundamental research methodology covering the steel sample heating and melting programme, as well as the execution of the deformation process itself, is analogous to the experimental-modelled research based upon a modelling concept using axially symmetrical models. Steel S355 was the tested material. A new type of hexahedral samples was used in the tests:

- type A samples ($10 \times 10 \times 76$ mm),
- type B samples ($10 \times 10 \times 100$ mm),
- type C samples ($10 \times 10 \times 125$ mm).

The sample length, which is different for each sample type, largely determines the actual length of the heating zone in the simulator system, which in turn influences the width of the obtained remelting zone.

A new type of copper grips, adopted to the new sample shape, was used in the tests. In addition, the quartz shield, which was primarily to protect the simulator inside against an accidental leak of liquid metal during testing, was given up. This approach allowed one to limit the disturbances influencing the heat transfer mechanism between the sample and the environment (the simulator inside). The experience gained during the tests with cylindrical samples enabled a precise experiment schedule to be developed, allowing a safe course and full control over the experiment to be ensured.

Figure 9.1 presents the view of the Gleeble 3800 simulator with a type C hexahedral sample installed and a control thermocouple in the middle of the sample heating zone. Additionally, during the basic tests, an additional thermocouple was installed near the contact place of the sample with the copper holder.

On the basis of the determined characteristic temperatures of the steel tested (see Chap. 7), and bearing in mind that as a result of resistance heating the highest temperatures exist in the sample core, an experiment programme was proposed, which was appropriate for all sample types (A, B and C), presented in detail in Table 9.1.

The temperature programme consisted of heating a sample to a temperature of 1400 °C at a constant rate of 20 °C/s, and then to a temperature of 1450 °C at a rate of 1 °C/s. The next stage was holding at the constant temperature for 10 s and cooling to the nominal deformation temperature at a rate of 10 °C/s. Before the deformation process, also holding for 10 s to stabilise the temperature in the sample volume was introduced. The tests were performed at a constant tool stroke velocity of 1 mm/s. For type A samples, due to the shortest free zone, the ram stroke length was 1.2 mm. In other cases, for type B and C samples, the ram stroke length was 5 mm. During the tests, the temperature, force, voltage and electrical current were recorded.



Fig. 9.1 The view of the Gleeble 3800 simulator with a type C hexahedral sample and a control thermocouple installed

Table 9.1 Experiment programme of heating and deforming type A, B and C samples

Heating				
Heating temperature (°C)		Heating rate (°C/s)		Holding time (s)
1	1400	20		–
2	1450	1		10
Deformation parameters				
Cooling rate to the deformation temperature (°C/s)		Holding time (s)		
10		10		
Deformation temperature		Deformation parameters		Sample type
No.	T _d (°C)	Stroke (mm)	Grip velocity (mm/s)	
1	1450	–1.2	1	Type A
2	1440	–1.2	1	Type A
3	1435	–1.2	1	Type A
4	1450	5	1	Type B
5	1440	5	1	Type B
6	1435	5	1	Type B
7	1450	5	1	Type C
8	1440	5	1	Type C
9	1435	5	1	Type C

The resistance heating method was applied for heating and remelting of samples. The energy necessary to remelt a certain zone width (depending on the type of samples used for the tests) is released inside the sample, due to the electrical current flow, as Joule's heat. The process of steel sample remelting itself is characterised by considerable complexity. During changes in the temperature of the heated sample, its physical, thermal and electrical properties change continuously, and furthermore, in critical process times, phase transformations occur with an abrupt change in these parameters. The heat dissipation into the environment accompanying the remelting process and the heterogeneity of the temperature field additionally hinder the modelling of the steel deformation process in the conditions of liquid and solid phase coexistence. The resistance heating method is a complex physico-chemical process. In accordance with Joule-Lenz law, the source of energy is the heat Q liberated in each conductor during the electrical current flow with the electrical current of I . This heat is proportional to the square of the current intensity and the conductor resistance R . However, the simplicity of this dependence is ostensible. In fact, both the current intensity and the resistance of the medium analysed depend on other parameters, in particular on temperature T and time τ . During the process, the internal structure changes, and thus the heat and electricity conduction conditions change. In effect, a steel sample is characterised by different thermo-physical properties before and after remelting. It is accompanied by a change in the physical

(density, state of aggregation), thermal (specific heat, thermal conductivity) and electrical properties (change in resistance). Some of these conditions may be tracked by numerical analysis. It concerns in particular the impact of effects related to the heat transfer in the sample being remelted. Therefore, the main objective of the fundamental research was to determine the prevailing thermal effects, or to determine the zones where sample heating is heterogeneous, or to compare the influence of the application of three types of samples on the obtained size of the remelting zone. The numerical analyses were performed with some restrictions. The necessary thermo-physical characteristics were determined on the basis of the chemical composition using the commercial software JMatPro, version 8. The calculated thermo-physical properties of the steels analysed were attached as an annex to this monograph (Appendix A). During the steel sample remelting process, the electric current flows between the grips through the sample. As the copper grips in the simulator system—compared to other system components conducting electricity—are intensively cooled with water, during the electrical current flow the heat liberation within the sample is the most intensive.

9.2 Resistance Heating Model

From the perspective of thermal problem classification in the numerical model described, the problem of transient heat conduction was considered with the present internal, voluminal heat source. The problem of this class is described in the general case, for a rectangular system of coordinates, by the Fourier-Kirchhoff differential equation (see Chap. 6). The numerical model of the system analysed and the boundary conditions are similar to heating cylindrical samples with long contact zone grips (see Chap. 8). In the variant with the “cold” grips five heat transfer zones were defined, which were denoted from Γ_0 to Γ_4 respectively (Fig. 9.2). Different boundary conditions must be defined for each zone. Zones identified as Γ_0 , Γ_2 and Γ_4 define the free area of the sample. Zones Γ_1 and Γ_3 define the contact area of the sample with the copper grips. From the perspective of the numerical model it is one of the key zones, where heat is intensively discharged to the tool. The last zones are Γ_{d1} , Γ_{d2} which defines grips free heat transfer zones.

The heat source efficiency Q in the model discussed is a function of resistance R , which in turn depends on temperature T and function A which represents intensify of heating:

$$Q = f(A(\tau)I^2(\tau)R(T)) \quad (9.1)$$

It corresponds to resistance changing in the actual model, and the internal heat source efficiency changes together with the resistance. When modelling the Joule heat generation, it was assumed that its equivalent in the numerical model will be the voluminal heat source with its power related to the resistance R and the square of electric current I during simulation time τ . During the numerical analyses, the

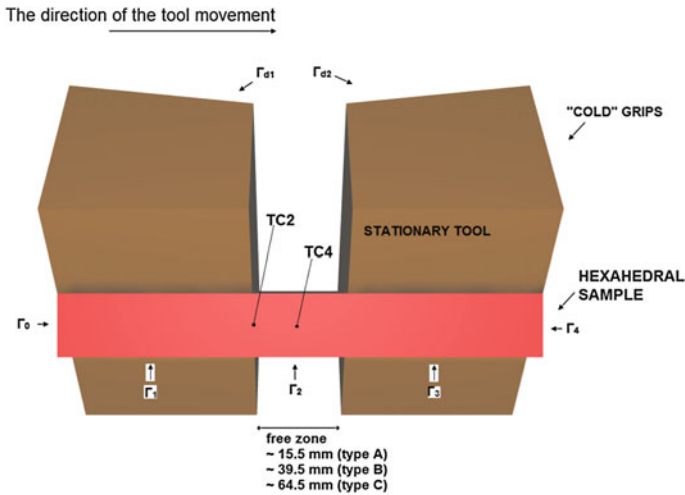


Fig. 9.2 The numerical model divided into heat transfer zones, along with the location of numerical sensors (TC4, TC2) for the “cold” grips

Joule heat liberated in other components of the electrically conductive simulator system was skipped as it was negligible. It arises from the above description that heat is liberated in the small volume of the sample subjected to the remelting process. A hexahedral sample remelted in the Gleeble 3800 simulator is surrounded by a massive system built of good electrical and thermal conductors (Fig. 9.1). An increase in the voluminal heat source power in the numerical model corresponding to the increase of electrical current in the actual system causes an increase of the temperature in the volume of the sample remelted. In view of the heat transfer conditions presented in detail in Chap. 6, the energy from the sample is transferred to the adjacent structural components of the Gleeble 3800 simulator, and next, by radiation, to the environment (simulator inside). Because of the large dimensions (large thermal capacity) of the whole system compared with the sample dimensions, the heat source power in the sample must reach the level of kilowatts to ensure the conditions necessary to transform the solid phase and obtain the liquid phase. The method of input function execution, that is the intensity of electrical current flowing through the analysed system versus time, is the essential problem. However the determination, by numerical modelling, of the temperature field in the sample and the difference between the highest and lowest temperature zones may be useful for the selection of the optimal method of input function (heating-remelting), bearing in mind the risk of high local temperature increases. As part of the numerical analyses, the intensity of the current flowing through the system was input on the basis of actual courses measured during the execution of physical simulations with the thermo-mechanical Gleeble 3800 simulator. Depending on the sample type (A, B or C), the current intensity variability as a function of time ranged between 600 A and 2500 A. For type A samples the maximum current values close to 2500 A were

reached, whereas for type B and C, 1400 A and 1200 A respectively. Significant differences in the current intensity measurement subject to the applied sample type arise primarily from the thermal conditions in the simulator system. For type A samples (length 76 mm), with the shortest heating/remelting zone, the heat discharge from the heated sample to the intensively cooled metal grips is the most intensive. In order to maintain the assumed experiment plan (the heating schedule), more energy should be supplied to the system. On the basis of the temperature reading from the control thermocouple and the assumed heating schedule, the Gleeble 3800 simulator automatics adjusts the current automatically. The boundary conditions for heating and deforming hexahedral samples were assumed similar to the cylindrical samples and the applied long contact zone holders (see Chap. 8).

9.3 Modelling the Resistance Heating Process

As mentioned above, the experience gained during the tests with cylindrical samples enabled a precise experiment schedule to be developed, allowing its safe course and full control. Figure 9.3 presents an example of a photo of a type C sample, for which the second stage of the experiment was not performed, which was its deformation. In this case, the basic heating was performed to a temperature of 1460 °C, just below the determined solidus temperature $T_s = 1465$ °C. Additionally, bearing in mind that a substantial temperature gradient occurs on the sample cross-section, one may conclude that when the sample is heated a significant amount of the liquid phase will be present in its volume. By analysing the type C sample photo presented in Fig. 9.3, one may notice the areas of distinct remelting of the sample present in half of the heating zone length. These areas were identified in all four side surfaces of the sample.

The conducted numerical analyses of heating to the nominal temperature of 1460 °C show a substantial temperature gradient on the sample cross-section and intensive heat discharge in the direction perpendicular to the sample side surface. Figure 9.4 presents temperature distributions on the sample cross-section for nine selected stages of the controlled cooling process. The visualisation was limited to the temperature range from 1465 °C (calculated in the test on the sample surface) to the maximum calculated temperature in the sample core of 1511 °C. The analysis of the obtained temperature field distributions indicates, as in the conducted experiment for the type C sample, the occurrence on the sample side surfaces of the areas slightly exceeding the solidus temperature $T_s = 1465$ °C (step 1). The subsequent simulation stages (step 2 to step 9) show that the mushy zone disappears.

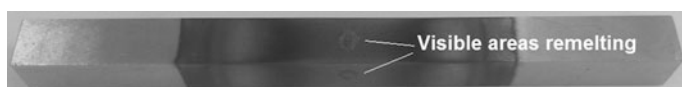


Fig. 9.3 The view of a type C sample heated to the nominal temperature $T = 1460$ °C

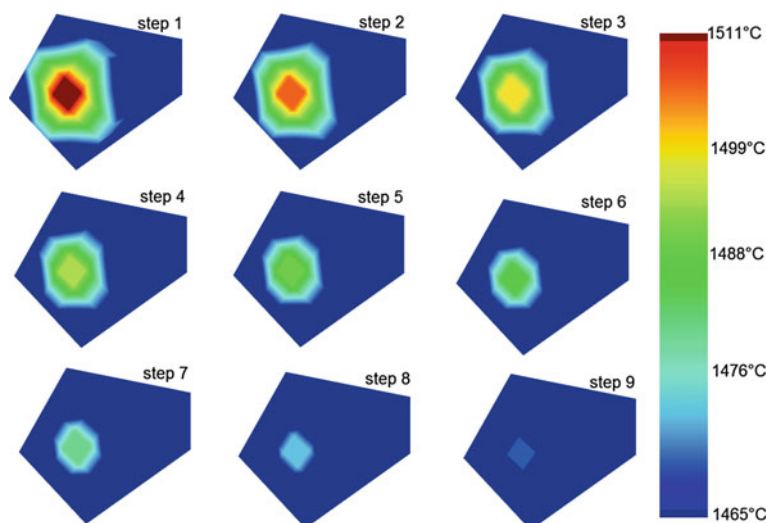


Fig. 9.4 The temperature distributions on the cross-section of the sample heated to the nominal temperature of 1460 °C for the selected stages of controlled cooling

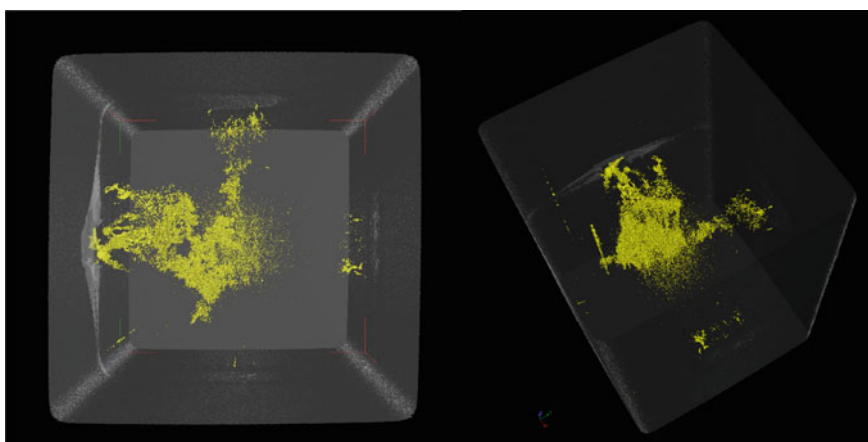


Fig. 9.5 The view of the 3D porous zone (type C sample)

As part of supplementary tests, additional tomographic tests were conducted on the basis of the methodology presented in Chap. 8 [2]. Figures 9.5 and 9.6 presents a three-dimensional view of the porous zone formed as a result of heating and remelting of a type C sample at the nominal temperature of 1460 °C, along with the performed projections of this zone on planes YX, ZY and YX.

The biggest area of the porous zone is located in the middle of the sample volume, at a place with the highest measured, and calculated temperatures. The

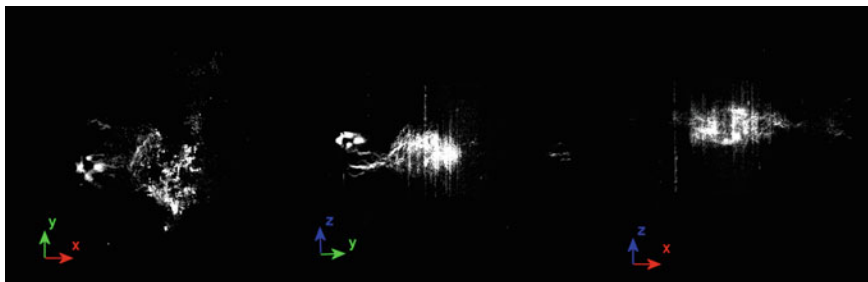


Fig. 9.6 The projections of the 3D porous zone on planes YX, ZY, YX (type C sample)

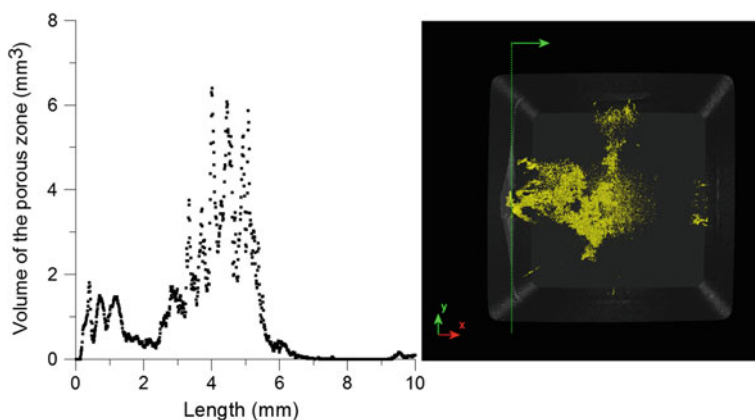


Fig. 9.7 The change in the porous zone volume with respect to the coordinates for the cross-section in the X direction

porous zone further propagates in directions perpendicular to the side surfaces of the sample. The measured area of the porous zone (yellow colour in Fig. 9.5) for the analysed type C sample was 1018.200 mm^3 . Figures 9.7, 9.8 and 9.9 present the results of measurements of changes in the porous zone volume with respect to the coordinates for individual axes of the coordinate system. Measurements for directions X and Y were made exactly in the cross-section at $\frac{1}{2}$ of the length of the heating zone of the type C sample (Figs. 9.7 and 9.8). The maximum measured porous zone volume for both measurements oscillated within 7 mm^3 (sample core).

For measurements along the Z axis (along the sample heating zone), the measurement was made on the whole length of the visible porous zone (Fig. 9.9). The obtained width of the porous zone was about 2.2 mm , and the porous zone volume at $\frac{1}{2}$ of the sample heating zone length was 8 mm^3 .

For the analysis performed for the other sample types (A and B), it was observed that when the length of the free zone that is intensively heated decreases, the porous zone area decreases. Figure 9.10 presents the view of the central part of a type B

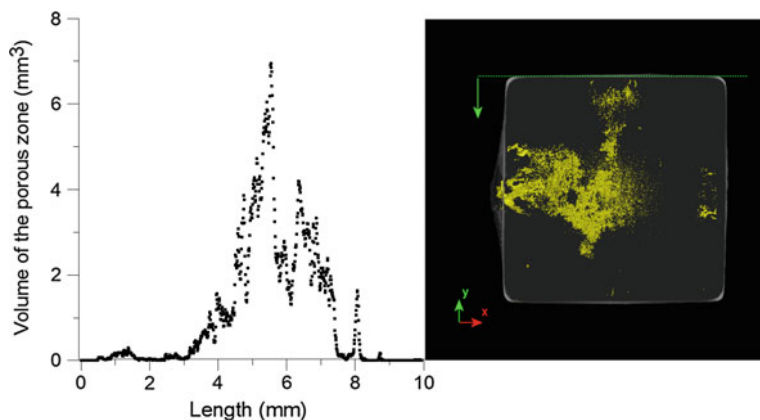


Fig. 9.8 The change in the porous zone volume with respect to the coordinates for the cross-section in the Y direction

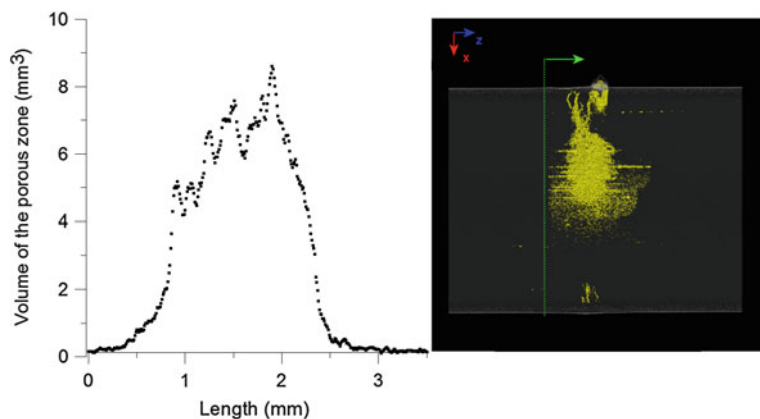


Fig. 9.9 The change in the porous zone volume with respect to the coordinates for the cross-section in the Z direction

sample heated to a temperature of 1460 °C, with a visible porous zone. Compared to the type C sample (Fig. 9.5), the porous zone form is different, and no characteristic remelting areas were observed on the sample side surfaces.

Analysis of the obtained results for type A samples indicates that in this case the share of the mushy zone in the sample volume is the smallest when compared to type B and C samples. Figure 9.11 presents cross-sections with the estimated mushy zone for three nominal temperatures of 1450, 1440 and 1435 °C. It is not the actual mushy zone shape, but its contour obtained as a result of the visualisation of the mesh temperature values for the colour scale assumed on the basis of the minimum determined temperature and the maximum calculated temperature.

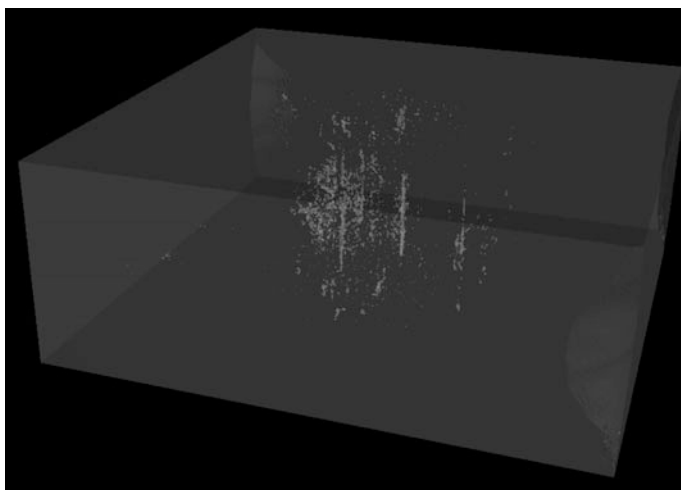


Fig. 9.10 The view of the porous zone (type B sample)

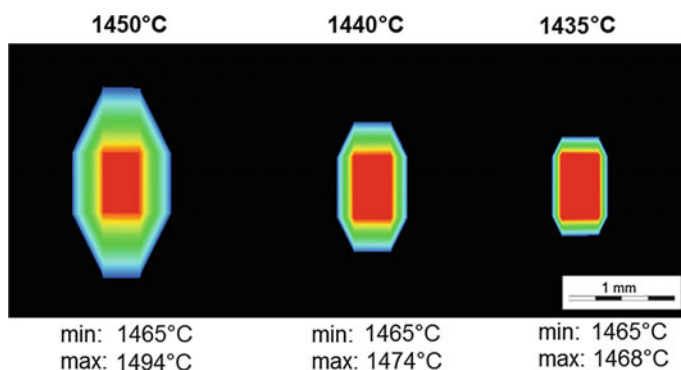


Fig. 9.11 The cross-section with an estimated mushy zone (type A sample)

Bearing in mind the values of the solidus ($T_s = 1465\text{ }^{\circ}\text{C}$) and liquidus ($T_l = 1513\text{ }^{\circ}\text{C}$) temperatures of the steel tested, all defined ranges are within T_s - T_l . For heating to the nominal temperature of $1450\text{ }^{\circ}\text{C}$, the maximum temperature value reached in the core sample was $1494\text{ }^{\circ}\text{C}$. The estimated range of the mushy zone for the sample cross-section is small and decreases when the nominal test temperature decreases.

To estimate the 3D shape of the mushy zone more accurately, numerical calculations were made with the use of a CAFE model (see Chap. 6). Figure 9.12 presents the evolution of the mushy zone shape changes during the consecutive selected free cooling steps along with the solid phase share distribution in the selected cross-sections of a type C sample. The mushy zone decreases in the next

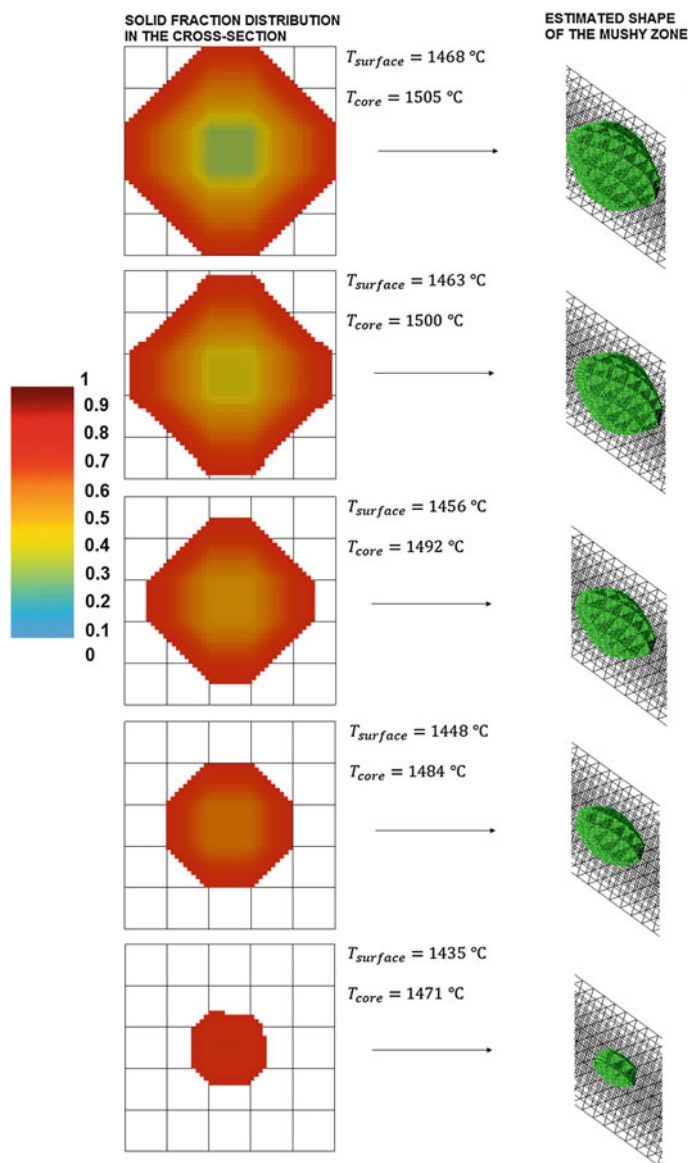


Fig. 9.12 The evolution of the mushy zone shape changes during the free cooling, along with the solid phase share distribution in the cross-section (type C sample)

steps, and the calculated solid phase itself is the smallest in the sample core and increases towards the sample surface.

Figures 9.13, 9.14, 9.15, 9.16, 9.17 and 9.18 present the calculated temperature fields for 10 and 25 s of the heating process. The analysis of the obtained results

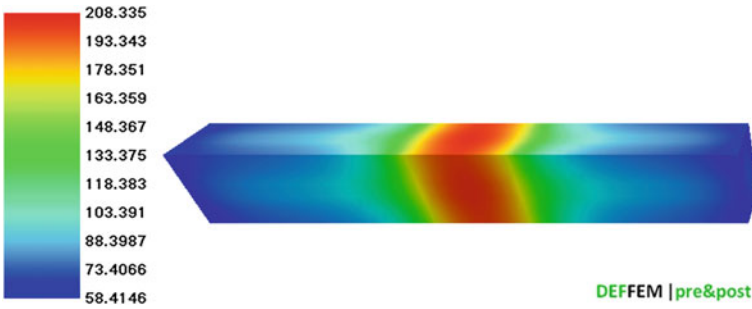


Fig. 9.13 The temperature field after the10th second of heating (type A sample)

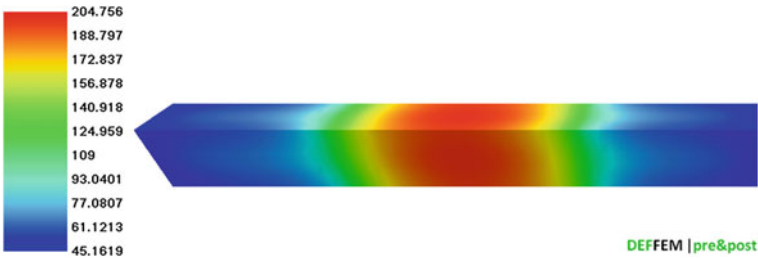


Fig. 9.14 The temperature field after the 10th second of heating (type B sample)



Fig. 9.15 The temperature field after the 10th second of heating (type C sample)

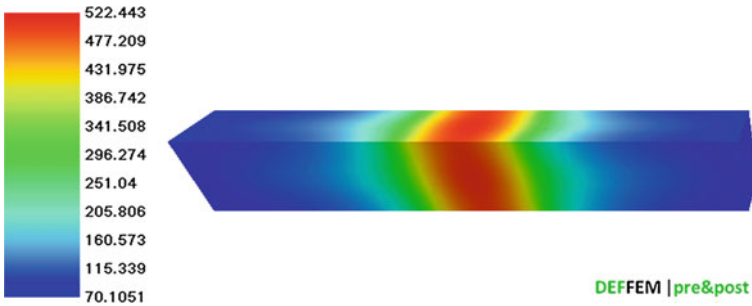


Fig. 9.16 The temperature field after 25 s of heating (type A sample)

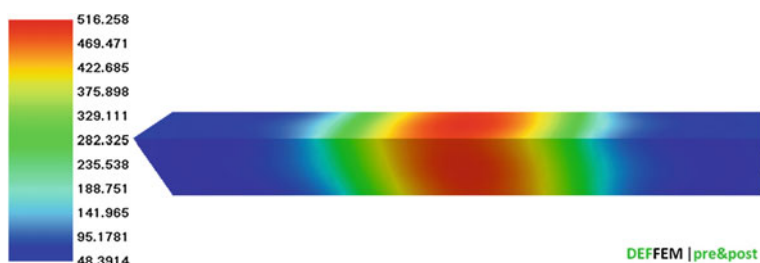


Fig. 9.17 The temperature field after 25 s of heating (type B sample)



Fig. 9.18 The temperature field after 25 s of heating (type C sample)

indicates that the type of the applied samples has a big impact on the obtained width of the remelting zone. This zone extends when the sample free zone length increases. In accordance with the heating schedule presented in Table 9.1, the numerical control sensor defined at the same place as the control thermocouple during the experiment after 10 and 25 s of heating, should indicate 200 and 500 °C respectively, regardless of the selected sample type. After 10 s of heating, the difference between the calculated temperature on the sample surface (numerical sensor 1) and the sample core temperature (numerical sensor 2) for the type A sample was 8 °C (Fig. 9.13) and increased to 22 °C after 25 s of heating (Fig. 9.16). For the other samples the differences in indications of both sensors after 10 s of heating were smaller and were 5 and 4 °C for type B and C samples respectively (Figs. 9.14 and 9.15), and then after 25 s of heating increased to 16 and 14 °C respectively (Figs. 9.17 and 9.18).

The final temperature fields (for the deformation test performed at the nominal temperature of 1450 °C) are presented in Figs. 9.19, 9.20 and 9.21. The computed difference between the calculated temperature on the sample surface (numerical sensor 1) and the sample core temperature (numerical sensor 2) for a type A sample was 44 °C (Fig. 9.19). For the other two types of samples (B and C), the obtained differences were 46.5 °C (Fig. 9.20) and 48 °C (Fig. 9.21) respectively. When comparing the amount of energy released in Joule's effect with the amount of energy needed to remelt a sample, it occurs that the amount of energy needed to heat the

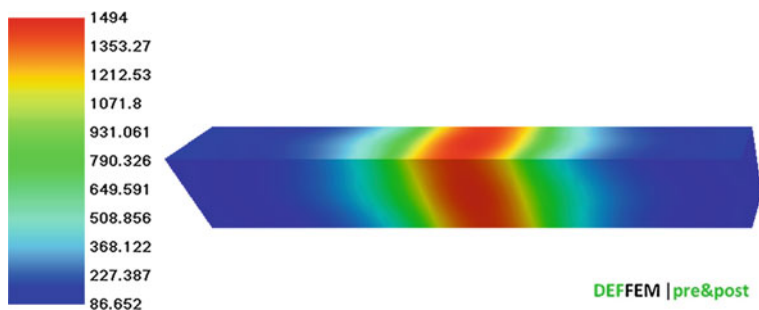


Fig. 9.19 The temperature distribution just before deformation at the nominal temperature of 1450 °C (type A sample)

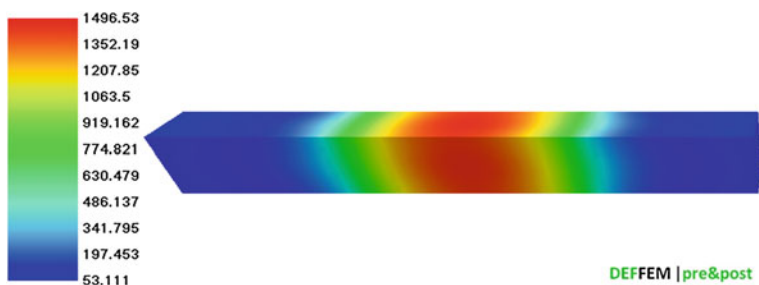


Fig. 9.20 The temperature distribution just before deformation at the nominal temperature of 1450 °C (type B sample)

structural components of the Gleeble 3800 simulator system is much bigger than the amount necessary to remelt the sample. More of the source heat is lost to the environment. The volume where the transition of the solid phase into the liquid state is the first is located approximately in one half of the heating zone. When the power increases, the zone develops towards the face surfaces. As a result, the maximum temperature and the time of maintaining the phase in the liquid state differs in individual sample zones. Near the zone of contact with the copper grips, the heat loss is so big that remelting the sample is generally difficult to obtain. For the free zone this effect is less intensive and it is possible to remelt the sample surface locally (Fig. 9.2). It is an argument that a restriction of the heat flux dissipated into the environment could improve the effectiveness of impact of internal heat sources and homogenise the temperature distribution within the sample volume.

During the tests a thermovision measurement module was used to record the courses of the selected heating process simulations. On the basis of the indications of the control thermocouple and an additional thermocouple installed near the sample-grip contact, thermograms were calibrated and developed. Next, they were used to estimate the course of the temperature change along the heating zone. Figures 9.22, 9.23 and 9.24 present an example of a temperature change profile



Fig. 9.21 The temperature distribution just before deformation at the nominal temperature of 1450 °C (type C sample)

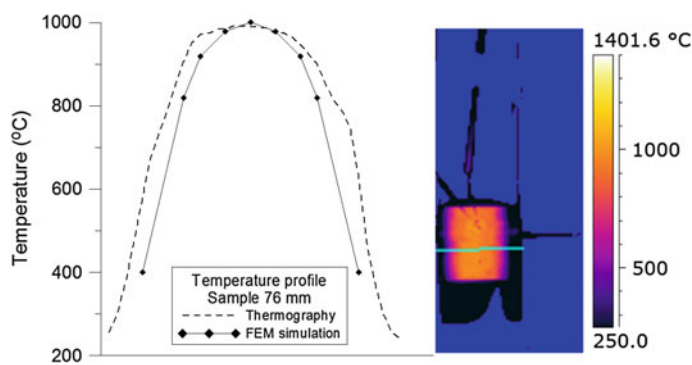


Fig. 9.22 A temperature change profile obtained from a computer and physical simulation for the 50th second of heating (type A sample)

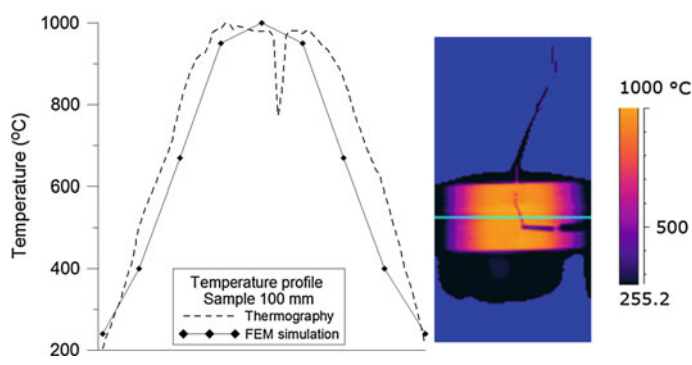


Fig. 9.23 A temperature change profile obtained from a computer and physical simulation for the 50th second of heating (type B sample)

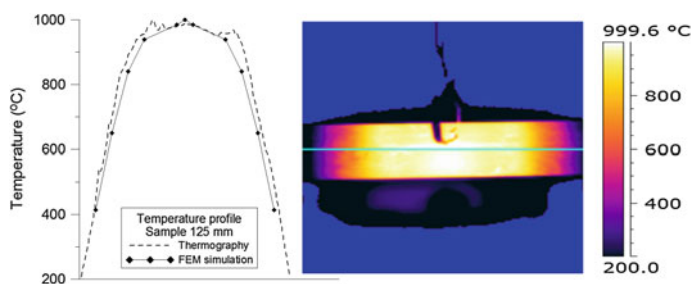


Fig. 9.24 A temperature change profile obtained from a computer and physical simulation for the 50th second of heating (type C sample)

obtained from a computer and physical simulation for the 50th second of heating for type A, B and C samples, respectively. The obtained temperature change profiles for the experiment and computer simulation are characterised by a similar course and acceptable compatibility. The maximum relative errors for type A, B and C sample were 7.21, 9.98 and 3.58 %, respectively. In all cases the temperature change course is parabolic. When assessing the differences occurring between the measured and computed temperature values, one should bear in mind that they were calculated with a few simplifying assumptions. At the present stage of implementation work on the DEFFEM simulation system, the couplings of the temperature field and the electrical field were not considered directly. It was modelled by an internal voluminal heat source. Therefore, the influence of the varying electrical properties of the heated sample on the electrical charge density and local voluminal heat source power could not be analysed. At the present stage of implementation work, it is difficult to state that taking into account the thermo-electrical impact would constitute significant progress and would allow more precise results to be obtained. If formulating such a conclusion is possible, it would be a fundamental argument to focus the software development work on a thermo-electrical impact module.

9.4 Deformation Process

After the first stage, which is the heating process, in accordance with the experiment programme (Table 9.1), the deformation process is performed. The rheological model of deformed steel S355, which was the basis for the conducted computations, was presented in detail in the other monograph co-authored by the author [3] and journals [4, 5]. Figures 9.25, 9.26, 9.27 and 9.28 present the strain distributions ε_z for tests performed at the nominal deformation temperature of 1450 and 1440 °C for type A and C samples respectively. For experiments conducted with type C samples, a wider range of the deformed zone was obtained (Fig. 9.27 and 9.28), compared to the experiments conducted with type A samples (Figs. 9.25 and 9.26).

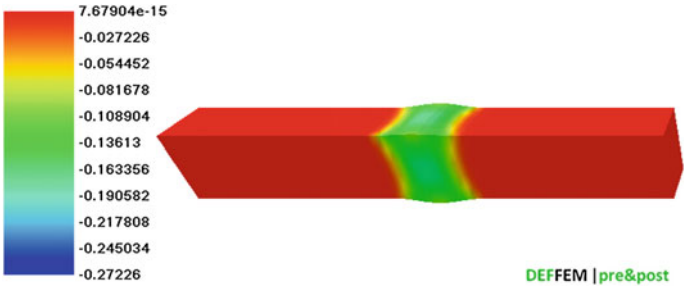


Fig. 9.25 The strain ε_z distribution after deformation at the nominal temperature of 1450 °C (type A sample)

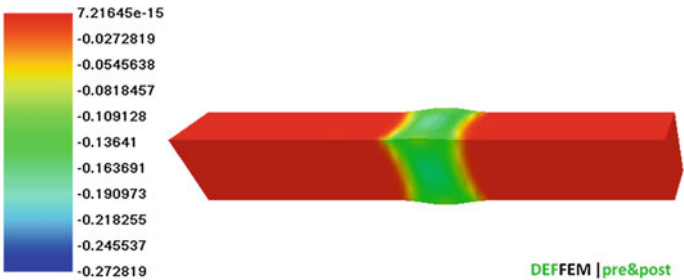


Fig. 9.26 The strain ε_z distribution after deformation at the nominal temperature of 1440 °C (type A sample)

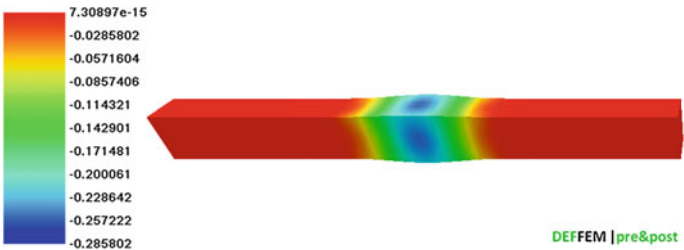


Fig. 9.27 The strain ε_z distribution after deformation at the nominal temperature of 1450 °C (type C sample)

With reference to the applied sample types, the maximum strain values are similar, however the nature of their distribution is different. For type A samples the maximum strain values are achieved mainly in the sample core, in the volume with a small fraction of the liquid phase. For a type C sample, where the liquid phase volume is bigger than that for a type A sample, the maximum strain accumulate virtually in the whole volume on the cross-section.

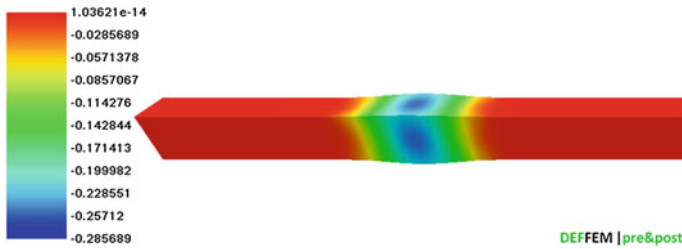


Fig. 9.28 The strain ε_z distribution after deformation at the nominal temperature of 1440 °C (type C sample)

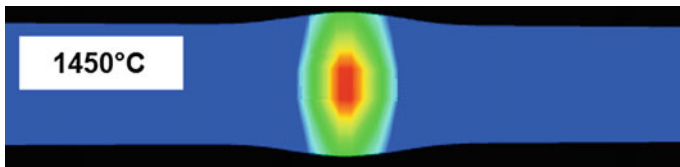


Fig. 9.29 The longitudinal section with the estimated mushy zone after the deformation process (type C sample)

As a result of the deformation work, heat is also generated. This has a considerable impact on the mushy zone area obtained. Figure 9.29 presents a longitudinal section with the estimated mushy zone after the deformation process for the nominal temperature of 1450 °C. The adopted range of temperature field visualisation was based upon the maximum calculated value in the sample core of 1555 °C and the minimum of 1466 °C. The obtained mushy zone exists practically in the whole volume on the cross-section of the sample analysed. A similar estimated mushy zone area was identified in the macrostructural tests.

Analysing the macrostructure of type C samples (Fig. 9.30) deformed at nominal temperatures of 1450, 1440 and 1435 °C, one can notice a visible concentration of the mushy zone in the sample core (the brightest areas) and the formed porous zone in the subsurface areas. This zone decreases when the nominal deformation temperature declines. This tendency, although less intensive, also occurred for type B samples (Fig. 9.31). For type A samples, where the mushy zone fraction is the smallest compared to the other types, indicating the mushy zone areas directly on the basis of the macrostructure is difficult (Fig. 9.32).

The following was adopted as an additional criterion of the qualitative assessment:

- comparison of lengths of non-deformed zones obtained as a result of the experiment and the computer simulation,
- comparison of the maximum measured cross-sections in half of the length of the heating/remelting zone, at a place of the highest strain accumulation. The measurement was made for both planes, and then averaged. After the conducted

Fig. 9.30 The macrostructure on the longitudinal section after the deformation process at the nominal temperature of 1450, 1440 and 1435 °C (type C sample)

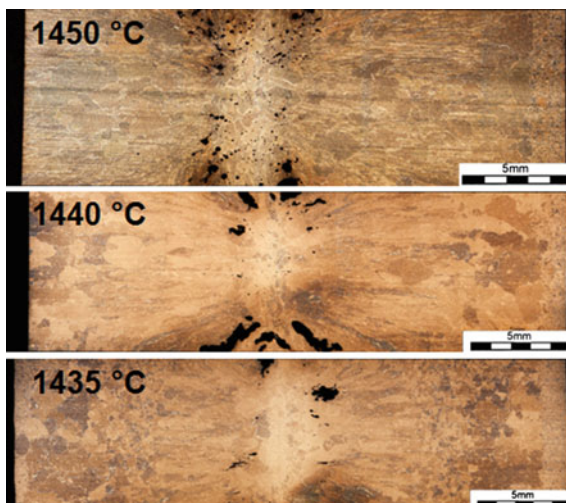
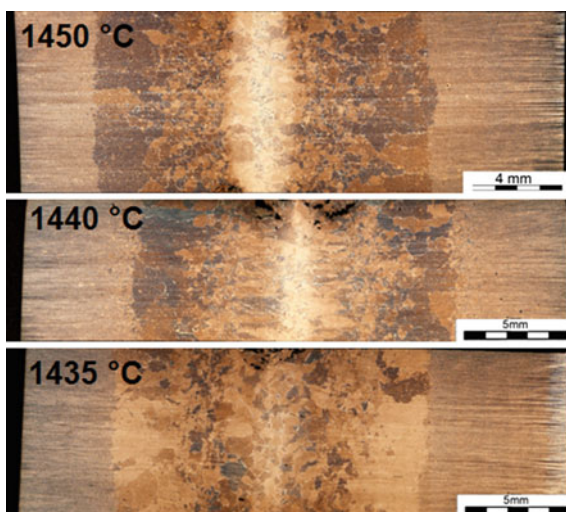


Fig. 9.31 The macrostructure on the longitudinal section after the deformation process at the nominal temperature of 1450, 1440 and 1435 °C (type B sample)



experimental tests with samples of type A, B and C, a slight increase of the deformation zone cross-section was observed, as well as insignificant extension of the sample zone that was not subject to deformation (shortening of the deformation zone) as the nominal test temperature increased (Fig. 9.33). A similar tendency was observed for computer simulations.

The conducted measurements on the basis of both criteria showed slight differences between individual measurements. For instance, for a type A sample deformed at a nominal temperatures of 1450, 1440 and 1435 °C the maximum measured cross-sections were 11.49, 11.18 and 11.14 mm respectively. However,

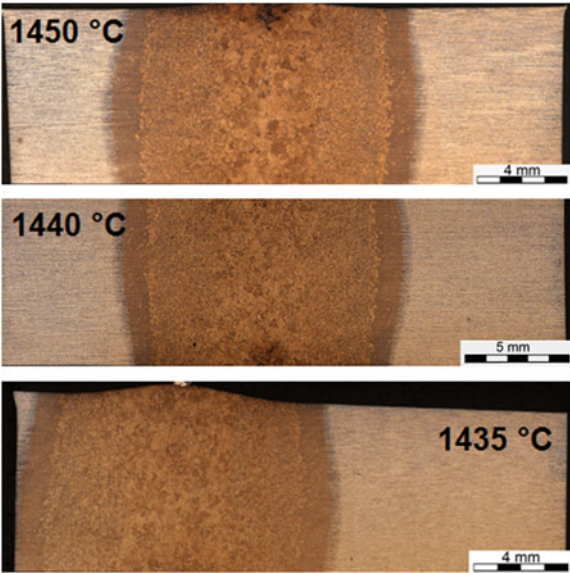


Fig. 9.32 The macrostructure on the longitudinal section after the deformation process at the nominal temperature of 1450, 1440 and 1435 °C (type A sample)

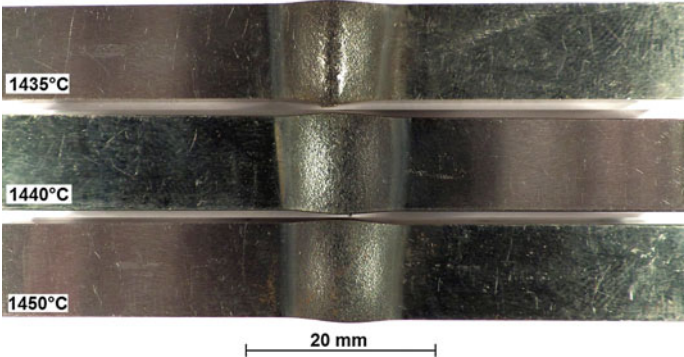


Fig. 9.33 Sample pictures after the deformation process at a nominal temperature of 1450, 1440 and 1435 °C (type A sample)

the results obtained from the simulation were 10.78, 10.65 and 10.63 mm respectively. The obtained absolute error was 6.17 %, 4.74 % and 4.57 % respectively. A similar range of errors was obtained for the second criterion, as well as for two other sample types. The occurring differences may be caused by the simplified

rheological model adopted for computing and determined on the basis of the Simple Interval Methodology (SintM) presented in details [4, 5]. Difficulties with

maintaining the convergence of the solution itself were an additional problem from the numerical implementation side, as well as the simulation performance itself. The assumed simplest type of finite elements and the occurring large local mesh deformation lead to conclusions focusing future implementation work on mathematical model development with the use of e.g. higher order elements, or the application of special remeshing algorithms. An alternative approach may be taking advantage of the meshless methods combined with the finite element method. It will allow one to elaborate the effects that occur within the deformation zone, while avoiding problems related to the finite element method.

9.5 Microstructure

The microstructural tests were performed for all types of samples that were deformed for three selected areas of the deformed sample (Fig. 9.34).

Area number one (the top deformation zone) identified hereinafter as “peak”, area number 2 (sample core) identified as “centre”, and zone number 3 (transition zone) identified as “transition zone”. Figures 9.35, 9.36, 9.37, 9.38, 9.39, 9.40, 9.41, 9.42 and 9.43 present the obtained microstructures for type A samples, deformed at temperatures of 1450, 1440 and 1435 °C respectively. The following letters designate individual phases in the presented figures: F (ferrite), M (martensite), P (perlite), B (bainite). The sample centre microstructure is formed by finer grains of the former austenite (transformed into martensite and/or lower bainite), decorated with very fine ferrite and/or bainite (probably upper bainite). The ferrite is acicular because of its high cooling rate. In the peak deformation zone, one can detail large grains of the former austenite decorated with white (slightly acicular) ferrite and/or bainite. The former austenite is primarily martensite formed after quenching to the ambient temperature. Martensite is light brown in the presented microstructures. The former austenite grain is distinctly smaller when moving towards the transition zone. The martensite share declines in favour of bainite and ferrite (white). The ferrite morphology changes from acicular to grainy—and more precisely the ferrite grains have a polygonal (equiaxed) shape. In the zone where the material temperature does not exceed A_{c1} , we have a banded ferritic-perlitic structure with a certain amount of



Fig. 9.34 Identification of the microstructural test areas (1-peak, 2-centre, 3-transition zone)

Fig. 9.35 The microstructure of a type A sample deformed at the nominal temperature of 1450 °C (center)

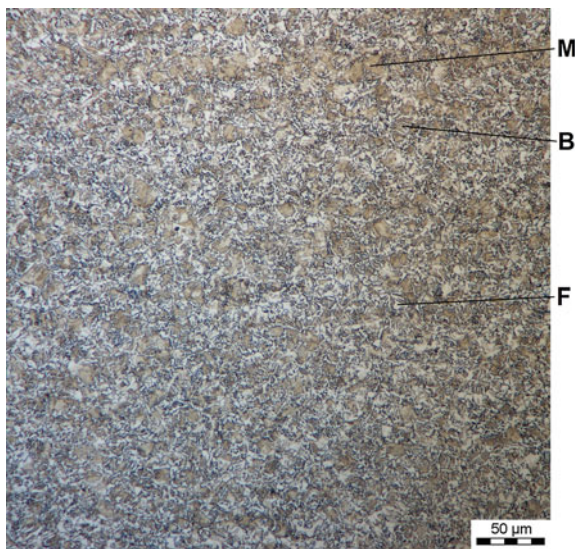
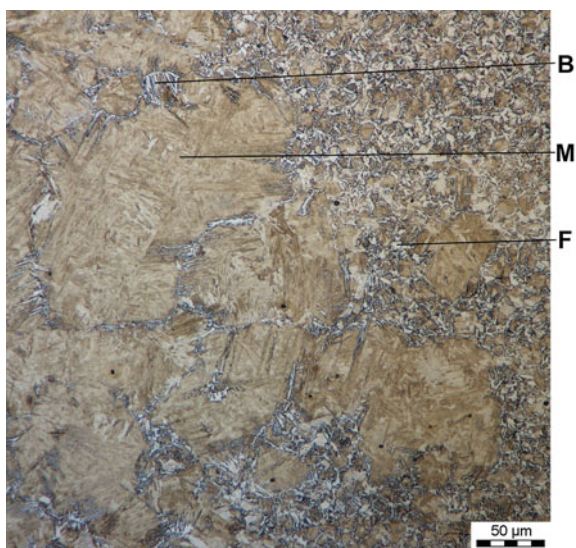


Fig. 9.36 The microstructure of a type A sample deformed at the nominal temperature of 1450 °C (peak)



bainite. The perlite colour depends on the etching degree and may change from dark brown to black. Bright brown fields may represent martensite or perlite with a different crystallographic orientation. It can be unambiguously shown with e.g. scanning electron microscopy (SEM).

The microstructure for a type B sample deformed at the nominal temperatures of 1450, 1440 and 1435 °C is presented in Figs. [9.44](#), [9.45](#), [9.46](#) [9.47](#), [9.48](#) and [9.49](#)

Fig. 9.37 The microstructure of a type A sample deformed at the nominal temperature of 1450 °C (transition zone)

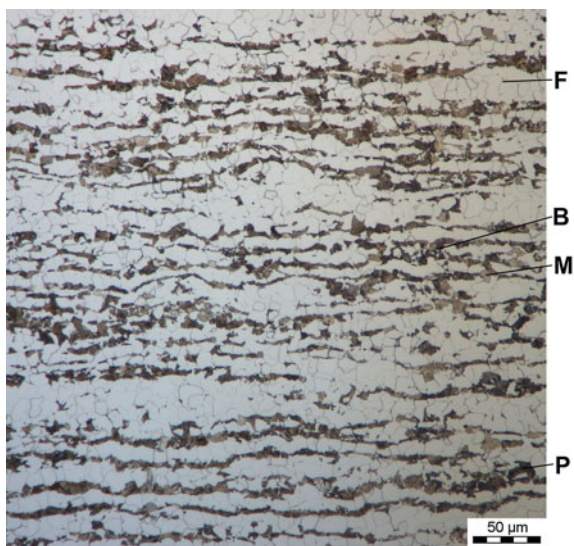
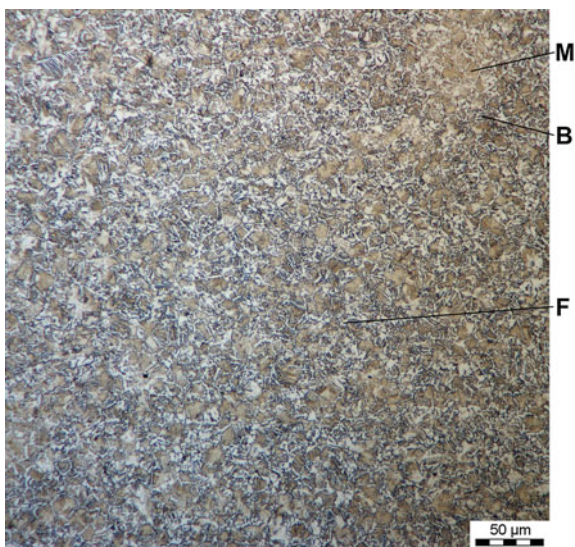


Fig. 9.38 The microstructure of a type A sample deformed at the nominal temperature of 1440 °C (center)



respectively. The sample centre (centre) and the top deformation zone (peak) are large grains of former austenite decorated with white (slightly needle-shaped) ferrite and/or bainite, which “comes” deep into the grain. Generally, bainite prevails in these samples. Probably in the direct vicinity of ferrite (between the needles) there is perlite (dark brown or black). This can only be confirmed by tests with the electron

Fig. 9.39 The microstructure of a type A sample deformed at the nominal temperature of 1440 °C (peak)

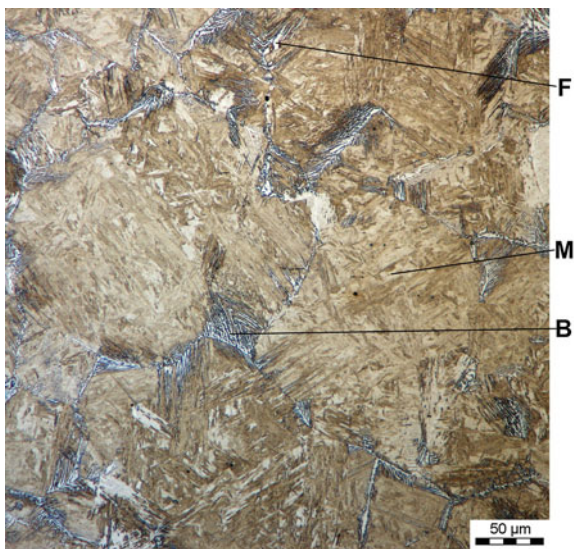
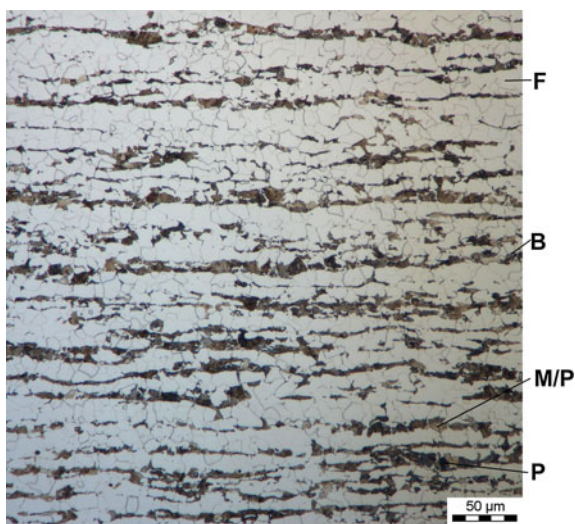


Fig. 9.40 The microstructure of a type A sample deformed at the nominal temperature of 1440 °C (transition zone)



microscopy method. The martensite share (brown) is bigger in the areas of the so-called “peak”.

Figures 9.50, 9.51, 9.52, 9.53, 9.54, 9.55 and 9.56 present the obtained microstructure for type C samples, deformed at temperatures of 1450, 1440 and

Fig. 9.41 The microstructure of a type A sample deformed at the nominal temperature of 1435 °C (center)

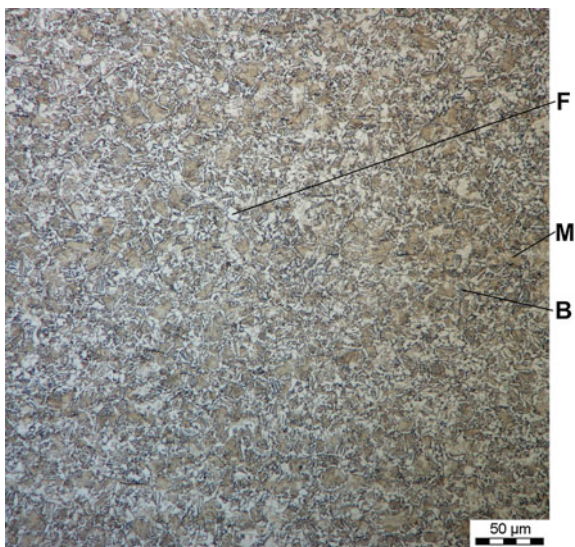
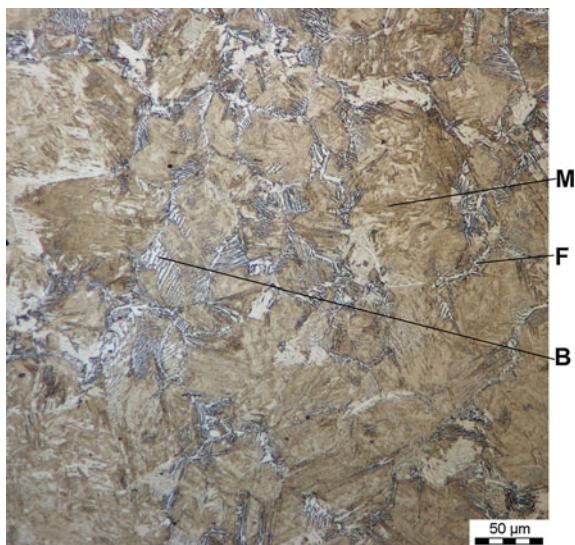


Fig. 9.42 The microstructure of a type A sample deformed at the nominal temperature of 1435 °C (peak)



1435 °C respectively. The analysis of the sample centre shows primarily the bainitic structure with local martensite areas (brown). The former austenite grain boundaries are decorated with white ferrite. The top deformation zone is characterised more by martensite, as well as ferrite. It is possible that the darkest (brown) areas near ferrite is perlite. However, the structure was more etched and its interpretation in favour of perlite is less substantiated here (it seems that verification with the electron microscopy is necessary).

Fig. 9.43 The microstructure of a type A sample deformed at the nominal temperature of 1435 °C (transition zone)

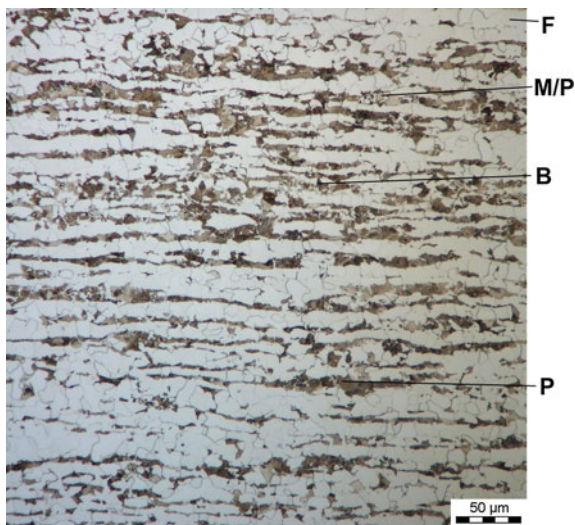


Fig. 9.44 The microstructure of a type B sample deformed at the nominal temperature of 1450 °C (center)

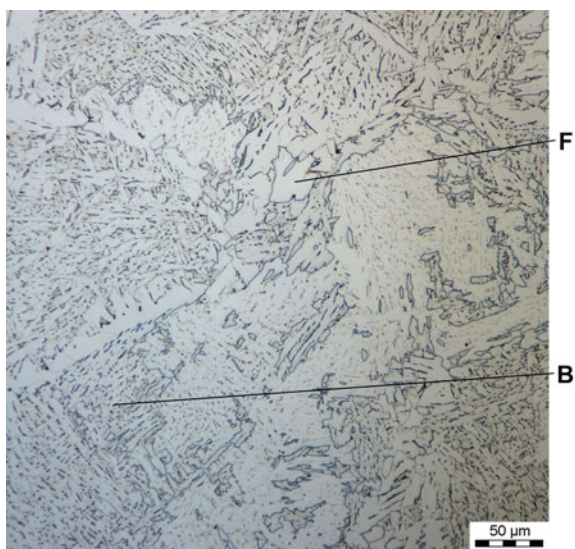


Fig. 9.45 The microstructure of a type B sample deformed at the nominal temperature of 1450 °C (peak)

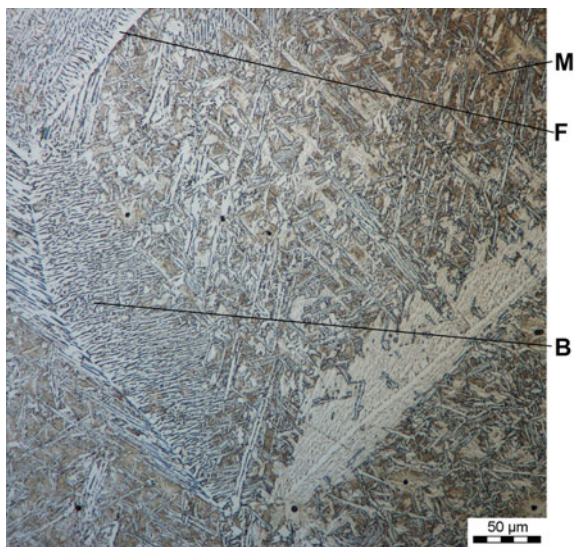


Fig. 9.46 The microstructure of a type B sample deformed at the nominal temperature of 1440 °C (center)

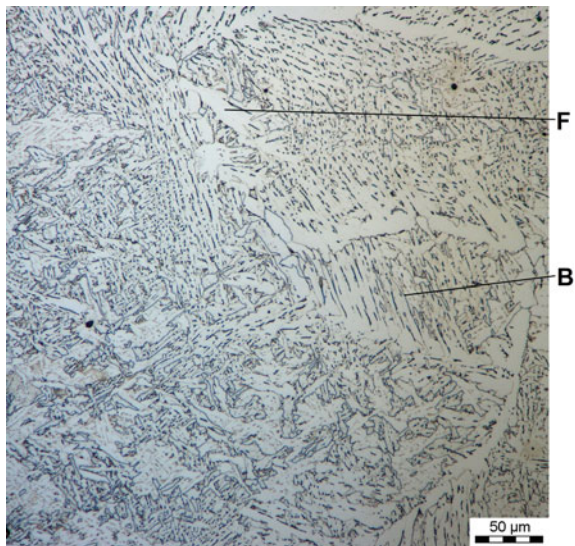


Fig. 9.47 The microstructure of a type B sample deformed at the nominal temperature of 1440 °C (peak)

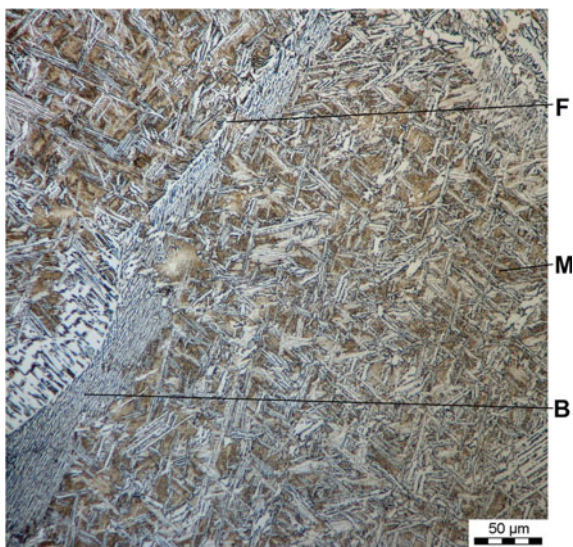


Fig. 9.48 The microstructure of a type B sample deformed at the nominal temperature of 1435 °C (center)

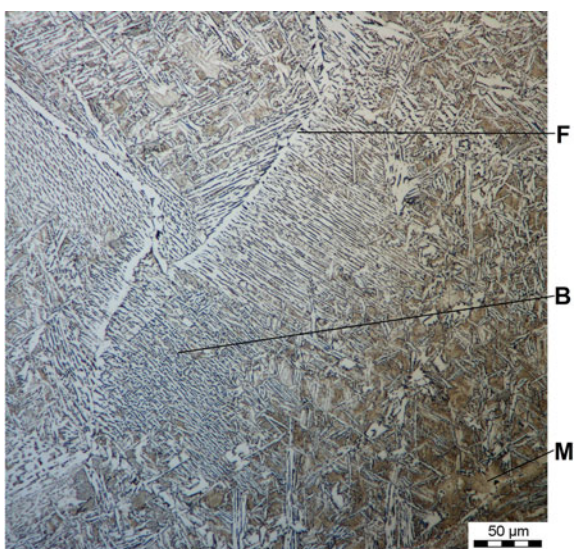


Fig. 9.49 The microstructure of a type B sample deformed at the nominal temperature of 1435 °C (peak)

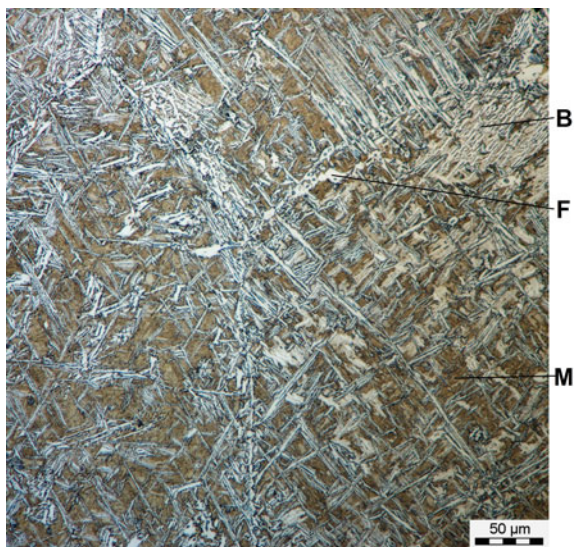


Fig. 9.50 The microstructure of a type C sample deformed at the nominal temperature of 1450 °C (center)

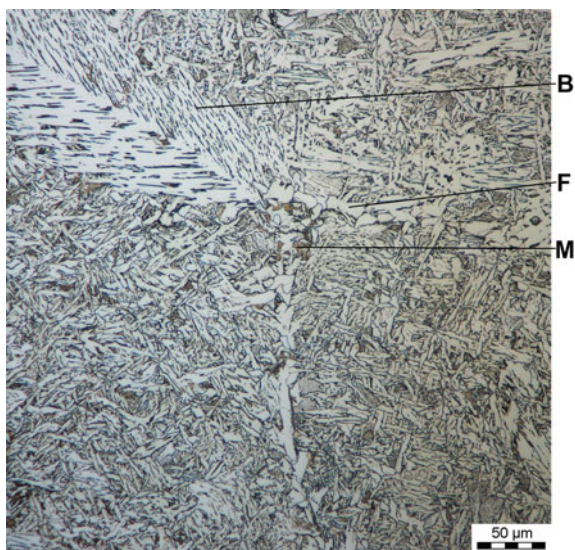


Fig. 9.51 The microstructure of a type C sample deformed at the nominal temperature of 1450 °C (peak)

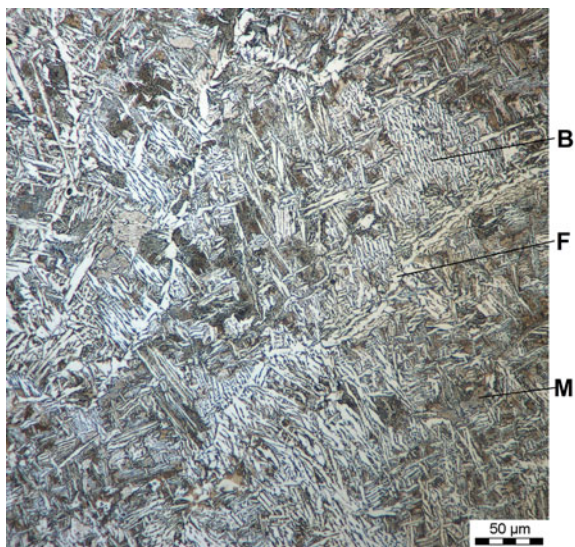


Fig. 9.52 The microstructure of a type C sample deformed at the nominal temperature of 1450 °C (transition zone)

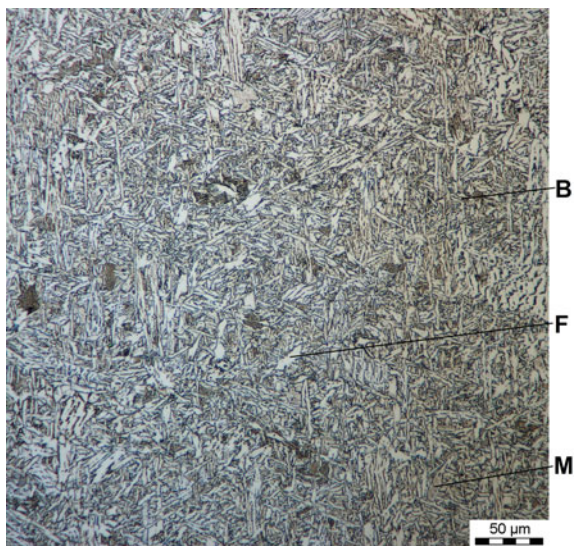


Fig. 9.53 The microstructure of a type C sample deformed at the nominal temperature of 1440 °C (center)

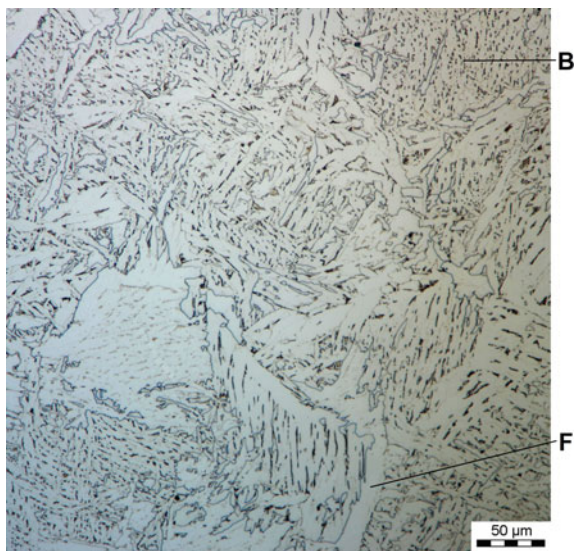


Fig. 9.54 The microstructure of a type C sample deformed at the nominal temperature of 1440 °C (peak)

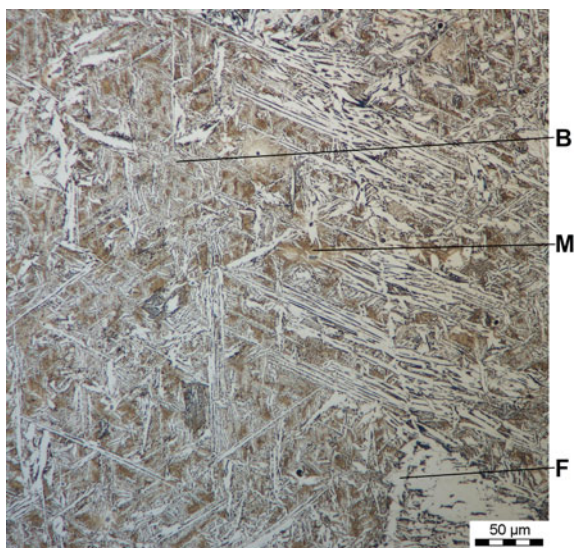


Fig. 9.55 The microstructure of a type C sample deformed at the nominal temperature of 1435 °C (center)

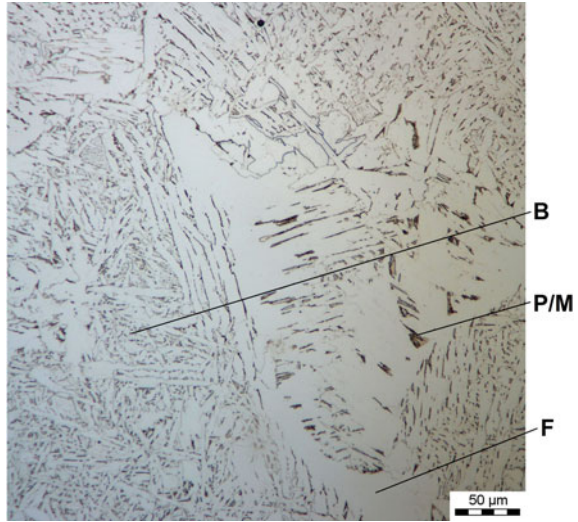
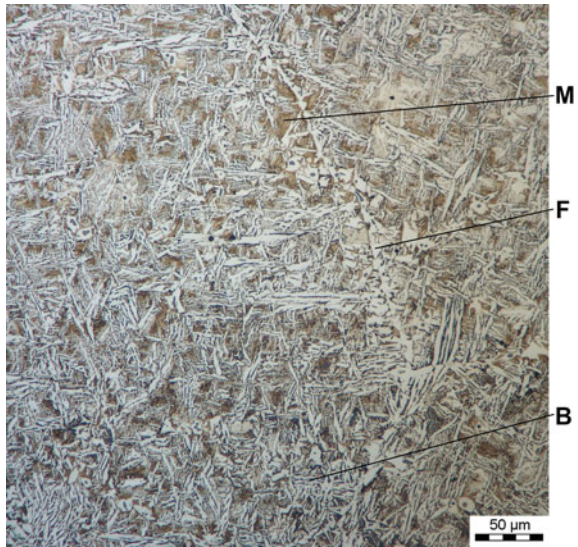


Fig. 9.56 The microstructure of a type C sample deformed at the nominal temperature of 1435 °C (peak)



9.6 Summary

The presented chapter presents the selected research of computer and physical simulations combined with macro- and microstructural tests. The conducted model tests, based upon the developed new research concept with three-dimensional models, lead to the following main conclusions:

- The developed new research methodology with square cross-section samples and simultaneous precise control of the heating and deformation process after giving up the quartz shield causes that fairly uniform (symmetrical) shape of the remelting zone (tomographic tests) is obtained. It leads to a supplementary conclusion that the application of a similar approach (giving up the quartz shield + precise process control) with cylindrical samples should lead to obtaining more precise results if the modelling concept based upon axially symmetrical models (obtaining the symmetricalness of the remelting zone) is applied.
- Regardless of the sample type applied, a significant temperature gradient occurs on the cross-section. The maximum temperature values are achieved in the sample core, and the differences between the sample surface temperature and the temperature calculated in the sample core may reach a maximum of 48 for type C samples.
- The type of applied samples directly influence the size of the maximum attainable remelting zone, and thus the mushy zone size. For a type C sample, the mushy zone and the remelting zone shares are the biggest. This fact was confirmed by macrostructural tests.
- The formulated numerical model of the heating/remelting process is characterised by substantial compliance of the obtained results with the experiment and may be practically used for virtual simulations of heating/remelting on the basis of new modified temperature programmes. The occurring differences between the measured and computed temperature values result, among others, from the fact that the couplings of the temperature field and the electrical field were not directly considered in the numerical model. It was modelled by an internal voluminal heat source. Therefore, the influence of the varying electrical properties of the heated sample on the electrical charge density and local voluminal heat source power could not be analysed.
- The formulated numerical model of the deformation process is characterised by the correct compliance of the obtained results with the experiment on the basis of the proposed verification criteria (the cross-section dimensions or the length of the non-deformed zone). The differences between the experiment and simulation result among others from the rheological model of steel S355 assumed for computing on the basis of the modelling concept using Simple Interval Methodology (SintM) presented in details [4, 5].
- With regard to the applied sample types, the maximum strain values are similar, however the nature of their distribution is different. For type A samples, the maximum strain values are achieved mainly in the sample core, in the volume with a small share of the liquid phase. For type C samples, where the liquid phase share is bigger than type A, the accumulation of maximum strains occur virtually in the whole volume on the cross-section.
- The application of a CAFE model allows the mushy zone shape to be more precisely estimated, and, among others, the solid and liquid phase fraction in the sample volume to be determined. Information about the distribution and share of

individual phases may then be used to develop new constitutive models, considering the change in the individual phase share as one of their parameters.

References

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Chapter 10

Summary and Future Work

The presented findings of simulation and experimental research, in the author's opinion, have proved the thesis proposed in this study, and the DEFFEM simulation system developed during the research, performing the role of a modern tool for computer aided test procedures carried out with thermo-mechanical Gleeble series simulators, allowed the author to accomplish the assumed objective of the study. The presented steel deformation simulation results, both in extra-high temperatures, and in the semi-solid state, showed the capability of models to predict changes in parameters such as temperature, strain, process force parameters or to estimate the shape of the mushy zone, and to determine the distribution of the liquid/solid phase fraction.

On the basis of the description of mathematical models presented in this study, the carried out simulation calculations, and a comparison of the findings with the results of the experimental research, one may formulate the following main conclusions:

1. The experimental research has shown vast possibilities for the application of the Gleeble 3800 simulator for physical simulations of the process of integrated casting and rolling, and to determine the material characteristics and process characteristics necessary to build and verify the developed mathematical models.
2. In the temperature range close to the solidus temperature, one should apply specific methods during the modelling of the deformation process, due to rapid changes in the plastic and mechanical properties of the metal. Therefore, the computer simulation presented in this study is fully suitable.
3. The numerical models of deformation of samples with a solidifying core formulated as part of this study, enable the plastic flow kinetics, changes in strains and temperature during deformation under the conditions of the liquid and solid phase coexistence to be predicted.
4. Not only may the presented numerical models be successfully applied to simulate the deformation of cylindrical or hexahedral samples with a semi-solid

core, but also to model another class of issues, where during deformation the solidification occurs simultaneously.

5. The DIM (Direct Identification Methodology) and NIM (Numerical Identification Methodology) methodologies for determining the parameters of the function describing the dependence of stress on strain, developed as part of the study, are unique on the global scale. They are unique methodology, among others, because the developed NIM methodology is based upon a hybrid numerically-analytical model of the deformation of axially symmetrical samples with a semi-solid core.

To conclude, one should state that the developed modelling concepts, integrating the areas of physical and computer simulation, may constitute a sound foundation for the theoretical design of new processes of casting and rolling of strands with a semi-solid core. Performing simulation calculations is the foundation for learning mechanisms of flow to a much higher degree than can be obtained with traditional methods. Work on the DEFFEM simulation system was long and painstaking, as the mere specificity of the analysed process caused many problems. The problems encountered during the implementation and modelling work, for instance with three-dimensional solutions (problems with the solution convergence, a very big mesh deformation within the deformation zone) has directed further research towards searching for new solutions and methods allowing us to elaborate on the effects occurring within the deformation zone, while omitting limitations, imposed by the adopted numerical methods of solving a specific class of problems, and to ensure a sufficient computation accuracy. Hence, the idea of developing a hybrid model based upon three-dimensional solutions was conceived. This model combines the advantages of the finite element method (FEM) and the smoothed particle method (SPH), which at the same time is the direction of the ongoing work by the author. The first stage of work aiming at developing and implementing numerically a hybrid model was the formulation of the grounds for a model of fluid flow for the meso-scale in the area of the porous structure. The examples of test results presented in Chap. 5 show that the utilization of the SPH method is very promising for the further development of numerical models in order to elaborate effects that occur in the deformation zone.

The most important scientific achievements presented in this monograph include:

1. Developing the advanced simulation system DEFFEM, unique in the global scale, to implement the formulated mathematical models of processes, along with the advanced engineering data visualization tools.
2. Developing an axially symmetrical sample resistance heating model and identifying the boundary conditions in the Gleeble 3800 thermo-mechanical simulator system.
3. Developing the structural model concept and experimental research methodology for the possibilities for determining material characteristics, and physical

simulations of industrial processes of integrated casting and rolling, with a modern thermo-mechanical Gleeble 3800 simulator.

4. Developing the fundamental research methodology with the use of the Gleeble 3800 simulator for the purposes of identification of the model parameters and verification of the formulated mathematical models.
5. Developing test methodology for application of computer tomography for the needs of analysis and estimation of the obtained shape of the porous zone.
6. Developing the DIM (Direct Identification Methodology) for determining parameters of the function describing the dependence of stress on strain, and utilizing data obtained directly from the Gleeble 3800 simulator.
7. Developing an alternative NIM (Numerical Identification Methodology) utilizing data obtained directly from the Gleeble 3800 simulator, as well as the capabilities of the developed DEFFEM simulation system to determine parameters of the function describing the dependence of stress on strain.
8. Developing the methodology for the construction of the rheological model of steel deformation at extra-high temperatures and in the semi-solid state.
9. Developing a mathematical model based upon the meshless method to simulate the fluid flow in the porous structure meso-scale.
10. Developing a 3D hexahedral sample resistance heating/cooling model and identifying the boundary conditions in the Gleeble thermo-mechanical simulator system.
11. Developing a 3D thermo-mechanical model of deformations of hexahedral steel samples at extra-high temperatures, and under the conditions of liquid and solid phase coexistence.

The developed methodologies and models constitute the foundation of the formulated innovative modelling concepts integrating the areas of physical and computer simulation and at the same time to providing full or partial exchange of information between those areas.

Appendix A

Thermo-physical Properties of the S355 Steel

T (°C)	Fraction liquid (wt%)	Density (g/cm ³)	Thermal conductivity (W/(m K))	Electrical resistivity (10e−6 Ohm m)	Young's modulus (GPa)
1600	100	6.91218	34.91665	1.31434	0
1580	100	6.92858	34.54952	1.31412	0
1560	100	6.94487	34.18239	1.3139	0
1540	100	6.96107	33.81526	1.31367	0
1520	100	6.97717	33.44813	1.31344	0
1513.7	99.99996	6.98222	33.33249	1.31337	1.13E−24
1500	46.85386	7.13721	36.00007	1.20672	6.38733
1486.24	25.80748	7.20396	37.09981	1.16187	25.52687
1483.93	10.7205	7.25349	35.0414	1.2285	46.73048
1480	6.46744	7.2678	35.1107	1.22334	57.04138
1465.4	0.19412	7.29098	35.10308	1.21341	76.17767
1465.22	4.91E−05	7.29142	35.10561	1.2132	76.81795
1460		7.29426	35.03964	1.21183	77.25785
1420		7.31594	34.53488	1.20117	80.62455
1400		7.32673	34.28274	1.19571	82.30757
1360		7.34827	33.77882	1.18453	85.67304
1340		7.35903	33.52701	1.17882	87.35554
1300		7.38052	33.02361	1.16711	90.72018
1280		7.39127	32.772	1.16112	92.40234
1240		7.41278	32.26891	1.14885	95.76642
1200		7.43433	31.76595	1.13619	99.13026
1180		7.44512	31.5145	1.12971	100.8121
1140		7.46675	31.01165	1.11642	104.1757
1120		7.47759	30.76024	1.10962	105.8575
1080		7.49932	30.25745	1.09567	109.221
1040		7.52113	29.75469	1.08125	112.5844

(continued)

(continued)

T (°C)	Fraction liquid (wt%)	Density (g/cm ³)	Thermal conductivity (W/(m K))	Electrical resistivity (10e-6 Ohm m)	Young's modulus (GPa)
1020		7.53206	29.50331	1.07385	114.2661
980		7.55399	29.00056	1.05868	117.6295
940		7.57599	28.49781	1.04296	120.9929
900		7.59809	27.99507	1.02669	124.3563
880		7.60917	27.7437	1.01833	126.0379
840		7.6314	27.24096	1.00115	129.4013
822.87		7.64095	27.02563	0.99359	130.8419
820		7.63921	27.19745	0.98473	131.7515
780		7.62239	29.24646	0.88223	141.6961
760		7.61956	30.00841	0.8435	145.3467
720		7.62059	31.21428	0.77952	151.2662
706.93		7.62221	31.54512	0.7612	152.9354
700		7.61719	32.55451	0.73238	155.6952
693.09		7.61436	33.32865	0.71029	157.8891
660		7.62712	33.61721	0.68007	160.5761
640		7.63474	33.8191	0.66152	162.1925
600		7.64982	34.2856	0.62394	165.4091
580		7.65727	34.55049	0.60497	167.0097
540		7.67204	35.14422	0.56687	170.1964
520		7.67936	35.47328	0.5478	171.7825
480.87		7.69356	36.1795	0.5106	174.8723
480		7.69389	36.20218	0.5097	174.9466
440		7.70932	37.31181	0.46827	178.4056
431.86		7.71246	37.54104	0.4601	179.0995
420		7.71658	37.80282	0.44923	180.0225
380		7.73035	38.74111	0.41305	183.1183
360		7.73716	39.24242	0.39529	184.6557
320		7.7506	40.3099	0.36051	187.7085
300		7.75724	40.87627	0.34353	189.2233
260		7.77033	42.07472	0.31045	192.2282
240		7.77678	42.70698	0.29438	193.7176
200		7.7895	44.03823	0.26323	196.6688
180		7.79577	44.73759	0.24816	198.1302
140		7.80812	46.2054	0.21907	201.0256
120		7.81421	46.97471	0.20505	202.4606
80		7.82621	48.58644	0.17808	205.3079
68.52		7.82962	49.06718	0.1706	206.1196
40		7.83811	50.27003	0.15262	208.119
25		7.84248	50.93719	0.14341	209.1696

T (°C)	Poisson's ratio	Liquid viscosity (mPa s)	Enthalpy (J/g)	Specific heat (J/(g K))	Latent heat (J/g)
1600	0.49992	5.66944	1341.7645	0.82688	
1580	0.49992	5.84298	1325.2278	0.82684	
1560	0.49992	6.0258	1308.6915	0.82682	
1540	0.49992	6.21856	1292.1556	0.82679	
1520	0.49992	6.42199	1275.7131	0.81806	
1513.7	0.49992	6.48841	1270.5687		50.97787
1500	0.42097	6.44337	1131.8002	6.05028	96.93005
1486.24	0.3882	6.40566	1072.0753		128.23126
1483.93	0.39375	6.40141	1015.0818		150.54388
1480	0.38815	6.38227	1001.5291	2.97105	167.01298
1465.4	0.37924	6.32939	975.70594		211.36935
1465.22	0.37898	6.32857	975.06483		241.82898
1460	0.37868		971.38423	0.70351	
1420	0.37633		943.38307	0.69556	
1400	0.37515		929.49892	0.69173	
1360	0.3728		901.9554	0.68431	
1340	0.37162		888.29294	0.6807	
1300	0.36925		861.18047	0.67365	
1280	0.36807		847.72861	0.67016	
1240	0.36571		821.03032	0.66333	
1200	0.36334		794.59762	0.65679	
1180	0.36216		781.47837	0.65355	
1140	0.35979		755.43174	0.64711	
1120	0.35861		742.50364	0.64393	
1080	0.35624		716.83646	0.63761	
1040	0.35387		691.41987	0.63129	
1020	0.35269		678.80514	0.62816	
980	0.35032		653.76217	0.62191	
940	0.34796		628.96727	0.61568	
900	0.34559		604.41988	0.60943	
880	0.3444		592.23888	0.60632	
840	0.34204		568.06213	0.60011	
822.87	0.34102		557.78226		
820	0.3401		554.9352	0.99814	
780	0.32991		514.98116	0.99243	
760	0.32655		495.06587	1.00289	
720	0.32173		452.16563	1.0585	
706.93	0.32051		438.48967		
700	0.31745		421.67167	2.16441	
693.09	0.3153		408.16114		

(continued)

(continued)

T (°C)	Poisson's ratio	Liquid viscosity (mPa s)	Enthalpy (J/g)	Specific heat (J/(g K))	Latent heat (J/g)
660	0.31401		377.71663	0.8885	
640	0.31324		360.24442	0.85654	
600	0.3117		327.04394	0.80251	
580	0.31093		311.19806	0.77943	
540	0.30939		280.78854	0.73914	
520	0.30862		266.15472	0.72132	
480.87	0.30712		238.49024		
480	0.30708		237.85883	0.72682	
440	0.3052		209.02962	0.70229	
431.86	0.30482		203.33605		
420	0.30436		195.61239	0.64602	
380	0.30281		170.2417	0.62038	
360	0.30203		157.93091	0.6083	
320	0.30047		134.01322	0.5859	
300	0.29969		122.39202	0.57492	
260	0.29813		99.79758	0.55366	
240	0.29735		88.81615	0.54331	
200	0.29579		67.46756	0.52339	
180	0.29501		57.09232	0.51364	
140	0.29345		36.9104	0.49522	
120	0.29267		27.08885	0.48655	
80	0.29112		7.95299	0.46994	
68.52	0.29067		2.58538		
40	0.28956			0.45329	
25	0.28897			0.44669	

Appendix B

Thermo-physical Properties of the C45 Steel

T (°C)	Fraction liquid (wt%)	Density (g/cm ³)	Thermal conductivity (W/(m K))	Electrical resistivity (10e-6 Ohm m)	Young's modulus (GPa)
1600	1	6.91435	35.34082	1.29856	0
1550	1	6.95495	34.4199	1.29771	0
1505	1	6.99096	33.59108	1.29691	0
1500	1	6.99493	33.49898	1.29682	0
1495	1	6.99889	33.40689	1.29673	0
1494.79	1	6.99906	33.40304	1.29672	0
1490	0.87841	7.03448	33.97108	1.27159	0.01651
1489.88	0.87555	7.03532	33.9845	1.271	0.018106
1489.88	0.87553	7.03534	33.98456	1.271	0.018101
1485	0.7273	7.07865	34.14199	1.26163	0.094192
1480	0.60769	7.11483	34.26067	1.25369	0.84088
1475	0.51111	7.14508	34.34632	1.24699	2.86007
1470	0.43136	7.17097	34.40652	1.24125	6.27462
1465	0.36426	7.19354	34.44713	1.23623	10.88971
1460	0.30683	7.2136	34.47117	1.23182	16.42427
1455	0.25701	7.23165	34.48333	1.22783	22.61462
1450	0.21335	7.24802	34.48592	1.22419	29.25093
1445	0.17473	7.26307	34.48068	1.22082	36.18725
1440	0.14025	7.277	34.46906	1.21768	43.32377
1435	0.10925	7.28997	34.45225	1.21472	50.59053
1430	0.081175	7.30214	34.43121	1.2119	57.94115
1425	0.055606	7.31363	34.40654	1.20921	65.33844
1420	0.032188	7.32452	34.37859	1.20663	72.758
1415	0.010638	7.33489	34.34723	1.20416	80.18024
1412.42	0.006122	7.34013	34.32971	1.20293	84.06567
1405		7.34391	34.23823	1.20084	84.69597

(continued)

(continued)

T (°C)	Fraction liquid (wt%)	Density (g/cm ³)	Thermal conductivity (W/(m K))	Electrical resistivity (10e-6 Ohm m)	Young's modulus (GPa)
1400		7.34646	34.17663	1.19942	85.12081
1370		7.36177	33.80816	1.19075	87.66882
1340		7.3771	33.44172	1.18182	90.21507
1310		7.39246	33.07744	1.17262	92.75958
1280		7.40785	32.71543	1.16313	95.30232
1250		7.42327	32.35579	1.15334	97.8433
1220		7.43871	31.99862	1.14324	100.3825
1190		7.45417	31.64402	1.13283	102.92
1160		7.46967	31.29205	1.12208	105.4556
1130		7.48519	30.9428	1.11099	107.9895
1100		7.50075	30.59631	1.09955	110.5216
1070		7.51633	30.25262	1.08775	113.0519
1040		7.53194	29.91177	1.07557	115.5804
1000		7.5528	29.46171	1.05874	118.9489
960		7.57372	29.01666	1.0412	122.3143
920		7.59469	28.57653	1.02294	125.6764
900		7.6052	28.35825	1.01354	127.3562
860		7.62625	27.92515	0.99416	130.7134
830		7.64208	27.60321	0.97913	133.2292
800		7.65795	27.28359	0.96366	135.7431
770		7.67385	26.96612	0.94775	138.2551
765		7.6765	26.91341	0.94506	138.6736
760		7.67915	26.86075	0.94235	139.0921
755		7.68181	26.80814	0.93963	139.5105
750		7.68446	26.75559	0.93689	139.9288
745		7.68712	26.70308	0.93415	140.3471
740		7.68978	26.65063	0.93139	140.7653
735		7.69244	26.59822	0.92862	141.1835
730		7.6951	26.54587	0.92584	141.6017
725		7.69776	26.49356	0.92304	142.0197
720		7.70042	26.4413	0.92023	142.4378
715		7.70308	26.38908	0.91741	142.8558
710		7.70575	26.33691	0.91458	143.2737
705		7.70841	26.28478	0.91173	143.6915
700		7.71108	26.23269	0.90887	144.1094
695		7.71374	26.18064	0.906	144.5271
690		7.71641	26.12863	0.90312	144.9449
685		7.71908	26.07666	0.90022	145.3625

(continued)

(continued)

T (°C)	Fraction liquid (wt%)	Density (g/cm ³)	Thermal conductivity (W/(m K))	Electrical resistivity (10e-6 Ohm m)	Young's modulus (GPa)
680		7.72175	26.02473	0.89731	145.7801
675		7.72442	25.97284	0.89438	146.1977
670		7.72709	25.92098	0.89145	146.6152
665		7.72977	25.86915	0.8885	147.0327
660		7.73244	25.81736	0.88553	147.4501
655		7.73511	25.7656	0.88256	147.8674
650		7.73779	25.71387	0.87957	148.2847
645		7.74047	25.66217	0.87657	148.7019
640		7.74314	25.6105	0.87355	149.1191
635		7.74582	25.55885	0.87053	149.5363
630		7.7485	25.50723	0.86749	149.9534
615		7.75655	25.35252	0.85828	151.2043
610		7.75923	25.30099	0.85519	151.6212
600		7.7646	25.19799	0.84896	152.4548

T (°C)	Poisson's ratio	Liquid viscosity (mPa s)	Enthalpy (J/g)	Specific heat (J/(g K))	Latent heat (J/g)
1600	0.49968	5.44574	1351.003		
1550	0.49968	5.87455	1309.562	0.8288	
1505	0.49968	6.31224	1272.547	0.814	
1500	0.49968	6.36427	1268.489	0.8116	
1495	0.49968	6.41703	1264.442	0.8094	
1494.79	0.49968	6.41926	1264.274	0.80371	
1490	0.48196	6.40787	1229.413	7.2764	28.871
1489.88	0.48155	6.40771	1228.587		29.554
1489.88	0.48154	6.40771	1228.638		29.502
1485	0.46441	6.37848	1184.669	8.9488	67.637
1480	0.45033	6.35021	1148.982	7.1374	98.081
1475	0.43876	6.32358	1119.988	5.7988	122.357
1470	0.42905	6.29814	1095.888	4.82	142.121
1465	0.42075	6.27418	1075.471	4.0834	158.489
1460	0.41354	6.25124	1057.88	3.5182	172.255
1455	0.40719	6.22958	1042.516	3.0728	183.969
1450	0.40155	6.20922	1028.956	2.712	194.021
1445	0.39648	6.18996	1016.866	2.418	202.715
1440	0.39189	6.17154	1005.992	2.1748	210.288
1435	0.38771	6.15421	996.137	1.971	216.921
1430	0.38386	6.13801	987.143	1.7988	222.76

(continued)

(continued)

T (°C)	Poisson's ratio	Liquid viscosity (mPa s)	Enthalpy (J/g)	Specific heat (J/(g K))	Latent heat (J/g)
1425	0.38031	6.1227	978.883	1.652	227.919
1420	0.37701	6.10826	971.257	1.5252	232.494
1415	0.37393	6.09474	964.18	1.4154	236.562
1412.42	0.3724	6.06324	960.689	1.35151	238.52
1405	0.37197		955.515	0.69759	
1400	0.37169		952.036	0.6958	
1370	0.36997		931.247	0.691	
1340	0.36825		910.595	0.6864	
1310	0.36654		890.077	0.682	
1280	0.36482		869.693	0.6776	
1250	0.3631		849.442	0.6732	
1220	0.36139		829.321	0.6688	
1190	0.35967		809.328	0.6648	
1160	0.35795		789.463	0.6604	
1130	0.35624		769.721	0.6564	
1100	0.35452		750.102	0.6522	
1070	0.3528		730.6	0.6484	
1040	0.35109		711.212	0.6448	
1000	0.3488		685.531	0.64	
960	0.34651		660.03	0.6356	
920	0.34422		634.687	0.632	
900	0.34308		622.067	0.6304	
860	0.34079		596.902	0.6284	
830	0.33908		578.066	0.6278	
800	0.33736		559.217	0.6288	
770	0.33564		540.288	0.633	
765	0.33536		537.119	0.6338	
760	0.33507		533.878	0.6482	
755	0.33479		530.629	0.6498	
750	0.3345		527.391	0.6476	
745	0.33421		524.166	0.645	
740	0.33393		520.952	0.6428	
735	0.33364		517.748	0.6408	
730	0.33336		514.556	0.6384	
725	0.33307		511.374	0.6364	
720	0.33278		508.203	0.6342	
715	0.3325		505.042	0.6322	
710	0.33221		501.891	0.6302	
705	0.33193		498.749	0.6284	

(continued)

(continued)

T (°C)	Poisson’s ratio	Liquid viscosity (mPa s)	Enthalpy (J/g)	Specific heat (J/(g K))	Latent heat (J/g)
700	0.33164		495.617	0.6264	
695	0.33135		492.495	0.6244	
690	0.33107		489.382	0.6226	
685	0.33078		486.277	0.621	
680	0.3305		483.182	0.619	
675	0.33021		480.095	0.6174	
670	0.32993		477.017	0.6156	
665	0.32964		473.947	0.614	
660	0.32935		470.886	0.6122	
655	0.32907		467.832	0.6108	
650	0.32878		464.787	0.609	
645	0.3285		461.75	0.6074	
640	0.32821		458.72	0.606	
635	0.32792		455.698	0.6044	
630	0.32764		452.684	0.6028	
615	0.32678		443.686	0.5984	
610	0.32649		440.701	0.597	
600	0.32592		434.753	0.5942	

Appendix C

Complete Source Code: Steady Heat Flow

As an example, let's consider the area presented in Fig. C.1, which is a cross-section of e.g. a rolled strand with dimensions of 0.5×0.5 m. The left, right and top surface of the cast strand are heated by the medium with a temperature $T = 500$ °C. On the other hand the bottom surface of the cast strand is cooled by the medium with a temperature $T = 20$ °C. The heat transfer coefficient for all boundary conditions assumes the same value of $\alpha = 100$ W/m²K, and heat transfer coefficients of $\lambda_x = \lambda_y = 78$ W/mK. The power of heat sources referred to the volume unit in the analysed case $q_{vol} = 0$ W/m³.

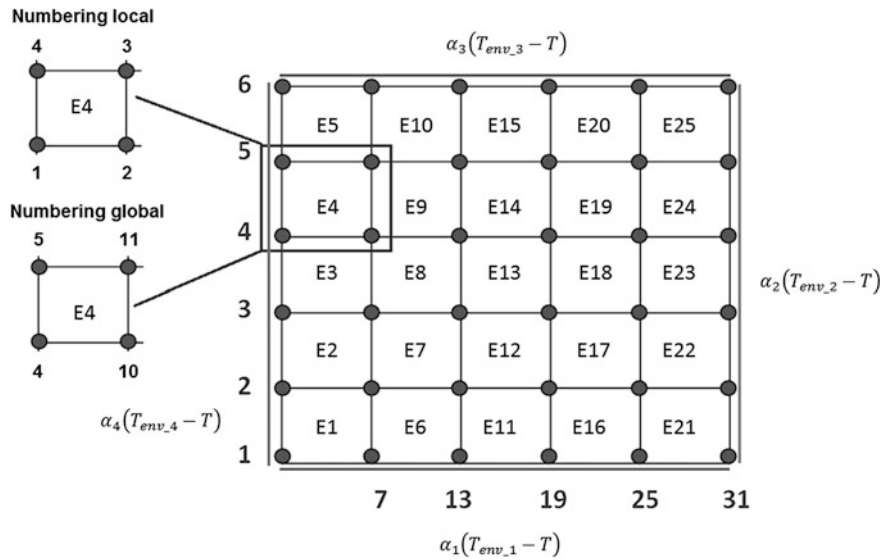


Fig. C.1 A cross-section of a cast strand with defined third type boundary conditions

Below find a complete print-out of the source code written in the C++ language, simulating the steady state condition of heat transfer in the cross-section. The comments placed within the code will enable the reader to analyse the numerical code individually, and will be helpful during potential modifications implemented by the user, or when creating original solutions. The program code may be compiled with any C++ compiler (e.g. Dev-C++ 5.11). The final result will be the temperature field distribution for the steady state condition (test data) (Fig. C.2).

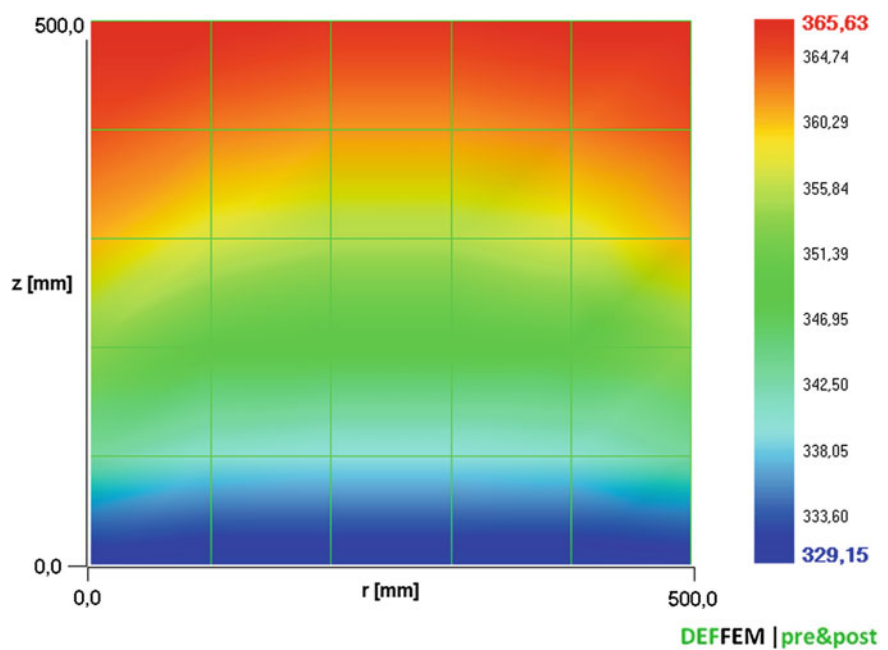


Fig. C.2 The temperature field distribution for the case analysed (steady state condition)

```

#include <iostream>
#include <fstream>

main()
{
float a[220][220],x_w[251],zamiana,stala,b,max;
int nlh,nlv,nw,ne,ie[1000][5];
int l,licznik,k,i,j,u,ii,jj;
float r,h,lambdax,lambday,moc_zrodel,strumien;
float t_czynnika1, t_czynnika2, t_czynnika3, t_czynnika4;
float alfa1,alfa2,alfa3,alfa4;
float dx,dy,dv,dh,wx[1000],wy[1000],x[1000],y[1000],xe[500],ye[500];
float Kc_e[5][5],Kalfa_e[5][5];
float Kc[251][251],Kalfa[251][251],K[251][251],f[251][2];
float fq_duze[251][2],fq_duze_e[5][2],falfa_e[5][2],falfa[251][2];
float x1,x2,x3,x4,y1,y2,y3,y4;
float czlon_lambda_x,czlon_lambda_y,czlon_alfa_bok23,czlon_alfa_bok41;
float czlon_alfa_bok12,czlon_alfa_bok34;
float czlon_fq_duze,czlon_falfa,czlon_q;
int n,imax,spr=1;
//-----INPUT PARAMETERS-----
//nlh-the number of horizontal lines in the mesh
//nlv-the number of vertical lines in the mesh
//nw,ne-number of mesh nodes, number of elements
//h,r-height, width section
//dv,dh-increases the length of elements for h and r
//dx,dy-operating variables

```

```

//wx[],wy[]-tables containing the coordinates of the mesh
//x[],y[]-coordinates x and y nodes of the mesh
//-----INPUT DATA-----
nlh=6;
nlv=6;
h=500;
r=500;
h=h/1000;
r=r/1000;           //conversion of centimeters to meters
lambdaX=78;         //thermal conductivity, x-direction, W/(m*K)
lambdaY=78;         //thermal conductivity, y-direction, W/(m*K)
alfa1=100;          //heat transfer coefficient, bottom section, W/(m2*K)
alfa2=100;          //heat transfer coefficient, right section, W/(m2*K)
alfa3=100;          //heat transfer coefficient, top section, W/(m2*K)
alfa4=100;          //heat transfer coefficient, left section, W/(m2*K)
moc_zrodel=0;       //power sources of heat per unit volume, (W/m3)
t_czynnika1=20;     //the temperature of the cooling medium, bottom section, [st. C]
t_czynnika2=500;    //the temperature of the cooling medium, right section, [st. C]
t_czynnika3=500;    //the temperature of the cooling medium, top section, [st. C]
t_czynnika4=500;    //the temperature of the cooling medium, left section, [st. C]
//-----
dx=0;
dy=0;
dv=h/(nlh-1);
dh=r/(nlv-1);
nw=nlh*nlv;
ne=(nlh-1)*(nlv-1);
std::cout<<"Parameters the generated mesh:"<<std::endl;
std::cout<<"Number of elements:"<<" "<<ne<<std::endl;
std::cout<<"Number of nodes:"<<" "<<nw<<std::endl;
std::cout<<std::endl;
std::cout<<"ENTER-START CALCULATION";
std::cin.get();
//----- DETERMINATION OF THE MESH COORDINATES-----
for(int i=1;i<=nlv;i++)
{
    wx[i]=dx;
    dx=dx+dh;
}
for(int j=1;j<=nlh;j++)
{
    wy[j]=dy;
    dy=dy+dv;
}
//----- DETERMINING COORDINATES OF A GRID NODES -----
licznik=1;
l=0;
for(int i=1;i<=nw;i++)
{
    x[i]=wx[licznik];
    l++;

```

```

if(l==nlh)
{
licznik++;
l=0;
}}
licznik=1;
for(int i=1;i<=nw;i++)
{
y[i]=wy[licznik];
licznik++;
if(licznik==nlh+1)
{
licznik=1;
}}
//----- DETERMINATION OF MATRIX CONNECTION -----
k=1;
i=1;
for(int w=1;w<=ne;w++)
{
ie[w][1]=i;
ie[w][2]=i+nlh;
ie[w][3]=1+i+nlh;
ie[w][4]=1+i;
k++;
i++;
if(k==nlh)
{
k=1;
i=i+1;
}}
//-----
//Calculation of the thermal conductivity of the matrix
//Kc_e for one single element and global matrix conductivity Kc
//-----
for (k=1;k<=250;k++)
{
for (l=1;l<=250;l++)
{
Kc[k][l]=0;
}}
//----- the beginning of the loop elements -----
for(u=1;u<=ne;u++)
{
for(j=1;j<=4;j++)
{
xe[j]=x[ie[u][j]];
ye[j]=y[ie[u][j]];
}
x1=xe[1];x2=xe[2];x3=xe[3];x4=xe[4]; //determining coordinates of a single element
y1=ye[1];y2=ye[2];y3=ye[3];y4=ye[4];
for (k=1;k<=4;k++) //resetting single array Kc_e

```

```

{
for (l=1;l<=4;l++)
{
Kc_e[k][l]=0;
}
czlon_lambda_x= (lambdaX/6)*(((y4-y1))/((x2-x1)));
czlon_lambda_y= (lambdaY/6)*(((x2-x1))/((y4-y1)));
Kc_e[1][1]=(czlon_lambda_x)*2+(czlon_lambda_y)*2;
Kc_e[1][2]=(czlon_lambda_x)*-2+(czlon_lambda_y)*1;
Kc_e[1][3]=(czlon_lambda_x)*-1+(czlon_lambda_y)*-1;
Kc_e[1][4]=(czlon_lambda_x)*1+(czlon_lambda_y)*-2;
Kc_e[2][1]=(czlon_lambda_x)*-2+(czlon_lambda_y)*1;
Kc_e[2][2]=(czlon_lambda_x)*2+(czlon_lambda_y)*2;
Kc_e[2][3]=(czlon_lambda_x)*1+(czlon_lambda_y)*-2;
Kc_e[2][4]=(czlon_lambda_x)*-1+(czlon_lambda_y)*-1;
Kc_e[3][1]=(czlon_lambda_x)*-1+(czlon_lambda_y)*-1;
Kc_e[3][2]=(czlon_lambda_x)*1+(czlon_lambda_y)*-2;
Kc_e[3][3]=(czlon_lambda_x)*2+(czlon_lambda_y)*2;
Kc_e[3][4]=(czlon_lambda_x)*-2+(czlon_lambda_y)*1;
Kc_e[4][1]=(czlon_lambda_x)*1+(czlon_lambda_y)*-2;
Kc_e[4][2]=(czlon_lambda_x)*-1+(czlon_lambda_y)*-1;
Kc_e[4][3]=(czlon_lambda_x)*-2+(czlon_lambda_y)*1;
Kc_e[4][4]=(czlon_lambda_x)*2+(czlon_lambda_y)*2;
std::cout<<std::endl;
for(i=1;i<=4;i++)          //the creation of a global matrix Kc
{
ii=ie[u][i];
for(j=1;j<=4;j++)
{
jj=ie[u][j];
if(jj>0)
Kc[ii][jj]=Kc[ii][jj]+Kc_e[i][j];
}}
//----- the end of the loop elements -----
//Calculation of matrix thermal conductivity taking into account the convective boundary
//conditions Kalfa_e for single element and global matrix Kalfa
//-----
for (k=1;k<=250;k++)
{
for (l=1;l<=250;l++)
{
Kalfa[k][l]=0;
}}
//----- the beginning of the loop elements -----
for(u=1;u<=ne;u++)
{
for(j=1;j<=4;j++)
{
xe[j]=x[ie[u][j]];
ye[j]=y[ie[u][j]];
}
}

```

```

x1=xe[1];x2=xe[2];x3=xe[3];x4=xe[4]; //determining coordinates of a single element
y1=ye[1];y2=ye[2];y3=ye[3];y4=ye[4];
for (k=1;k<=4;k++) //resetting single array Kalfa_e
{
for (l=1;l<=4;l++)
{
Kalfa_e[k][l]=0;
}}
if (u==21 || u==22 || u==23 || u==24 || u==25) //boundary condition, right section
{
//exchange heat on the side 2-3 according to the local numbering nodes
czlon_alfa_bok23= (alfa2*(y4-y1))/6;
Kalfa_e[1][1]= 0;
Kalfa_e[1][2]= 0;
Kalfa_e[1][3]= 0;
Kalfa_e[1][4]= 0;
Kalfa_e[2][1]=0;
Kalfa_e[2][2]=czlon_alfa_bok23*2;
Kalfa_e[2][3]=czlon_alfa_bok23*1;
Kalfa_e[2][4]=0;
Kalfa_e[3][1]=0;
Kalfa_e[3][2]=czlon_alfa_bok23*1;
Kalfa_e[3][3]=czlon_alfa_bok23*2;
Kalfa_e[3][4]=0;
Kalfa_e[4][1]=0;
Kalfa_e[4][2]=0;
Kalfa_e[4][3]=0;
Kalfa_e[4][4]=0;
}
if (u==1 || u==2 || u==3 || u==4 || u==5) //boundary condition, left section
{
//exchange heat on the side 4-1 according to the local numbering nodes
czlon_alfa_bok41= (alfa4*(y4-y1))/6;
Kalfa_e[1][1]= czlon_alfa_bok41*2;
Kalfa_e[1][2]= 0;
Kalfa_e[1][3]= 0;
Kalfa_e[1][4]= czlon_alfa_bok41*1;
Kalfa_e[2][1]=0;
Kalfa_e[2][2]=0;
Kalfa_e[2][3]=0;
Kalfa_e[2][4]=0;
Kalfa_e[3][1]=0;
Kalfa_e[3][2]=0;
Kalfa_e[3][3]=0;
Kalfa_e[3][4]=0;
Kalfa_e[4][1]=czlon_alfa_bok41*1;
Kalfa_e[4][2]=0;
Kalfa_e[4][3]=0;
Kalfa_e[4][4]=czlon_alfa_bok41*2;
}
if (u==1 || u==6 || u==11 || u==16 || u==21) //boundary condition, bottom section

```

```

{
//exchange heat on the side 1-2 according to the local numbering nodes
czlon_alfa_bok12= (alfa1*(x2-x1))/6;
Kalfa_e[1][1]= czlon_alfa_bok12*2;
Kalfa_e[1][2]= czlon_alfa_bok12*1;
Kalfa_e[1][3]= 0;
Kalfa_e[1][4]= 0;
Kalfa_e[2][1]=czlon_alfa_bok12*1;
Kalfa_e[2][2]=czlon_alfa_bok12*2;
Kalfa_e[2][3]=0;
Kalfa_e[2][4]=0;
Kalfa_e[3][1]=0;
Kalfa_e[3][2]=0;
Kalfa_e[3][3]=0;
Kalfa_e[3][4]=0;
Kalfa_e[4][1]=0;
Kalfa_e[4][2]=0;
Kalfa_e[4][3]=0;
Kalfa_e[4][4]=0;
}
if (u==5 || u==10 || u==15 || u==20 || u==25)    //boundary condition, top section
{
//exchange heat on the side 3-4 according to the local numbering nodes
czlon_alfa_bok34= (alfa3*(x2-x1))/6;
Kalfa_e[1][1]= 0;
Kalfa_e[1][2]= 0;
Kalfa_e[1][3]= 0;
Kalfa_e[1][4]= 0;
Kalfa_e[2][1]=0;
Kalfa_e[2][2]=0;
Kalfa_e[2][3]=0;
Kalfa_e[2][4]=0;
Kalfa_e[3][1]=0;
Kalfa_e[3][2]=0;
Kalfa_e[3][3]=czlon_alfa_bok34*2;
Kalfa_e[3][4]=czlon_alfa_bok34*1;
Kalfa_e[4][1]=0;
Kalfa_e[4][2]=0;
Kalfa_e[4][3]=czlon_alfa_bok34*1;
Kalfa_e[4][4]=czlon_alfa_bok34*2;
}
if (u==7 || u==8 || u==9 || u==12 || u==13 || u==14 || u==17 || u==18 || u==19)
{
Kalfa_e[1][1]=0;Kalfa_e[1][2]=0;Kalfa_e[1][3]=0;Kalfa_e[1][4]=0;
Kalfa_e[2][1]=0;Kalfa_e[2][2]=0;Kalfa_e[2][3]=0;Kalfa_e[2][4]=0;
Kalfa_e[3][1]=0;Kalfa_e[3][2]=0;Kalfa_e[3][3]=0;Kalfa_e[3][4]=0;
Kalfa_e[4][1]=0;Kalfa_e[4][2]=0;Kalfa_e[4][3]=0;Kalfa_e[4][4]=0;
}
for(i=1;i<=4;i++)    //the creation of a global matrix Kalfa
{
ii=ie[u][i];

```

```

for(j=1;j<=4;j++)
{
jj=ie[u][j];
if(jj>0)
Kalfa[ii][jj]=Kalfa[ii][jj]+Kalfa_e[i][j];
}}
//----- the end of the loop elements -----
//-----
//Determination of the final matrix K = Kc+Kalfa
//-----
for (k=1;k<=nw;k++)          //matrix addition Kc i Kalfa
{
for (l=1;l<=nw;l++)
{
K[k][l]=Kc[k][l]+Kalfa[k][l];
}}
//-----
//Calculation of the free vector fq_duze_e for single element
//and global vector taking into account the power sources of heat per unit volume
//-----
for (k=1;k<=250;k++)          //resetting vector fq_duze
{
for (l=1;l<=2;l++)
{
fq_duze[k][l]=0;
}}
//----- the beginning of the loop elements -----
for(u=1;u<=ne;u++)
{
for(j=1;j<=4;j++)
{
xe[j]=x[ie[u][j]];
ye[j]=y[ie[u][j]];
}
x1=xe[1];x2=xe[2];x3=xe[3];x4=xe[4];    //determining coordinates of a single element
y1=ye[1];y2=ye[2];y3=ye[3];y4=ye[4];
for (k=1;k<=4;k++)          //resetting vector fq_male_e for single element
{
for (l=1;l<=1;l++)
{
fq_duze_e[k][l]=0;
}}
czlon_fq_duze=((moc_zrodel)*((x2-x1)*(y4-y1)))/4;
fq_duze_e[1][1]= czlon_fq_duze*1;fq_duze_e[2][1]= czlon_fq_duze*1;
fq_duze_e[3][1]= czlon_fq_duze*1;fq_duze_e[4][1]= czlon_fq_duze*1;
for(i=1;i<=4;i++)          //the creation of a global fq_duze
{
ii=ie[u][i];
if(jj>0)
fq_duze[ii][1]=fq_duze[ii][1]+fq_duze_e[i][1];
}}

```

```

//----- the end of the loop elements -----
//-----
//Calculation of the free vector falfa_e for single element
//and global vector falfa taking into account convection heat transfer
//-----
for (k=1;k<=250;k++)          //resetting vector falfa
{
for (l=1;l<=2;l++)
{
falfa[k][l]=0;
}}
//----- the beginning of the loop elements -----
for(u=1;u<=ne;u++)
{
for(j=1;j<=4;j++)
{
xe[j]=x[ie[u][j]];
ye[j]=y[ie[u][j]];
}
x1=xe[1];x2=xe[2];x3=xe[3];x4=xe[4]; //determining coordinates of a single element
y1=ye[1];y2=ye[2];y3=ye[3];y4=ye[4];
for (k=1;k<=4;k++)          //resetting vector falfa_e for single element
{
for (l=1;l<=1;l++)
{
falfa_e[k][l]=0;
}}
if (u==21 || u==22 || u==23 || u==24 || u==25) //boundary condition, right section
{
czlon_falfa= ((alfa2*t_czynnika2)*(y4-y1))/2;
falfa_e[1][1]=0;
falfa_e[2][1]=czlon_falfa*1;
falfa_e[3][1]=czlon_falfa*1;
falfa_e[4][1]=0;
}
if (u==1 || u==2 || u==3 || u==4 || u==5) //boundary condition, left section
{
czlon_falfa= ((alfa4*t_czynnika4)*(y4-y1))/2;
falfa_e[1][1]=czlon_falfa*1;
falfa_e[2][1]=0;
falfa_e[3][1]=0;
falfa_e[4][1]=czlon_falfa*1;
}
if (u==1 || u==6 || u==11 || u==16 || u==21) //boundary condition, bottom section
{
czlon_falfa= ((alfa1*t_czynnika1)*(x2-x1))/2;
falfa_e[1][1]=czlon_falfa*1;
falfa_e[2][1]=czlon_falfa*1;
falfa_e[3][1]=0;
falfa_e[4][1]=0;
}
}

```

```

if (u==5 || u==10 || u==15 || u==20 || u==25)    //boundary condition, top section
{
    czlon_falfa= ((alfa3*t_czynnika3)*(x2-x1))/2;
    falfa_e[1][1]=0;
    falfa_e[2][1]=0;
    falfa_e[3][1]=czlon_falfa*1;
    falfa_e[4][1]=czlon_falfa*1;
}
if (u==7 || u==8 || u==9 || u==12 || u==13 || u==14 || u==17 || u==18 || u==19)
{
    falfa_e[1][1]=0;falfa_e[2][1]=0;
    falfa_e[3][1]=0;falfa_e[4][1]=0;
}
for(i=1;i<=4;i++)    //the creation of a global falfa
{
    ii=ie[u][i];
    if(jj>0)
    falfa[ii][1]=falfa[ii][1]+falfa_e[i][1];
}
//----- the end of the loop elements -----
//-----
// Determination of the End vector f= falfa+fq_duze
//-----
for (k=1;k<=nw;k++)    //adding a vector
{
    for (l=1;l<=1;l++)
    {
        f[k][l]=fq_duze[k][l]+falfa[k][l];
    }
}
//-----
// The solution of equations using Gaussian elimination
//-----
    for(i=0;i<nw;i++)
    {
        for(j=0;j<nw;j++)
        {
            a[i][j]=a[i][j]+K[i+1][j+1];
        }
        a[i][nw]=f[i+1][1];
    }
    i=-1;
    while (i<nw-1 && spr)
    {
        i++;
        max=a[i][i]*a[i][i];
        imax=i;
        for (j=i+1;j<nw;j++)
        {
            if (max<a[j][i]*a[j][i])
            {
                max=a[j][i]*a[j][i];
            }
        }
    }

```

```

                                imax=j;
                                }
                            }
        if (imax!=i)
        {
            for (j=0;j<nw+1;j++)
            {
                zamiana=a[imax][j];
                a[imax][j]=a[i][j];
                a[i][j]=zamiana;
            }
        }
        for(j=i+1;j<nw;j++)
        {
            if (!a[i][i]) spr=0;
            stala=a[j][i]/a[i][i];
            for(k=i+1;k<nw;k++) a[j][k]=a[j][k]-stala*a[i][k];
        }
        for (i=nw-1;i>-1;i--)
        {
            b=0;
            for (j=nw-1;j>i;j--) b=b+a[i][j]*x_w[j];
            x_w[i]=(a[i][nw]-b)/a[i][i];
            if(!a[i][i]) spr=0;
        }
        std::ofstream stream("Output.txt");
        if (spr)
        {
            std::cout<<std::endl;
            std::cout<<"Results"<<std::endl;

            for (i=0;i<nw;i++)
            {
                std::cout<<"X["<<i+1<<"] = "<<x_w[i]<<std::endl;
                stream<<1000*x[i+1]<<"\t"<<1000*y[i+1]<<"\t"<<x_w[i]<<std::endl;
            }
        }
        else
        {
            std::cout<<" Method Gaussian used in the algorithm solver ";
            std::cout<<"\n it does not give an unambiguous solution in this case ";
            std::cout<<"\n or the equations does not give an unambiguous solution \n";
        }
        getchar();
    }
}

```

Appendix D

Subroutine: Gauss Method

```

PROGRAM gauss_program
IMPLICIT NONE
INTEGER, PARAMETER :: rozmiar = 3
DOUBLE PRECISION, DIMENSION(rozmiar,rozmiar) :: A
DOUBLE PRECISION, DIMENSION(rozmiar) :: b
! Predefined matrix A
A(1,1)=-1.0
A(1,2)=2.0
A(1,3)=1.0
A(2,1)=1.0
A(2,2)=-3.0
A(2,3)=-2.0
A(3,1)=3.0
A(3,2)=-1.0
A(3,3)=-1.0
! Predefined vector b
b(1)=-1
b(2)=-1
b(3)=4
! Call Gauss method
CALL Gauss_method(A,b,rozmiar)
END PROGRAM gauss_program

SUBROUTINE Gauss_method(A,b,n)
INTEGER :: n, i_max, Maks_bezw_calk
DOUBLE PRECISION, DIMENSION(n,n) :: A, AMatrix
DOUBLE PRECISION, DIMENSION(n) :: b, bVector, xVector
AMatrix = A
bVector = b
xVector(:) = -1
do i = 1, n
  if (AMatrix(i,i) == 0) then
    i_max = Maks_bezw_calk(AMatrix(i:n,i),(n-i+1)) + i - 1
    if(AMatrix(i_max,i) /= 0) then
      CALL Podmien_wiersz(i, i_max, AMatrix, n)
      CALL Podmien_elem_vec(i, i_max, bVector, n)
    else
      if (AMatrix(Maks_bezw_calk(AMatrix(:,i),n),i) /= 0) then
        STOP 'Impossible to calculate the roots'
      else
        xVector(i) = 0
      end if
    end if
  end if
end if
  if (AMatrix(i,i) /= 0) then
    do j = (i+1), n

```

```

        do k = (i+1), n
            AMatrix(j,k) = AMatrix(j,k) - AMatrix(i,k) * ( AMatrix(j,i) / AMatrix(i,i) )
        end do
        bVector(j) = bVector(j) - bVector(i) * ( AMatrix(j,i) / AMatrix(i,i) )
        AMatrix(j,i) = 0
    end do
end if
end do
do i = n, 1, -1
    if(xVector(i) /= 0) then
        xVector(i) = bVector(i) - SUM( xVector((i+1):n) * AMatrix(i,(i+1):n) )
        if(AMatrix(i,i) /= 0) xVector(i) = xVector(i) / AMatrix(i,i)
    end if
end do
print*, 'xVector='
print*, xVector
END SUBROUTINE Gauss_method

SUBROUTINE Podmien_wiersz(r1, r2, A, n)
INTEGER :: r1, r2, n
DOUBLE PRECISION, DIMENSION(n,n) :: A
do i = 1, n
    CALL Zamiana( A(r1,i) , A(r2,i) )
end do
END SUBROUTINE Podmien_wiersz

SUBROUTINE Podmien_elem_vec(i1, i2, A, n)
INTEGER :: n, i1, i2
DOUBLE PRECISION :: swap
DOUBLE PRECISION, DIMENSION(n) :: A
swap = A(i1)
A(i1) = A(i2)
A(i2) = swap
END SUBROUTINE Podmien_elem_vec

FUNCTION Maks_bezw_calk(A, n)
INTEGER :: Maks_bezw_calk, n
DOUBLE PRECISION, DIMENSION(n) :: A
Maks_bezw_calk = 1
do i = 2, n
    if(ABS(A(i)) > ABS(A(Maks_bezw_calk))) Maks_bezw_calk = i
end do
END FUNCTION Maks_bezw_calk

SUBROUTINE Zamiana(v1, v2)
DOUBLE PRECISION :: v1, v2, swap
swap = v1
v1 = v2
v2 = swap
END SUBROUTINE Zamiana

```

Appendix E

Subroutine: Transformation and Integration (3D)

```

subroutine TRANSFORM_INTEGRATION
  use globalvariables !in this module define global variables
  implicit REAL*8 (A-H,O-Z)
  integer(kind=8), dimension( 8) :: node_local

  !WFACTOR - Weighting factor (each Gaussian point)
  !COORD - Coordinates
  !PKSI - Derivative of shape function by KSI(each Gaussian point)
  !PETA - Derivative of shape function by ETA(each Gaussian point)
  !PZETA - Derivative of shape function by ZETA(each Gaussian point)
  !NO_ELEMENTS - Number of elements in solution domain
  !LAMBDA - Thermal conductivity factor W/mK
  !DPX - Derivative of shape function by X(each Gaussian point)
  !DPY - Derivative of shape function by Y(each Gaussian point)
  !DPZ - Derivative of shape function by Z(each Gaussian point)

  COORD(1)= -0.5773502692D+00
  COORD(2)= +0.5773502692D+00
  WFACTOR(1)= +1.0000000000D+00
  WFACTOR(2)= +1.0000000000D+00
  do kpnt= 1, 2
  do jpnt= 1, 2
  do ipnt= 1, 2

  !Shape function
  SHAPE_FUN(ipnt,jpnt,kpnt,1)= 0.125 * (1.d0 - COORD(ipnt)) *
    &(1.d0 - COORD(jpnt)) * (1.d0 - COORD(kpnt))
  SHAPE_FUN(ipnt,jpnt,kpnt,2)= 0.125 * (1.d0 + COORD(ipnt)) *
    &(1.d0 - COORD(jpnt)) * (1.d0 - COORD(kpnt))
  SHAPE_FUN(ipnt,jpnt,kpnt,3)= 0.125 * (1.d0 + COORD(ipnt)) *
    &(1.d0 + COORD(jpnt)) * (1.d0 - COORD(kpnt))
  SHAPE_FUN(ipnt,jpnt,kpnt,4)= 0.125 * (1.d0 - COORD(ipnt)) *
    &(1.d0 + COORD(jpnt)) * (1.d0 - COORD(kpnt))
  SHAPE_FUN(ipnt,jpnt,kpnt,5)= 0.125 * (1.d0 - COORD(ipnt)) *
    &(1.d0 - COORD(jpnt)) * (1.d0 + COORD(kpnt))
  SHAPE_FUN(ipnt,jpnt,kpnt,6)= 0.125 * (1.d0 + COORD(ipnt)) *
    &(1.d0 - COORD(jpnt)) * (1.d0 + COORD(kpnt))
  SHAPE_FUN(ipnt,jpnt,kpnt,7)= 0.125 * (1.d0 + COORD(ipnt)) *
    &(1.d0 + COORD(jpnt)) * (1.d0 + COORD(kpnt))
  SHAPE_FUN(ipnt,jpnt,kpnt,8)= 0.125 * (1.d0 + COORD(ipnt)) *
    &(1.d0 + COORD(jpnt)) * (1.d0 + COORD(kpnt))

  !Derivative of shape function
  PKSI(jpnt,kpnt,1)= - 0.125 * (1.d0 - COORD(jpnt)) *
    &(1.d0 - COORD(kpnt))
  PKSI(jpnt,kpnt,2)= + 0.125 * (1.d0 - COORD(jpnt)) *

```

```

&(1.d0 - COORD(kpnt))
PKSI(jpnt,kpnt,3)= + 0.125 * (1.d0 + COORD(jpnt)) *
&(1.d0 - COORD(kpnt))
PKSI(jpnt,kpnt,4)= - 0.125 * (1.d0 + COORD(jpnt)) *
&(1.d0 - COORD(kpnt))
PKSI(jpnt,kpnt,5)= - 0.125 * (1.d0 - COORD(jpnt)) *
&(1.d0 + COORD(kpnt))
PKSI(jpnt,kpnt,6)= + 0.125 * (1.d0 - COORD(jpnt)) *
&(1.d0 + COORD(kpnt))
PKSI(jpnt,kpnt,7)= + 0.125 * (1.d0 + COORD(jpnt)) *
&(1.d0 + COORD(kpnt))
PKSI(jpnt,kpnt,8)= - 0.125 * (1.d0 + COORD(jpnt)) *
&(1.d0 + COORD(kpnt))
PETA(ipnt,kpnt,1)= - 0.125 * (1.d0 - COORD(ipnt)) *
&(1.d0 - COORD(kpnt))
PETA(ipnt,kpnt,2)= - 0.125 * (1.d0 + COORD(ipnt)) *
&(1.d0 - COORD(kpnt))
PETA(ipnt,kpnt,3)= + 0.125 * (1.d0 + COORD(ipnt)) *
&(1.d0 - COORD(kpnt))
PETA(ipnt,kpnt,4)= + 0.125 * (1.d0 - COORD(ipnt)) *
&(1.d0 - COORD(kpnt))
PETA(ipnt,kpnt,5)= - 0.125 * (1.d0 - COORD(ipnt)) *
&(1.d0 + COORD(kpnt))
PETA(ipnt,kpnt,6)= - 0.125 * (1.d0 + COORD(ipnt)) *
&(1.d0 + COORD(kpnt))
PETA(ipnt,kpnt,7)= + 0.125 * (1.d0 + COORD(ipnt)) *
&(1.d0 + COORD(kpnt))
PETA(ipnt,kpnt,8)= + 0.125 * (1.d0 - COORD(ipnt)) *
&(1.d0 + COORD(kpnt))
PZETA(ipnt,jpnt,1)= - 0.125 * (1.d0 - COORD(ipnt)) *
&(1.d0 - COORD(jpnt))
PZETA(ipnt,jpnt,2)= - 0.125 * (1.d0 + COORD(ipnt)) *
&(1.d0 - COORD(jpnt))
PZETA(ipnt,jpnt,3)= - 0.125 * (1.d0 + COORD(ipnt)) *
&(1.d0 + COORD(jpnt))
PZETA(ipnt,jpnt,4)= - 0.125 * (1.d0 - COORD(ipnt)) *
&(1.d0 + COORD(jpnt))
PZETA(ipnt,jpnt,5)= + 0.125 * (1.d0 - COORD(ipnt)) *
&(1.d0 - COORD(jpnt))
PZETA(ipnt,jpnt,6)= + 0.125 * (1.d0 + COORD(ipnt)) *
&(1.d0 - COORD(jpnt))
PZETA(ipnt,jpnt,7)= + 0.125 * (1.d0 + COORD(ipnt)) *
&(1.d0 + COORD(jpnt))
PZETA(ipnt,jpnt,8)= + 0.125 * (1.d0 - COORD(ipnt)) *
&(1.d0 + COORD(jpnt))
enddo
enddo
enddo

```

```

do i= 1, NO_ELEMENTS
!Global number for each element
node1= CONNECT_MATRIX(i,1)
node2= CONNECT_MATRIX(i,2)
node3= CONNECT_MATRIX(i,3)
node4= CONNECT_MATRIX(i,4)
node5= CONNECT_MATRIX(i,5)
node6= CONNECT_MATRIX(i,6)
node7= CONNECT_MATRIX(i,7)
node8= CONNECT_MATRIX(i,8)

write (*,*) 'Global numbers for element:', i
write (*,*) '-----'
write (*,*) node1
write (*,*) node2
write (*,*) node3
write (*,*) node4
write (*,*) node5
write (*,*) node6
write (*,*) node7
write (*,*) node8
!XYZ coordinates for each element
X1= XYZ(node1,1)
X2= XYZ(node2,1)
X3= XYZ(node3,1)
X4= XYZ(node4,1)
X5= XYZ(node5,1)
X6= XYZ(node6,1)
X7= XYZ(node7,1)
X8= XYZ(node8,1)
Y1= XYZ(node1,2)
Y2= XYZ(node2,2)
Y3= XYZ(node3,2)
Y4= XYZ(node4,2)
Y5= XYZ(node5,2)
Y6= XYZ(node6,2)
Y7= XYZ(node7,2)
Y8= XYZ(node8,2)
Z1= XYZ(node1,3)
Z2= XYZ(node2,3)
Z3= XYZ(node3,3)
Z4= XYZ(node4,3)
Z5= XYZ(node5,3)
Z6= XYZ(node6,3)
Z7= XYZ(node7,3)
Z8= XYZ(node8,3)

write (*,*) 'Coordinates of nodes of element:', i
write (*,*) '-----'
write (*,*) X1,Y1,Z1
write (*,*) X2,Y2,Z2

```

```

write (*,*) X3,Y3,Z3
write (*,*) X4,Y4,Z4
write (*,*) X5,Y5,Z5
write (*,*) X6,Y6,Z6
write (*,*) X7,Y7,Z7
write (*,*) X8,Y8,Z8

call JACOBIAN (iflaga1, iflaga2,detJ, DPX, DPY, DPZ, PKSI, PETA,
& PZETA, X1, X2, X3, X4, X5, X6, X7, X8,
& Y1, Y2, Y3, Y4, Y5, Y6, Y7, Y8,
& Z1, Z2, Z3, Z4, Z5, Z6, Z7, Z8 )

!Integration
wspij= 0.d0
do iii= 1, 8
do jjj= 1, 8
do kpn= 1, 2
do jpn= 1, 2
do ipn= 1, 2

segment= abs(detJ(ipn,jpn,kpn))*WFACTOR(ipn)*WFACTOR(jpn)*WFACTOR(kpn)

wspij= wspij + LAMBDA *(DPX(ipn,jpn,kpn,iii)*
&DPX(ipn,jpn,kpn,jjj)
&+DPY(ipn,jpn,kpn,iii)*DPY(ipn,jpn,kpn,jjj)+DPZ(ipn,jpn,kpn,iii)*
&DPZ(ipn,jpn,kpn,jjj)) *segment

enddo
enddo
enddo
enddo
enddo
enddo
return
end

subroutine JACOBIAN (iflaga1, iflaga2,detJ, PX, DPY, DPZ, PKSI,
&PETA, PZETA,X1, X2, X3, X4, X5, X6, X7, X8, Y1, Y2, Y3, Y4, Y5,
&Y6, Y7, Y8,Z1, Z2, Z3, Z4, Z5, Z6, Z7, Z8 )

implicit REAL*8 (A-H,O-Z)
dimension detJ(2,2,2)
dimension PKSI(2,2,8), PETA(2,2,8), PZETA(2,2,8)
dimension DPX(2,2,2,8), DPY(2,2,2,8), DPZ(2,2,2,8)
do kpnt= 1, 2
do jpnt= 1, 2
do ipnt= 1, 2
DPX(ipnt,jpnt,kpnt,1)=0.d0
DPX(ipnt,jpnt,kpnt,2)=0.d0
DPX(ipnt,jpnt,kpnt,3)=0.d0
DPX(ipnt,jpnt,kpnt,4)=0.d0

```

```

DPX(ipnt,jpnt,kpnt,5)=0.d0
DPX(ipnt,jpnt,kpnt,6)=0.d0
DPX(ipnt,jpnt,kpnt,7)=0.d0
DPX(ipnt,jpnt,kpnt,8)=0.d0
DPY(ipnt,jpnt,kpnt,1)=0.d0
DPY(ipnt,jpnt,kpnt,2)=0.d0
DPY(ipnt,jpnt,kpnt,3)=0.d0
DPY(ipnt,jpnt,kpnt,4)=0.d0
DPY(ipnt,jpnt,kpnt,5)=0.d0
DPY(ipnt,jpnt,kpnt,6)=0.d0
DPY(ipnt,jpnt,kpnt,7)=0.d0
DPY(ipnt,jpnt,kpnt,8)=0.d0
DPZ(ipnt,jpnt,kpnt,1)=0.d0
DPZ(ipnt,jpnt,kpnt,2)=0.d0
DPZ(ipnt,jpnt,kpnt,3)=0.d0
DPZ(ipnt,jpnt,kpnt,4)=0.d0
DPZ(ipnt,jpnt,kpnt,5)=0.d0
DPZ(ipnt,jpnt,kpnt,6)=0.d0
DPZ(ipnt,jpnt,kpnt,7)=0.d0
DPZ(ipnt,jpnt,kpnt,8)=0.d0

DPXDPKSI =
& + PKSI(jpnt,kpnt,1) * X1 + PKSI(jpnt,kpnt,2) * X2
& + PKSI(jpnt,kpnt,3) * X3 + PKSI(jpnt,kpnt,4) * X4
& + PKSI(jpnt,kpnt,5) * X5 + PKSI(jpnt,kpnt,6) * X6
& + PKSI(jpnt,kpnt,7) * X7 + PKSI(jpnt,kpnt,8) * X8
DPYDPKSI =
& + PKSI(jpnt,kpnt,1) * Y1 + PKSI(jpnt,kpnt,2) * Y2
& + PKSI(jpnt,kpnt,3) * Y3 + PKSI(jpnt,kpnt,4) * Y4
& + PKSI(jpnt,kpnt,5) * Y5 + PKSI(jpnt,kpnt,6) * Y6
& + PKSI(jpnt,kpnt,7) * Y7 + PKSI(jpnt,kpnt,8) * Y8
DPZDPKSI =
& + PKSI(jpnt,kpnt,1) * Z1 + PKSI(jpnt,kpnt,2) * Z2
& + PKSI(jpnt,kpnt,3) * Z3 + PKSI(jpnt,kpnt,4) * Z4
& + PKSI(jpnt,kpnt,5) * Z5 + PKSI(jpnt,kpnt,6) * Z6
& + PKSI(jpnt,kpnt,7) * Z7 + PKSI(jpnt,kpnt,8) * Z8
DPXDPETA =
& + PETA(ipnt,kpnt,1) * X1 + PETA(ipnt,kpnt,2) * X2
& + PETA(ipnt,kpnt,3) * X3 + PETA(ipnt,kpnt,4) * X4
& + PETA(ipnt,kpnt,5) * X5 + PETA(ipnt,kpnt,6) * X6
& + PETA(ipnt,kpnt,7) * X7 + PETA(ipnt,kpnt,8) * X8
DPYDPETA =
& + PETA(ipnt,kpnt,1) * Y1 + PETA(ipnt,kpnt,2) * Y2
& + PETA(ipnt,kpnt,3) * Y3 + PETA(ipnt,kpnt,4) * Y4
& + PETA(ipnt,kpnt,5) * Y5 + PETA(ipnt,kpnt,6) * Y6
& + PETA(ipnt,kpnt,7) * Y7 + PETA(ipnt,kpnt,8) * Y8
DPZDPETA =
& + PETA(ipnt,kpnt,1) * Z1 + PETA(ipnt,kpnt,2) * Z2
& + PETA(ipnt,kpnt,3) * Z3 + PETA(ipnt,kpnt,4) * Z4
& + PETA(ipnt,kpnt,5) * Z5 + PETA(ipnt,kpnt,6) * Z6
& + PETA(ipnt,kpnt,7) * Z7 + PETA(ipnt,kpnt,8) * Z8

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DPXDPZETA =
& + PZETA(ipnt,jpnt,1) * X1 + PZETA(ipnt,jpnt,2) * X2
& + PZETA(ipnt,jpnt,3) * X3 + PZETA(ipnt,jpnt,4) * X4
& + PZETA(ipnt,jpnt,5) * X5 + PZETA(ipnt,jpnt,6) * X6
& + PZETA(ipnt,jpnt,7) * X7 + PZETA(ipnt,jpnt,8) * X8
DPYDPZETA =
& + PZETA(ipnt,jpnt,1) * Y1 + PZETA(ipnt,jpnt,2) * Y2
& + PZETA(ipnt,jpnt,3) * Y3 + PZETA(ipnt,jpnt,4) * Y4
& + PZETA(ipnt,jpnt,5) * Y5 + PZETA(ipnt,jpnt,6) * Y6
& + PZETA(ipnt,jpnt,7) * Y7 + PZETA(ipnt,jpnt,8) * Y8
DPZDPZETA =
& + PZETA(ipnt,jpnt,1) * Z1 + PZETA(ipnt,jpnt,2) * Z2
& + PZETA(ipnt,jpnt,3) * Z3 + PZETA(ipnt,jpnt,4) * Z4
& + PZETA(ipnt,jpnt,5) * Z5 + PZETA(ipnt,jpnt,6) * Z6
& + PZETA(ipnt,jpnt,7) * Z7 + PZETA(ipnt,jpnt,8) * Z8
detJ(ipnt,jpnt,kpnt)= DPXDPKSI*(DPYDPZETA*DPZDPZETA-DPZDPZETA*
DPYDPZETA) + DPYDPKSI*(DPZDPZETA*DPXDPZETA-DPXDPZETA*DPZDPZETA) +
&DPZDPKSI*(DPXDPZETA*DPYDPZETA-DPYDPZETA*DPXDPZETA)

segment= 1.d0 / detJ(ipnt,jpnt,kpnt)
w11= segment * ( DPYDPZETA*DPZDPZETA - DPZDPZETA*DPYDPZETA )
w12= segment * ( DPZDPKSI*DPYDPZETA - DPYDPKSI*DPZDPZETA )
w13= segment * ( DPYDPKSI*DPZDPZETA - DPZDPKSI*DPYDPZETA )
w21= segment * ( DPZDPZETA*DPXDPZETA - DPXDPZETA*DPZDPZETA )
w22= segment * ( DPXDPKSI*DPZDPZETA - DPZDPKSI*DPXDPZETA )
w23= segment * ( DPZDPKSI*DPXDPZETA - DPXDPKSI*DPZDPZETA )
w31= segment * ( DPXDPZETA*DPYDPZETA - DPYDPZETA*DPXDPZETA )
w32= segment * ( DPYDPKSI*DPXDPZETA - DPXDPKSI*DPYDPZETA )
w33= segment * ( DPXDPKSI*DPYDPZETA - DPYDPKSI*DPXDPZETA )

detJ(ipnt,jpnt,kpnt)= dabs(detJ(ipnt,jpnt,kpnt))

DPX(ipnt,jpnt,kpnt,1)= w11*PKSI(jpnt,kpnt,1) +
&w12*PETA(ipnt,kpnt,1) + w13*PZETA(ipnt,jpnt,1)
DPX(ipnt,jpnt,kpnt,2)= w11*PKSI(jpnt,kpnt,2) +
&w12*PETA(ipnt,kpnt,2) + w13*PZETA(ipnt,jpnt,2)
DPX(ipnt,jpnt,kpnt,3)= w11*PKSI(jpnt,kpnt,3) +
&w12*PETA(ipnt,kpnt,3) + w13*PZETA(ipnt,jpnt,3)
DPX(ipnt,jpnt,kpnt,4)= w11*PKSI(jpnt,kpnt,4) +
&w12*PETA(ipnt,kpnt,4) + w13*PZETA(ipnt,jpnt,4)
DPX(ipnt,jpnt,kpnt,5)= w11*PKSI(jpnt,kpnt,5) +
&w12*PETA(ipnt,kpnt,5) + w13*PZETA(ipnt,jpnt,5)
DPX(ipnt,jpnt,kpnt,6)= w11*PKSI(jpnt,kpnt,6) +
&w12*PETA(ipnt,kpnt,6) + w13*PZETA(ipnt,jpnt,6)
DPX(ipnt,jpnt,kpnt,7)= w11*PKSI(jpnt,kpnt,7) +
&w12*PETA(ipnt,kpnt,7) + w13*PZETA(ipnt,jpnt,7)
DPX(ipnt,jpnt,kpnt,8)= w11*PKSI(jpnt,kpnt,8) +
&w12*PETA(ipnt,kpnt,8) + w13*PZETA(ipnt,jpnt,8)
DPY(ipnt,jpnt,kpnt,1)= w21*PKSI(jpnt,kpnt,1) +
&w22*PETA(ipnt,kpnt,1) + w23*PZETA(ipnt,jpnt,1)
DPY(ipnt,jpnt,kpnt,2)= w21*PKSI(jpnt,kpnt,2) +

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&w22*PETA(ipnt,kpnt,2) + w23*PZETA(ipnt,jpnt,2)
DPY(ipnt,jpnt,kpnt,3)= w21*PKSI(jpnt,kpnt,3) +
&w22*PETA(ipnt,kpnt,3) + w23*PZETA(ipnt,jpnt,3)
DPY(ipnt,jpnt,kpnt,4)= w21*PKSI(jpnt,kpnt,4) +
&w22*PETA(ipnt,kpnt,4) + w23*PZETA(ipnt,jpnt,4)
DPY(ipnt,jpnt,kpnt,5)= w21*PKSI(jpnt,kpnt,5) +
&w22*PETA(ipnt,kpnt,5) + w23*PZETA(ipnt,jpnt,5)
DPY(ipnt,jpnt,kpnt,6)= w21*PKSI(jpnt,kpnt,6) +
&w22*PETA(ipnt,kpnt,6) + w23*PZETA(ipnt,jpnt,6)
DPY(ipnt,jpnt,kpnt,7)= w21*PKSI(jpnt,kpnt,7) +
&w22*PETA(ipnt,kpnt,7) + w23*PZETA(ipnt,jpnt,7)
DPY(ipnt,jpnt,kpnt,8)= w21*PKSI(jpnt,kpnt,8) +
&w22*PETA(ipnt,kpnt,8) + w23*PZETA(ipnt,jpnt,8)
DPZ(ipnt,jpnt,kpnt,1)= w31*PKSI(jpnt,kpnt,1) +
&w32*PETA(ipnt,kpnt,1) + w33*PZETA(ipnt,jpnt,1)
DPZ(ipnt,jpnt,kpnt,2)= w31*PKSI(jpnt,kpnt,2) +
&w32*PETA(ipnt,kpnt,2) + w33*PZETA(ipnt,jpnt,2)
DPZ(ipnt,jpnt,kpnt,3)= w31*PKSI(jpnt,kpnt,3) +
&w32*PETA(ipnt,kpnt,3) + w33*PZETA(ipnt,jpnt,3)
DPZ(ipnt,jpnt,kpnt,4)= w31*PKSI(jpnt,kpnt,4) +
&w32*PETA(ipnt,kpnt,4) + w33*PZETA(ipnt,jpnt,4)
DPZ(ipnt,jpnt,kpnt,5)= w31*PKSI(jpnt,kpnt,5) +
&w32*PETA(ipnt,kpnt,5) + w33*PZETA(ipnt,jpnt,5)
DPZ(ipnt,jpnt,kpnt,6)= w31*PKSI(jpnt,kpnt,6) +
&w32*PETA(ipnt,kpnt,6) + w33*PZETA(ipnt,jpnt,6)
DPZ(ipnt,jpnt,kpnt,7)= w31*PKSI(jpnt,kpnt,7) +
&w32*PETA(ipnt,kpnt,7) + w33*PZETA(ipnt,jpnt,7)
DPZ(ipnt,jpnt,kpnt,8)= w31*PKSI(jpnt,kpnt,8) +
&w32*PETA(ipnt,kpnt,8) + w33*PZETA(ipnt,jpnt,8)
enddo
enddo
enddo
return
end

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