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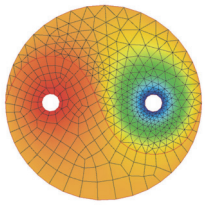

MODELLING OF TRANSIENT TEMPERATURE FIELD AND PHASE TRANSFORMATION CHANGE: A WAY FOR RESIDUAL STRESS MANAGEMENT IN LARGE SIZE FORGINGS

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Abstract

The paper is devoted to development of the modelling approach based on 3D finite-element (FE) analysis of the transient temperature fields and the thermally induced phase transformations as a way towards residual stress management in large size forgings. Heating, holding and cooling stages are under consideration and modelling of both the austenite formation and decomposition are taken into account. The thermal-mechanical FE model capable of taking into account changes in the specific volume during ferrite/austenite transformation is coupled with the relevant phase transformation model in order to allow simulation of the transient stresses due to both thermal contraction and the dilatometric effect. The model is capable of taking into account different boundary conditions for the heat transfer problem based on the available data. To improve the predictive abilities, the following two commercial FE codes, such as MSC Marc 2013.1.0 and Abaqus/Standard 6.12, are used for solving the non-steady state 3D problem of the metal expansion/contraction during consecutive heating, holding and cooling stages. Although all the mentioned process steps are considered, the model is dedicated to be used for modelling the cooling stages of large forgings and castings.

Key words: large ingot forging, finite element analysis, heating, holding and cooling, phase transformations

1. INTRODUCTION

Many of the steel manufactures, which supplies such industries like electric power companies or shipbuilders prefer to produce large single elements instead of numerously smaller ones in order to avoid many technical issues of connections between elements in large complex mechanical systems including stresses, difference of thermal expansion coefficients or complicated geometry of welding paths (Xiao-Xun Zhang et al., 2009; YoungDeak et al., 2011). The process of large ingots manufacturing is a long and complex operation. It usually takes months of engineering work to determine an appropriate chemical composition of the material, geometry and the relevant details of the forging and the heat treatment operations. The forged elements are used as very responsible parts working under very demanding conditions for a long times, for example shafts in nuclear reactors, rotors of the turbines of the wind power plants engines, nuclear powered submarines or reactor pressure vessels in the nuclear

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power plants. There is a strong demand for the materials of these products to have very high percent of purity in the whole cross section area. Even small inclusions could lead to disasters caused by internal cracking and propagation of stresses. Large dimensions of such ingots create extremely difficult conditions for carrying out any experimental work revealing the nature of the stress propagation during processing that makes it very expensive and sometimes impossible. Most of these tests are destructive for the element, many of them restricted to the surface areas of the product in terms of obtaining the relevant information about stresses (Carlone & Palazzo, 2011).

Mathematical modelling based on the finite element method seems to be an effective numerical tool allowing for minimization of the possibility of mistakes during the process and for investigation of the stress distribution during processing. Carlone and Palazzo presented an advanced thermo-mechanically coupled finite element model capable of taking into account the solid-solid phase transformation during steel cooling process (Carlone & Palazzo, 2011; Carlone et at., 2010). The presented approach, assuming the Johnson-Mehl-Avrami-Kolmogorov model with the Scheil's additivity rule, demonstrates good abilities in terms of stress distribution prediction within the steel samples during heating and holding stages. However, the approach does not consider the effects of transformation plasticity, phase change strain increment and stress induced phase transformation effects among others. Krzyzanowski et al. (2006) developed a thermal-mechanical finite element model capable of taking into account changes in the specific volume during austenite to ferrite transformation during cooling. The model can be coupled with any of the existing phase transformation models that allows for simulation of the sample contraction due to both thermal contraction and the dilatometric effect. YoungDeak Kim et al. (2011) used the finite element method to simulate the ultra – large ingot forging process to develop the finest stress distribution, which is significant in the inner void closing effect (Xiao-Xun Zhang et al., 2009; YoungDeak et al., 2011). Dye et al. (2004) developed the model that is capable of measuring the residual stresses in the 2-dimensional elements after quenching process. Bokota and Kulawik (2006) developed a numerical model of phase transformation during quenching low carbon steel elements, which takes into account the heat conduction equation, equilibrium equations. The macro-scale model are based on TTT diagrams and the mechanical phenomena influencing the hardening process.

As it has been mentioned above, there are several developments on void closure during forging of ultra-large size ingots. Although, there is still lack of the relevant material that refers to the technical problems influenced by residual stresses during heat treatment and phase transformations occurring in large forgings. The aim of this work is development of the numerical approach allowing for residual stress management in large size forgings and modelling of the transient temperature field and phase transformation change is the first stage of the project. An application of different and well established commercial software packages for the numerical calculations, such as Simulia Abaqus and MSC Marc, is also beneficial for achievement of the above mentioned goal.

2. THE MAIN COUPLING FACTORS

Temperature changes during heating, holding, quenching and tempering stages are the primary cause of the induced stresses because of the local differences in the specific volume within the part. Particular attention should be given to the large size parts where the temperature changes can be relatively high. At the beginning of the cooling from austenitic phase, the local contraction of the metallic material is higher for the areas with lower temperatures than in the areas having relatively higher temperatures. It already induces thermal stresses within volume of the part. At some temperature intervals, the temperature change leads to microstructural transformations within the workpiece during both heating, holding and cooling stages. As the local temperature exceeds the phase transformation temperature during heating, austenite formation from the preexisting structures is observed, while martensite, pearlite, bainite, ferrite and iron carbide is formed as a result of austenite decomposition during the cooling stage when the local temperature within the volume reaches the corresponding phase transformation temperature. Apart from the temperature, the formation is strongly influenced by the local chemical composition of the steel, the cooling rate and also by the induced stresses within the volume of the part. The complexity of the modelling is related to the reciprocal coupling between the heat transfer, the deformation and the phase transformations schematically presented in figure 1. When the stress exceeds

the yield strength, the material can be permanently deformed due to the combined effect of the differences in local temperature and the microstructure, which can even lead to destruction.

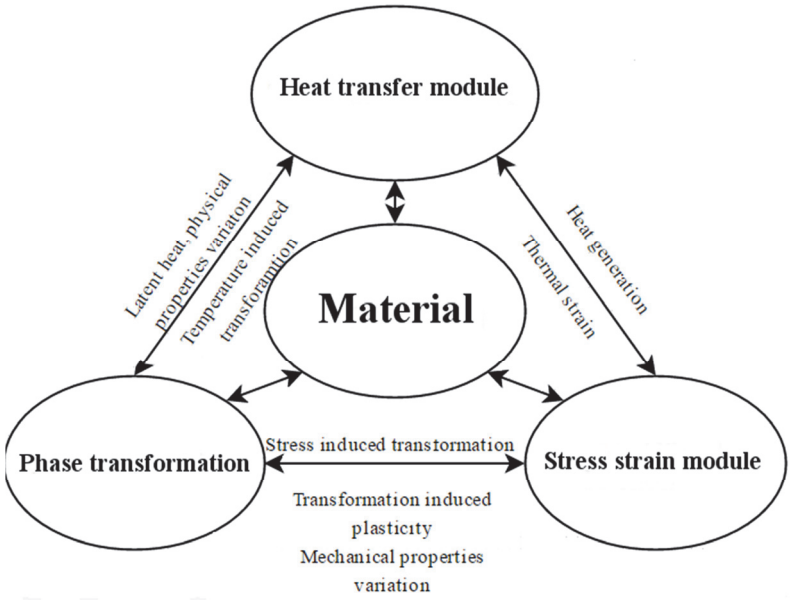

Fig. 1. *Schematic representation of reciprocal coupling between heat transfer, deformation and phase transformations during heating/cooling of large forgings.*

It can be seen in figure 1, the microstructure changes are temperature and stress dependent. The areas of the part characterized by the different microstructure will also have different mechanical and physical properties, influencing the temperature distribution. Formation of these areas having different specific volumes will result in mechanical strains leading to change of the stress distribution (Kulawik & Wróbel, 2013). Such phenomena as transformation induced plasticity when plastic strains are developed at stresses below the yield stress can also take place during this type of phase transformations depending on the transformation rate and the transient stress state. The thermal gradients within the processing part result in the different local thermal expansions generating stresses that can lead to plastic flow and part distortions. Generally, plastic deformations are characterized by heat generation that influence the temperature distribution. Finally, the distribution of the new appearing phase within the local volume of the processing part has its own effect on the expansion of this volume, which is added to the whole complexity of the events (Krzyzanowski et al., 2006).

All the above mentioned factors constitute an extensive, complicated system for modelling with many reciprocal connections between the different modules. It is unnecessary to implement all of mentioned elements into one single model. Overloading the FE model with unnecessary modules seems to be an ineffective approach since it can lead to instabilities and unnecessary increase of the computational time (Babeł & Kulawik, 2011). Only main co-operative relationships are considered at this stage of the investigation omitting the effects related to transformation induced plasticity and stress induced transformation. Although, the mentioned above factors may also impact the outcomes and are going to be taken into consideration in further analysis. The influence of the individual physical phenomena on the stress management will be accessed during further stages and progress of the project assuming particular geometry, the variation of technological parameters, chemical content and structural features of the processing parts. The aim of the first part of the work is to combine a 3D thermal mechanical finite element model capable of taking into account changes in the specific volume during solid-solid phase transformation model for simulation of the sample contraction due to both thermal contraction and the dilatometric effect. This solution will be used in the second part of the research as a model for investigation of size effects on dilatometric testing results carrying out in Sheffield Forgemasters RD26 Ltd, UK.

3. FE MODEL: PREDICTION OF THE SAMPLE EXPANSION/CONTRACTION

The coupled thermo-mechanical 3D numerical model is based on the FE method. The cubic section of the material is simulated at this stage of the investigation for simplification, while the shape of the model is going to be adjusted to the actual shape of the relevant part at later stages of the project. The 5.0 x 5.0 x 5.0 mm section has been divided into 125 3-D hexagonal full integration elements type with eight integration nodes.

The constraints are applied to displacements of the relevant nodes on the corresponding planes of the section, as it is shown in figure 2, while displacements of the rest of the nodes were allowed during contraction of the section. For instance, the displacements in *X* direction or rotations around the axes *Y* and *Z* was not allowed for the nodes situated on the plane *YZ*. The similar constraining conditions

were applied to *ZX* and *YX* planes of the section correspondingly:

$$\begin{aligned} u_1 = u_{r2} = u_{r3} = 0 \quad & for\ YZ\ plane \\ u_2 = u_{r1} = u_{r3} = 0 \quad & for\ XZ\ plane \\ u_3 = u_{r1} = u_{r2} = 0 \quad & for\ YX\ plane \end{aligned} \tag{1}$$

where u_i the displacement in i direction and u_{ri} is rotation around i axis (i = 1, 2, 3 and i = 1, 2 and 3 corresponds to *X*, *Y* and *Z* axis).

possible in different areas within the structure of the metal section, and it was assumed in the model that it can take place in randomly distributed elements within the area where the relevant condition are fulfilled. In other words, the elements, representing the new ferritic phase are randomly distributed within the corresponding area of the section, where the transformation start temperature is reached. The ratio between the number of transformed and untransformed elements within the area is determined

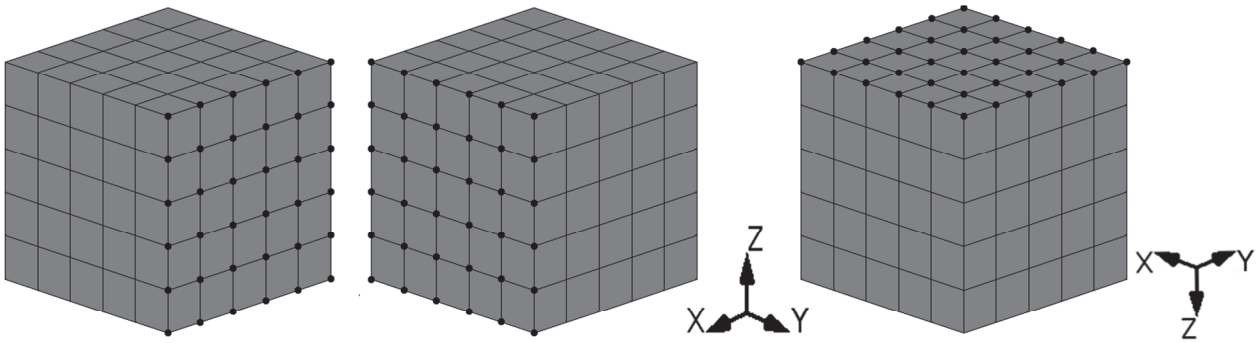

Fig. 2. *Schematic representation of the nodal constraints at the planes of symmetry.*

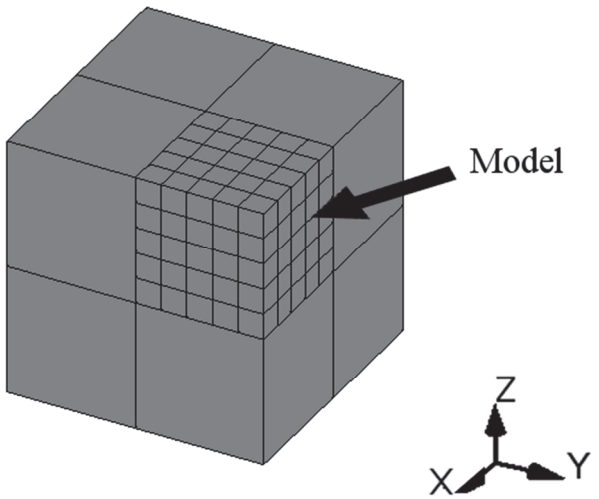

Fig. 3. *Schematic representation of the position of the modeled part in the whole element after application of the symmetry planes.*

The section underwent cooling by applying a cooling agent to the outer surfaces of the section. The cooling is simulated by prescribing the energy balance for the outer boundary surface:

$$\lambda \frac{\partial T}{\partial n} = \alpha (T_a - T) \tag{2}$$

where: λ is the thermal conductivity, n is a coordinate normal to the surface, α is the heat transfer coefficient, T_a and T are the ambient and the boundary surface temperature. The phase transformation is for every time step by the fraction of ferrite with respect to the whole volume of the material determined in the phase-transformation module for every time step. Each element of the model can be transformed from austenite into ferrite only once. The assumption of a random distribution of ferritic phase appearing within the section volume during phase transformation was introduced following earlier investigation results, where the contraction of the specimen during austenite-ferrite transformation corresponded to a gradual transformation within the whole material volume. It is assumed in the model that when an element is transformed from austenite into ferrite its volume is changed according to changes of atomic volumes of the corresponding phases. The details of the implemented procedure are presented elsewhere (Krzyzanowski et al., 2006). The components of the FE model are thermo-mechanically coupled and all the mechanical and thermal properties are included as functions of temperature. The relevant model parameters, such as thermal conductivity, specific heat and density of the steel, necessary for heat transfer calculation, were introduced on the basis of available experimental data. The mechanical properties of the steel were assumed to be similar to the those used in majority of FE models (Duffy, 2014; Sun et al., 2011; Pous-Romero et al., 2013; Francis et al., 2007; Lee et al.,

Table 1. *The thermal and mechanical parameters used in the model.*

Density [t/mm^3]	Young's modulus [MPa]	Poisson's ratio	Yield stress [MPa]	Conductivity* [mW/mm*K]	Specific heat* [kJ/kg*K]	Thermal expansion coefficient*
7,833e^{-09}	181135	0,3	345	23÷41	400e^{+06}÷1700 e^{+06}	10,8e^{-06} ÷ 22,3e^{-06}

*this data were assumed temperature dependent

2010; Jung et al., 2015; Keim et al., 2012) and are presented in the table 1.

Considering the effect of some stored energy in the unrecrystallised austenite, the transformation start temperature depends on the cooling rate, austenite grain size and retained strain. For the purpose of the current work, the following simplified equation was used describing the transformation start temperature as a function of just cooling rate:

$$T_F = 825 - 27.6 * \theta \qquad (3)$$

where T_F is the transformation start temperature and Θ is the cooling rate [ºC/s]. In the advanced physical models the austenite-ferrite transformation is divided into stages such as nucleation, growth and site saturation (Senuma et al., 1992). These models are connected with other models describing pearlitic, bainitic and martensitic transformations. Such models, being implemented into the FE code, allow for simulation of microstructural phenomena under varying thermal conditions showing good predictive capabilities (Pietrzyk & Kuziak, 1999). In the case of the simplified approaches, an Avrami-type equation describing the kinetics of phase transformation is often used (Campbell et al., 1992). As has been shown earlier by other authors (Roosz et al., 1983), the dilatometric transformation curves obtained under constant cooling rate can be described by an Avrami equation as a function of time (Gomez et al., 2003). The transformation curves present two differentiated zones that corresponds to the austenite to proeutectoid ferrite and remaining austenite into pearlite transformation. Assuming the above consideration, the following equation has been used in this part of the investigation taking into consideration that the amount of pearlite is significantly smaller than the amount of ferrite for relatively low cooling rates:

$$X_f = 1 - \exp\left[-\ln 2\left(\frac{t}{x_1}\right)^{x_2}\right] \qquad (4)$$

where X_f is the fraction of ferrite with respect to the whole volume of the material, x_1 and x_2 are the material parameters and t is defined as $t = [T_F\text{-}t(1)]/\Theta$, where $t(1)$ is the node temperature at the moment. The parameter x_1 corresponds to both the nucleation and growth rates and can also be a function of the cooling rate, austenite grain size, steel chemical composition and temperature (Sellars, 1980). The assumption of simplified Eq. (4) in order to predict the kinetics of the austenite–ferrite transformation significantly facilitates modelling and, at the same time, is sufficient to illustrate the formulation of the problem. The main advance in the new approach is made with the new thermo-mechanical finite element model, which simulates contraction of the modelling section during cooling through the austenite–ferrite temperature range.

4. RESULTS AND DISCUSSION

The following four representative nodes, illustrated in figure 4 and numbered as 1, 54, 66 and 216 have been chosen for the transient analysis. Node 1 is located in the middle of the cube while node 66 was chosen in the middle of the cube external edge. Node 216 represents the most remote from the middle of the cube point.

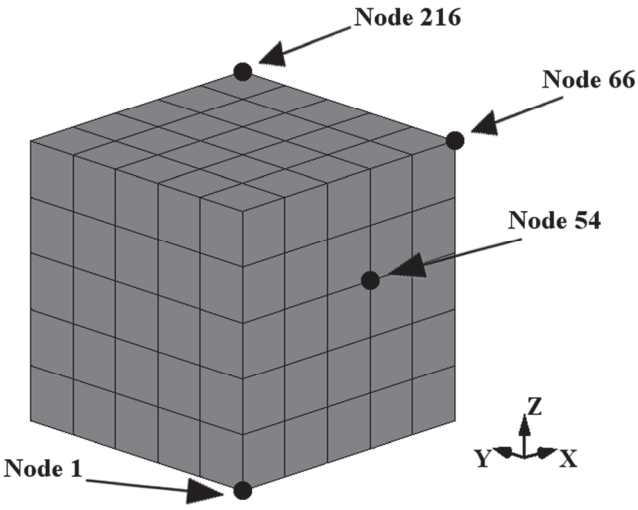

Fig. 4. *Representative nodes of the cube section chosen for the transient analysis.*

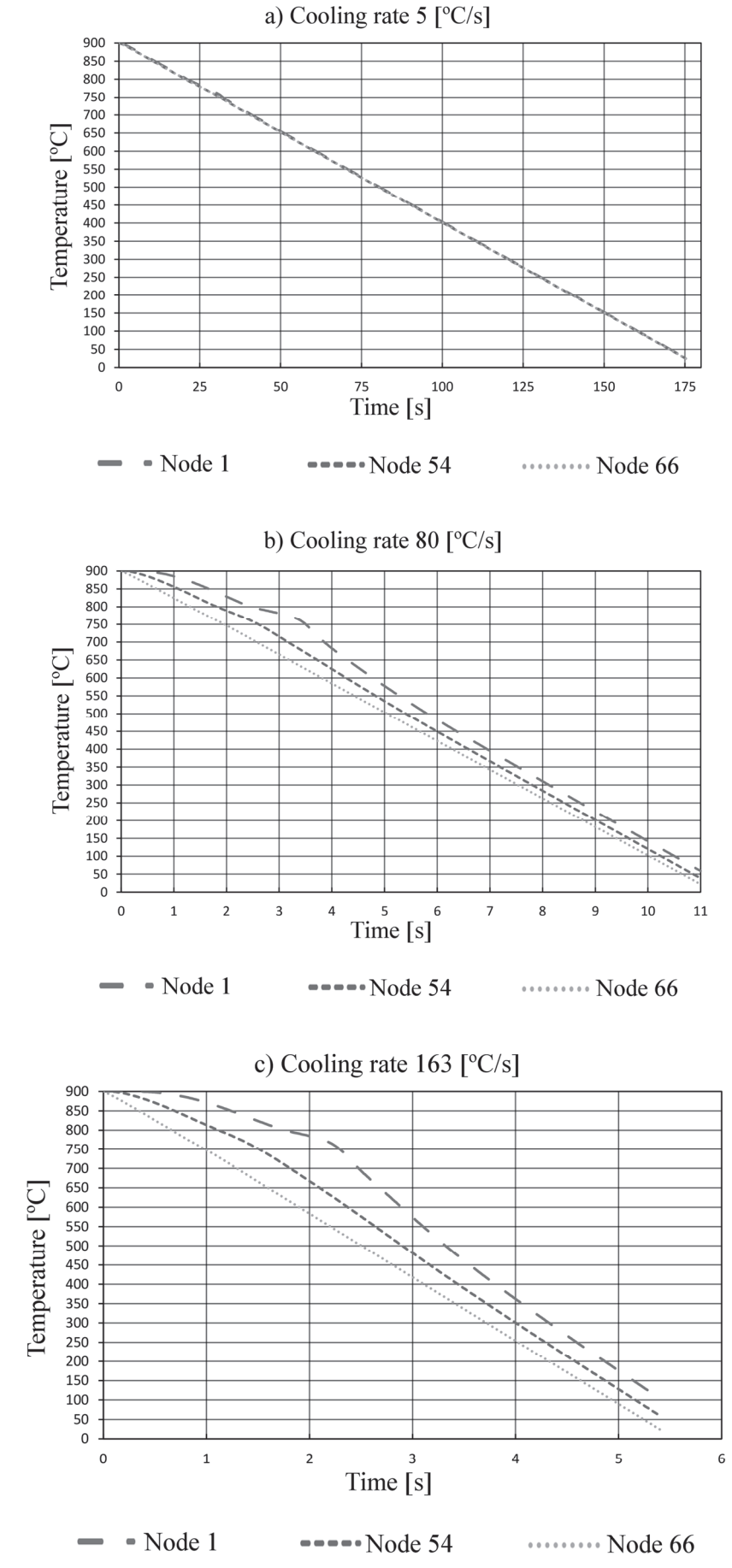

Fig. 5. *The change in temperature at the different nodes within the section predicted for the different cooling rates at the boundary surface: a) 5 [°C/s], b) 80 [°C/s], c) 163 [°C/s].*

To illustrate dependence of the temperature change within the section on the cooling rate, the boundary condition described by the energy balance, eq. (2), has been replaced by the prescription of the temperature change in time with different cooling rates at the corresponding boundaries, i.e. the boundary condition of the first kind. Figure 5 illustrates the time-temperature graphs presenting the temperature changes at different points of the section from start to finish of the cooling stage predicted for the three different cooling rates at the boundaries, which are referenced further in the text as cooling rates. The cooling stage takes significantly less time for the highest cooling rate, such as 163^{O}C. As can be seen in figure 5a, the differences in temperature predicted at the node located in the middle of the cube and the node in the middle of the cube external edge are very small when the cooling rate is low, about 5 ^{o}C/s. The actual cooling rate depends and can be controlled by the heat transfer coefficient (HTC) between the material and the ambient fluid. However, for higher HTCs, which influence cooling of the boundaries with cooling rates similar to the cases illustrated in figure 5b and 5c, the temperature distribution within the section is not homogeneous and the surface layers of the material cools down significantly faster than those situated deeper within volume of the section. The temperature inhomogeneity causes inhomogeneity in distribution of the corresponding element volumes within the section due to the differences in their thermal contraction that would inevitably result in development of internal stresses within the volume of the section.

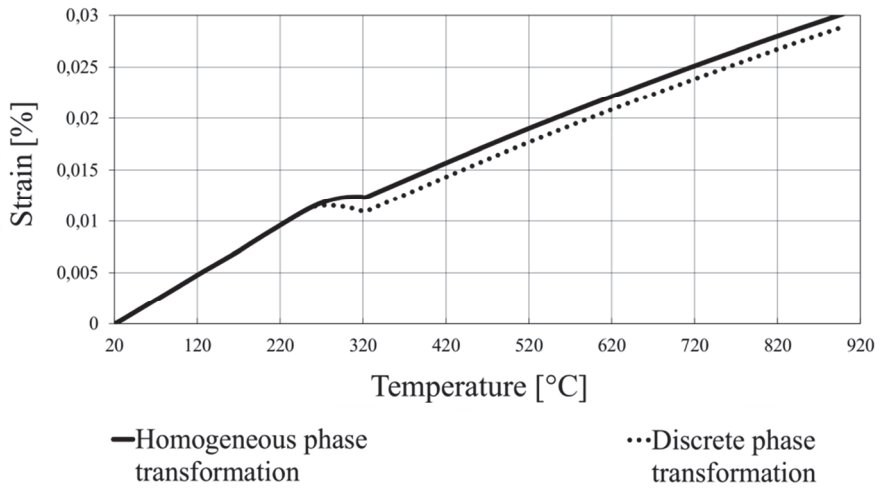

Fig. 6. *Dilatometric contraction curves predicted at node 216 for the cooling rate 5 [°C/s] assuming homogeneous and inhomogeneous appearance of the ferritic phase.*

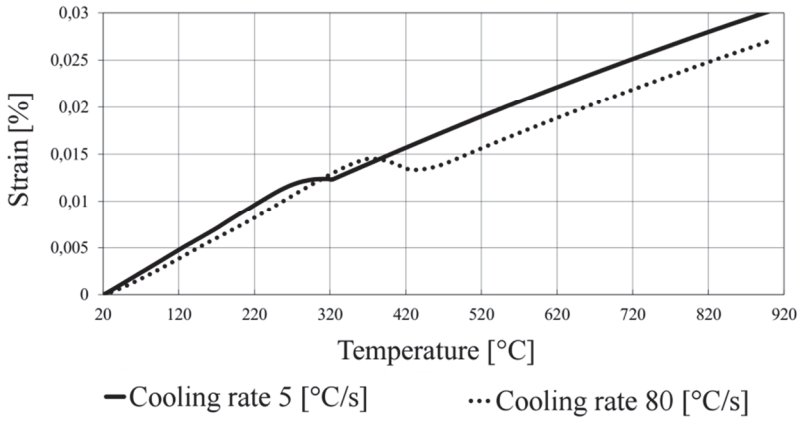

Fig. 7. *Dilatometric contraction curves predicted at node 216 for the different cooling rates.*

Figure 6 illustrates differences in the dilatometric curves predicted assuming a random distribution of the ferritic phase appearing within the volume of the section (discrete phase transformation) and assuming the conventional approach (homogeneous phase transformation). In the case of discrete transformation, it has been assumed that the phase transformation takes place in randomly distributed elements within the section and that the ratio between the number of ferrite and austenite elements during the phase transformation corresponds to the ferrite/austenite volume fractions at any time moment, according to eq. (4). The inhomogeneous discrete approach assumes that the ferrite phase appears within the specimen volume as randomly distributed elements having slightly expanded volumes relative to the remaining austenite elements, as follows from the changes in atomic volumes of the corresponding phases. The data were collected from the node 216, which is the most remote from the middle of the cube point located in its corner. The solid curve presents the strain response of the section registered at the same node 216 assuming the conventional approach representing homogeneous phase transformation modelled for the comparison. Implementing the random appearance of the new phase's elements, suggested in (Krzyzanowski et al., 2006), results in more gentle strain response of the section due to the constraints on strain induced by untransformed elements of austenite on that node. The difference between the deformation level occurs due to the position of the elements of the new phase. In homogenous approach all new ferrite elements appears on the edges of the model what divides the model into two near equal parts. The highest stress values occur between this two sections. In discrete phase transformation the randomly distributed lonely elements in the model causes higher stress level, stretching the surrounding elements almost always in three directions, because it is rare for the elements nearby to expand in the same direction together with the new phase elements. It is observed, that through the transformation order changes it is possible to make an influence on shapes of the strain curves in the very various ways.

The model of the homogenous phase transformation places new elements of the ferrite in some privileged places. Because of that some of the places are more deformed than the others, especially in the area near the origin of the coordinate system. This causes appearing of the region dependent results.

The differences in the predicted dilatometric curves due to the differences in cooling rates illustrated in figure 7. It can be noticed that the higher value of the cooling rate influences the delay in the transformation start temperature. This kind of inhomogeneity is taken into account by dividing the whole temperature range of the phase transformation into some temperature intervals, where temperature

within each interval can be characterised by some constant (characteristic) temperature. It is assumed, in terms of the austenite/ferrite transformation that the phase transformation occurs in elements randomly distributed within the corresponding regions of the equal characteristic temperature. The ratio between the number of transformed (ferrite) and untransformed (austenite) elements during the phase transformation period within such areas corresponds to the ferrite/austenite volume fractions for the characteristic temperature and is controlled by eq. (4).

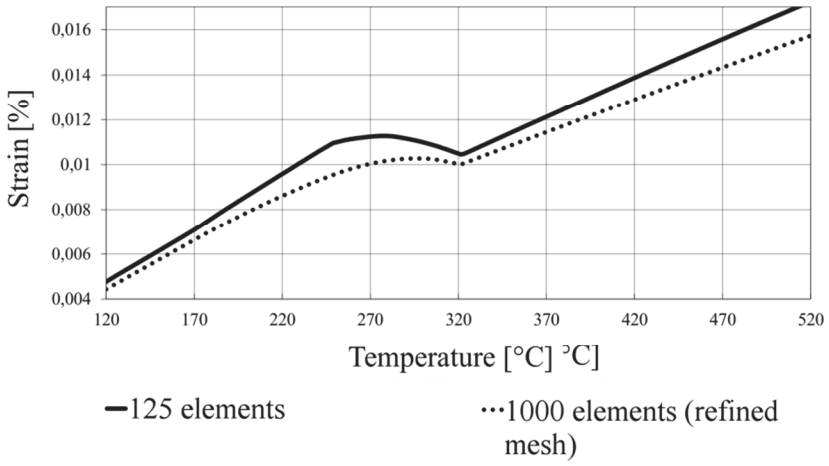

Fig. 8. Dilatometric contraction curves predicted at node 216 for the cooling rate of 5 [°C/s] assuming different mesh refinement of the section and discrete phase transformation.

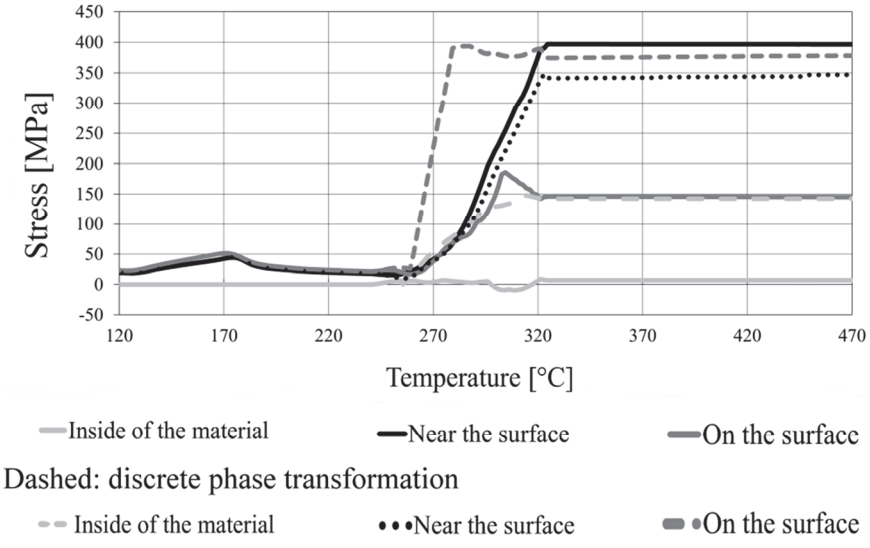

Fig. 9. Changes in the equivalent stress predicted at nodes 1, 54 and 66 located within the section for the different stages of austenite-ferrite phase transformation during cooling with 5 °C/s cooling rate assuming homogenous and discrete phase transformation.

This means, that not all elements at the given temperature are going to transform, because some of the austenite elements will not manage to change before the temperature change. This is dependent from the cooling ratio and at its higher rates the differences in the local volumes (elements) due to phase transformation and the differences due to higher temperature gradients results in the larger value of the deformation (figure 7).

The developed discrete approach assumes that the ferrite phase appears within the section volume as randomly distributed elements having slightly expanded volumes relative to the remaining austenite elements, as follows from the changes in atomic volumes of the corresponding phases. This produces differences in the predicted dilatometric curves during refinement of the finite element mesh even for the low cooling rates, such as 5 °C/s (figure 8). The effect has to be taken into consideration when the optimum mesh size is chosen for the direct model. This effect of the mesh refinement is more pronounced for cooling of the section at high cooling rates.

Figure 9 illustrates the equivalent stress predicted at different locations within the section for the cooling rate 5 °C/s. The dashed curves presents stress level after implementing the discrete transformation model. Before the randomizing the stress level inside the material during austenite-ferrite phase transformation occurred during the cooling process was very low and its value grew slow. It was the lowest among the corresponding stress predicted at areas near the surface of the section. The equivalent stress predicted on the surface was the highest because of the combination of the dilatometric effect and the local differences in volumes of the finite elements influenced by their inhomogeneous thermal contraction under higher temperature gradients at the surface regions. The elements situated closer to the surface of the section are exposed to the highest cooling rates. The highest residual stresses have been predicted in the middle

of the external edges of the cubic section, at node 66. It can be noticed that randomizing the phase transformation induced much more stresses inside the section. After randomizing it can be observed that the stresses on the surface were a little lower and the stresses inside the material and near the surface were closer to the themselves. The highest values of stresses were near the surface. This means that the randomizing the distribution of the phase transformation causes the stress distribution inside the material much more higher, but not higher than the previous stress level on the surface.

5. SUMMARY

A 3D thermomechanically coupled numerical model based on the finite element method has been developed capable of taking into account changes in the specific volume during both austenite-ferrite transformation and the local thermal contraction during cooling from austenite temperature region. The model is being developed with intention of residual stress management during cooling of large size forgings in further stages of the project. The model can be coupled with any of the available phase transformation models allowing simulation of the inhomogeneous metal part contraction due to both thermal contraction and the dilatometric effect. The model can also be used as a direct model during inverse calculations for identification of phase transformation model parameters on the basis of measurement of the dilatometric effect. The following two commercial FE codes, such as MSC Marc 2013.1.0 and Abaqus/Standard 6.12, are used for solving the non-steady state 3D problem of the metal expansion/contraction during cooling from the austenite region.

It has been shown that a discrete random distribution of the appearing ferritic phase within the sample cross section results in more gentle changes of the section contraction with time during cooling than that in the case of the conventional (homogeneous) approach. It is also observed that the changes in the order of the phase transformation influence the strain curve and can be used to achieve the more precise control on the transformation.

The temperature distribution within the volume of the section can be assumed as homogeneous for the low cooling rates, such as 5 ^{o}C/s. However, the temperature gradients within the volume are increased and are reflected in the dilatometric predictions at high cooling rates, 80 and 163 ^{o}C/s. It has been shown that additionally refinement of the finite element mesh can affect the model prediction and also has to be taken into account.

The numerical calculations have been performed for illustration of the predictive abilities of the developed thermal-mechanical finite element model. For this purpose, it was combined with the simplified phase transformation model. The more advanced physical phase transformation models validated using an inverse analysis are going to be used in the next stages of the work.

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MODELOWANIE ZMIAN NIESTACJONARNEGO POLA TEMPERATURY ORAZ PRZEMIANY FAZOWEJ; ANALIZA NAPRĘŻEŃ WŁASNYCH W ODKUWKACH WIELKOGABARYTOWYCH

Streszczenie

W artykule przedstawiono wyniki modelowania numerycznego 3D procesów obróbki cieplnej wielkogabarytowych odkuwek o masie 300÷600 ton. W celu obliczenia niestacjonarnego pola temperatur oraz zachodzących podczas procesu nagrzewania i chłodzenia zmian w przebiegu cieplnie indukowanej przemiany fazowej wykorzystano metodę elementów skończonych (MES). Zaproponowany zestaw modeli może stanowić narzędzie do badań naprężeń własnych, powstających podczas obróbki cieplnej odkuwek charakteryzujących się dużą masą i wymiarami. W modelu uwzględniono etapy nagrzewania, wytrzymania w danej temperaturze i chłodzenia materiału. Modelowanie przemian fazowych odbywa się w osobnym, powiązanym z proponowanym modelem podprogramie, gdzie przewidywane są zmiany objętości odkuwki podczas przemian ferrytycznej i austenitycznej. Umożliwia to odpowiednią symulację powstawania naprężeń chwilowych, wynikających z cieplnego skurczu materiału. Model może uwzględniać różne warunki brzegowe w celu dostosowania do danego problemu cieplnego. W celu poprawy dokładności uzyskiwanych wyników wykorzystano komercyjne oprogramowanie MES tj. MSC Marc 2013.1.0 oraz Abaqus/Standard 6.12. To oprogramowanie zostało wykorzystane w celu rozwiązania równań nieustalonego stanu materiału, tj zmian objętości podczas kolejnych stadiów nagrzewania, wytrzymania i chłodzenia. Efekty działania zaproponowanego modelu zostały przedstawione na przykładzie wybranego etapu chłodzenia.

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