

FEM simulation of microstructure refinement during severe deformation

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Abstract. The majority of methods of severe plastic deformation (SPD) used for producing ultra-fine grained (UFG) and nano materials involve the non-uniform distribution of strains in the workpiece. To make the refinement of grains uniform, interlinked operations are used in which either the orientation of the workpiece or the type of SPD is changed in some sequence. Each operation has its own set of control parameters affecting the output result. As a result, the optimization of the total chain of operations becomes very difficult, especially taking into account that each stage of material processing comes from the previous one with a certain non-uniformity of the structure. To deal with such types of problems the capability of tracing the transformation of the microstructure and accounting for its effect on mechanical properties in finite element modeling (FEM) is required. There are a number of detailed physical models of grain refinement and texture formation, but very often they are too complicated for practical engineering simulations. The mechanics of SPD are also studied and simulated in many works, but normally it is assumed that material is uniform, isotropic and its properties don't change during deformation. In this paper a microstructurally-coupled FE model of the SPD process is proposed. The question of selection and verification of macroscopic and microscopic constitutive relations is discussed. The results of a simulation made in QForm are analyzed and compared with some initial experimental data.

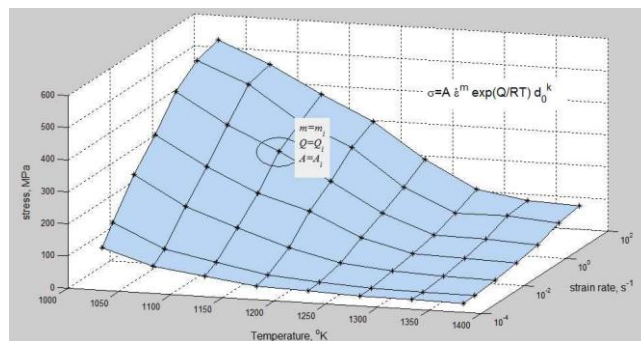
1. Introduction

The main purpose of the technological processes based on severe plastic deformation (SPD) is to obtain a good quality fine grained (FG) or ultra fine grained (UFG) microstructure, which is required for many applications [1]. It is well known that in principle any plastic deformation at low temperatures can result in refinement of the microstructure [2], but for obtaining grain sizes of 1 micron or less then the very high strains possible using SPD are required. The intention is to produce a preferably uniform grain structure, with the lowest possible content of defects [3]. It is evident that these requirements may contradict each other. Any large deformation, especially at relatively low temperatures, will tend to generate defects and non-uniformity of grain size. That is why, though a lot of progress is already achieved in SPD investigations, many methods are developed, but few technological processes are production-ready. Hence, there still remains a wide field for the optimization of SPD for the manufacture of commercial quantities of material.

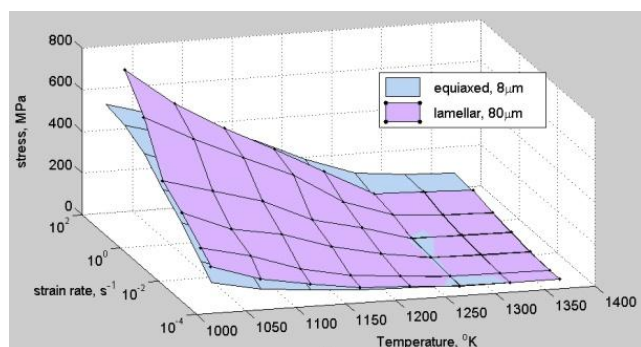
Optimization of SPD processes is especially complicated because it involves simultaneously three different areas – material science (related to microstructure transformation), the mechanics of solids (related to metal flow and its stability) and engineering (related to the heating, loading, friction, wear, die life, etc.) [4]. To solve all the problems is a complex task and tools involving relationships between these areas are required. Modern FEM software can successfully relate engineering with the mechanics of solids, but microstructure analysis is either not included into it or has a very complicated form which is difficult to use. However a very exact and complicated description of microstructure transformation is not always



necessary, sometimes simple assessment may be sufficient. One variant of such an assessment model which could be used for simulation and analysis of the SPD processes is discussed in this paper.



(a)



(b)

Figure 1. The stress surfaces for Ti-6Al-4V with a) equiaxed microstructure with average grain size 8 μm and b) lamellar (Widmanstätten) microstructure with average grain size 80 μm

2. Model description

Phenomenological models with internal variables first proposed by Yu.N. Rabotnov [5], whose 100-year jubilee is celebrated this year, are widely used to account for the changes of the structural state of materials during the deformation process. The internal variables used in such models can directly describe some elements of the microstructure or to be indirectly related to the microstructural state. They serve two main purposes: to characterize the microstructure state along with its transformation and to reflect the influence of the structural state on the mechanical behavior of the material. It is not necessary that each of the parameters is always of the same importance in both roles, e.g. some parameters critical for the stability of the microstructure may have negligible effect on the flow stress and some parameters responsible for hardening and softening may not be so relevant from the viewpoint of the microstructure state.

Unfortunately, while developing an internal variable based model it is impossible to include in it all the available characteristics of the microstructure. A balance between simplicity and accuracy is generally required. Besides that, the intention to utilize the model developed in an FEM simulation adds an extra limitation – all the equations used in the model must remain valid and stable across very wide range of temperatures, strain rates and strains. The attempt to use material constants that are only suitable for a narrow set of conditions, or the presence of non-smoothness or a discontinuity in the function used can cause problems with the convergence of the iteration process.

Taking into account all above mentioned considerations, the model development can be divided into a few steps. For the first approach the most significant internal variable is identified and included in the model. All the equations are thereafter calibrated and verified. Following that the analysis is carried out to identify the processing range over which this approximation is sufficient and can be used. For other problems, where the obtained level of accuracy is unsatisfactory, a list of the minimum necessary second level parameters has to be developed and included into the model at the next step of its modification.

Having the aim to simulate severe plastic deformation processes used for the development of FG and UFG microstructure, it is logical to choose, as a first level parameter, the variable related to the degree of the refinement of the microstructure – the effective grain size; ‘D’. At some stages of the process (when the microstructure has already become uniform without significant substructure) this may be equivalent to the average grain size, while at other stages of the process (e.g. at low strains when for a Widmanstatten type of microstructure it is difficult to specify what is meant by an average grain size) it can play the role of some assessment parameter [6].

This parameter is important both for tracing the microstructure transformation as well as for a more accurate description of the mechanical behavior of the material. As can be seen in Figure 1, constructed on the basis of the experimental results obtained by Prasad et. al.[7, 8], the flow stress significantly depends on the average grain size. Refinement of the microstructure from about 80 μm to 8 μm causes a temperature dependent softening that varies from about 1.2 times (at 750°C) up to about 1.6 (at 950°C). As a result of this data the main constitutive equation of the model was taken in the standard form for hot working simulation [9]:

$$\sigma = A\dot{\varepsilon}^m \exp\left(\frac{Q}{RT}\right)\left(\frac{D}{d_0}\right)^k \quad (1)$$

where σ is effective stress, $\dot{\varepsilon}$ is effective strain rate, T- temperature, R- the gas constant, D – effective grain size.

The main difference of this model from similar, previously proposed, versions is that material parameters A, m and Q are not constants, they are dynamic parameters varying during the process depending on the current thermal and loading conditions at points across the material. In another words for each state, characterized by the temperature and strain rate, a specific set of parameters is calculated suitable for approximation of the actual stress surface (Fig. 1a) with the mathematical expression shown in Eqn.1. Parameter d_0 refers to the average grain size of the material for which the basic stress surface is experimentally obtained (e.g. for Fig 1a $d_0=8\mu\text{m}$) i.e. the effective starting grain size. Parameter, ‘k’ is taken as a constant.

The kinetics of the refinement are described with the following equation [10]:

$$\dot{D} = \begin{cases} t_g \exp\left(-\frac{Q}{RT}\right) & \text{if } D \leq D_m & \text{for the static grain growth} \\ \left(c \frac{\sigma}{D^2} + t_d\right) \cdot \exp\left(-\frac{Q}{RT}\right) & \text{if } D_m \leq D \leq D_{cr} & \text{for the deformation grain growth} \\ 0, \quad D = 0.7 \cdot D_{cr}, & \text{if } D \geq D_{cr} & \text{for the integral refinement} \end{cases} \quad (2)$$

Here the main role is played by the parameter, D_{cr} which mainly depicts the refinement process. It is assumed here that the major mechanical characteristic controlling the refinement is the plastic work at a point (or, more accurately, the specific distortion energy):

$$D_{cr} = D_1 + D_{cr0} \exp\left(-B_1 \int \sigma \cdot \dot{\varepsilon} \cdot dt\right) \quad (3)$$

In equations (2) and (3) the parameters t_g , t_d , c , D_m , D_1 , D_{cr0} and B_1 are constants having empirical values found from experimental data.

The proposed model was programmed as a user sub-routine via the facilities of the QForm 7 FE metal forming simulation code and tested in the simulation of few standard SPD processes, which are described below.

3. Numerical simulation

The simulations were done for two main types of SPD processes: Multi-axial Forging (MF) and Equal Channel Angular Pressing (ECAP).

In all the types of simulations the microstructurally coupled problem was solved. It means changes of the refinement variable D were traced 'in-processor' and used for calculation of the stress at each iteration step. Both isothermal and non-isothermal processes were simulated. For all non-isothermal processes the heat transfer between workpiece and tooling was simulated as well as reheat due to friction and deformation [11]. Automatic remeshing was used for large strain deformations. All SPD processes were simulated as a sequence of operations, in which all the data about the workpiece state (temperature, accumulated strain, strain energy and microstructure refinement) developed at the end of one operation were used as the initial data for the following one. To take account of friction at contact surfaces the Levanov model was used with a friction factor of 0.1, Levanov coefficient of 1.25. The heat transfer coefficient was taken as 10000w/m²K, which is representative of using a glass coating. Such coatings are commonly used to provide both thermal insulation and lubrication.

3.1. Multiaxial Forging (MF)

Two main types of the multiaxial forging were simulated – triaxial forging of a cube and cogging of a cylindrical billet, see Fig. 2. For both process Ti-6Al-4V with the above described constitutive model was used. The dimensions of the cube were 80 x 80 x 80mm, while the diameter of the billet was also 80mm. At each operation the upset is done with the tool velocity of 1mm/s to give a tooling separation of 60mm. The MF in the open press was simulated with heated tools; the initial temperature of the workpiece was taken to be 900°C, the temperature of the tools at 400°C, and temperature of the air (locally) at 100°C.

As it was mentioned in the beginning, the main idea of the multiaxial forging is to change the direction of loading. The main purpose of it from the microstructural point of view is to change the direction of the working slip systems, which can help to transfer the low angle boundaries obtained by grain partitioning in the previous operation into the required high angular boundaries [12] (twinning effects are ignored in this paper). The change of the direction of loading also provides partial recovery of the developed defects [13]. From the mechanical point of view the change of the direction of deformation can be quantitatively described with the trajectories of the deformation steps constructed in the space of the strain deviator. These trajectories can be characterized by their internal geometry and classified depending on its complexity [14].

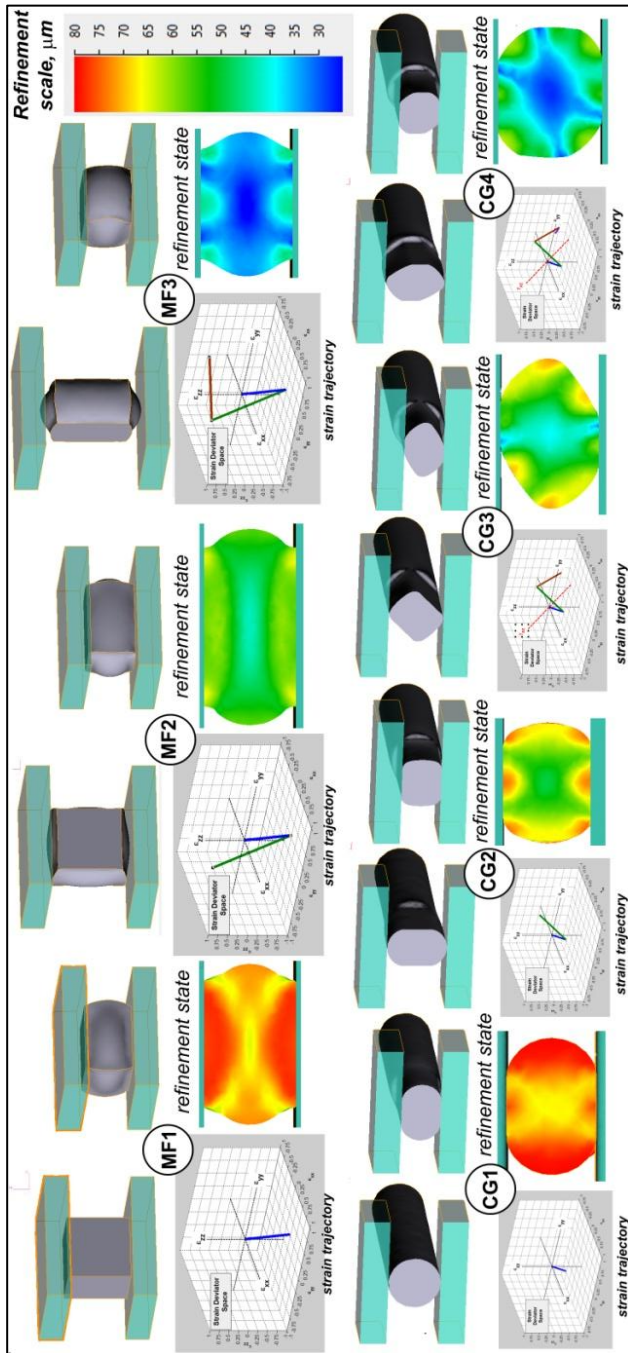


Fig. 2 The operations scheme of the simulated multidirectional forging (MF) and cogging (CG) with the strain trajectories (middle point of billet) and microstructure refinement.

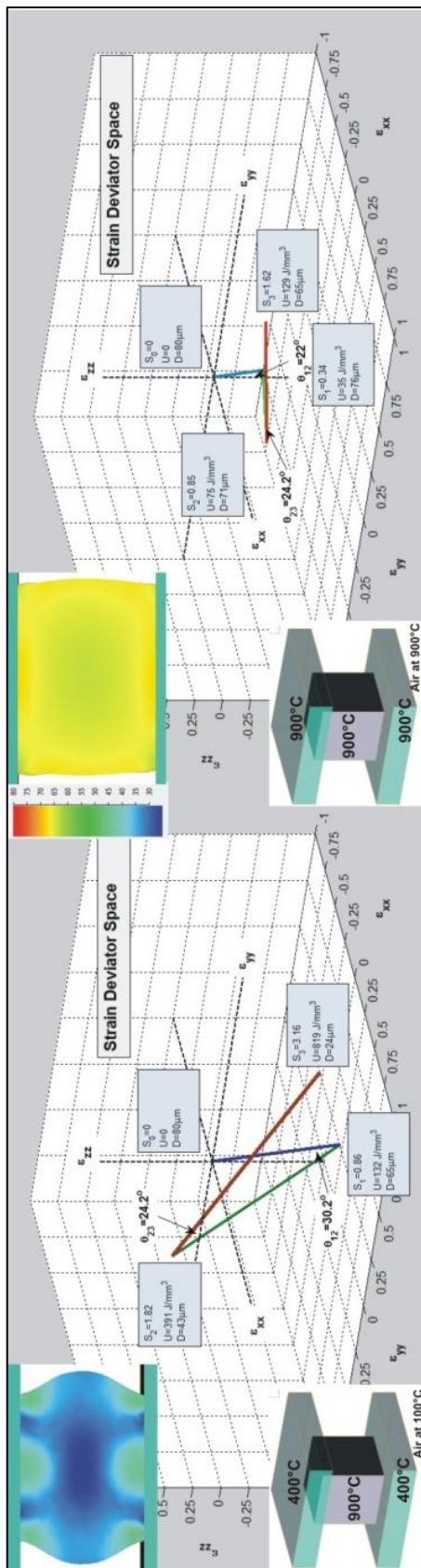


Fig. 3 The comparison of the strain path, mechanical parameters and refinement of the microstructure for the central point of the Ti6Al4V cube under triaxial forging. Here S is Odquist parameter, U – distortion energy, D – effective grain size.

As it can be seen in Figure 2, the deformation trajectories of the MF processes are represented by multi-polylines, characterized by the length of the links and the angles between them (Fig.3). These characteristics can be accompanied with the specific distortional energy and related to the microstructure transformation. In the work of Dmitriev [15] an attempt was made to find mathematically the optimal deformation trajectory. It was shown there that the best results can be achieved if corresponding trajectory is 6-dimensional (includes all 6 components of the deviator). However, by conducting triaxial forging only 3-dimensional trajectories (MF1-MF2-MF3, Fig 2) can be obtained. To get the other components along the shear axis rotation of the workpiece for angles different from 90° is required, which can be done by cogging (incrementally rotating and deforming) the cylindrical billet. If the rotation of the billet is not 90° , but, for example, 45° (CG3, Fig.2) the trajectory becomes 4-dimensional as the components related to shear strain γ_{xy} appear. In this way the technological process of SPD can be specially designed to obtain the most complicated trajectory within the practical limitations given by the forging equipment and the handling of the workpiece.

One more aspect has to be pointed out and taken into consideration. Even those SPD processes which are based on uniform loading, in practice at every operation may have to deal with non-isothermal conditions, friction, non-regularity of the shape and non-uniformity of the material after previous operations. All these factors cause the deformation process to be non-uniform and the strain trajectories will be different at different points (in the Figures 2 and 3 the trajectories are shown only for the center of the billets).

3.2. Isothermal and non-isothermal processes

A brief example of how the non-uniformity of the processing conditions affect the strain trajectories can be obtained by the comparison of isothermal and non-isothermal triaxial forging (Fig.3). Many SPD processes are designed to be isothermal (to be conducted using tooling that has the same temperature as the workpiece), but it is quite costly and complicated from the viewpoint of rotation of the billet and not always possible (e.g. for large scale billets). That is why the analysis of the non-isothermal processes with the intent to find some acceptable solutions is important.

It can be seen in Fig.3 that non-uniformity of the thermal conditions can completely change the picture of the strain trajectories as well as microstructure refinement. To some extent the refinement in the non-isothermal process is more efficient (refinement up to $24\ \mu\text{m}$ in the center of the cube versus $65\ \mu\text{m}$ in the case of isothermal conditions) though it is accompanied with significant variability across the volume of the billet. Some ideas concerning the possibility to utilizing these effects are discussed below.

3.3. Equal Channel Angular Pressing (ECAP)

ECAP is a very large class of SPD processes which require separate study and separate discussion [1,3,4,16]. The analysis of microstructure transformation during ECAP has been examined by a number of authors, for example the dislocation density-based model used by Baik & Estrin et al. [17] for simulation of the deformation of aluminum. Here ECAP is mentioned only to illustrate one of the options which is provided by the simulation of microstructurally coupled problems with a relatively simple assessment model (which can be used for two phase titanium alloys). One of the essential questions for ECAP is the choice of the optimal processing route (optimal sequence of rotations of the billet) and optimization of the channel geometry [18-19]. In order to attempt to fully map the effects of different processing routes on microstructure a complex crystal plasticity based methodology would be necessary. As noted, however, it is possible to simplify somewhat using neo-continuum models, as used here. The results of the simulations, depicted in the Fig.4, show that due to friction, mechanical softening and a few other specific features of the material flow the

microstructure refinement is non-uniform after the first pass. This will lead to further distortion of the deformation zone during following passes, i.e. the slip systems will vary from the idealized ones [20] (Fig. 4, c). Taking this into account as well as tracing the corresponding strain trajectories can help in solving the problem of optimization.

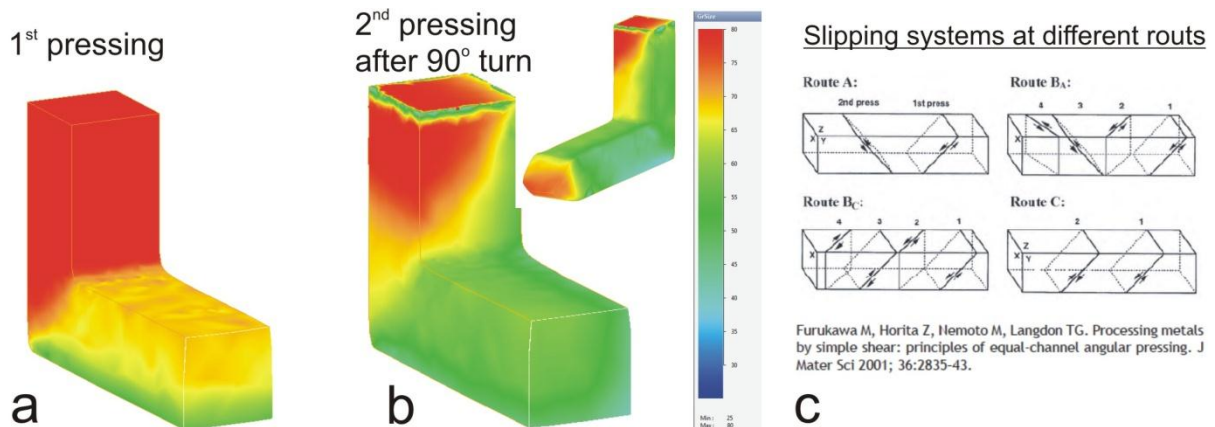


Fig. 4 The results of the simulation of microstructure refinement during ECAP: a) during 1st pressing, b) during the second pressing (after the turn of the workpiece 90 degrees counterclockwise), c) theoretical orientation of the slip systems for different processing routes [20].

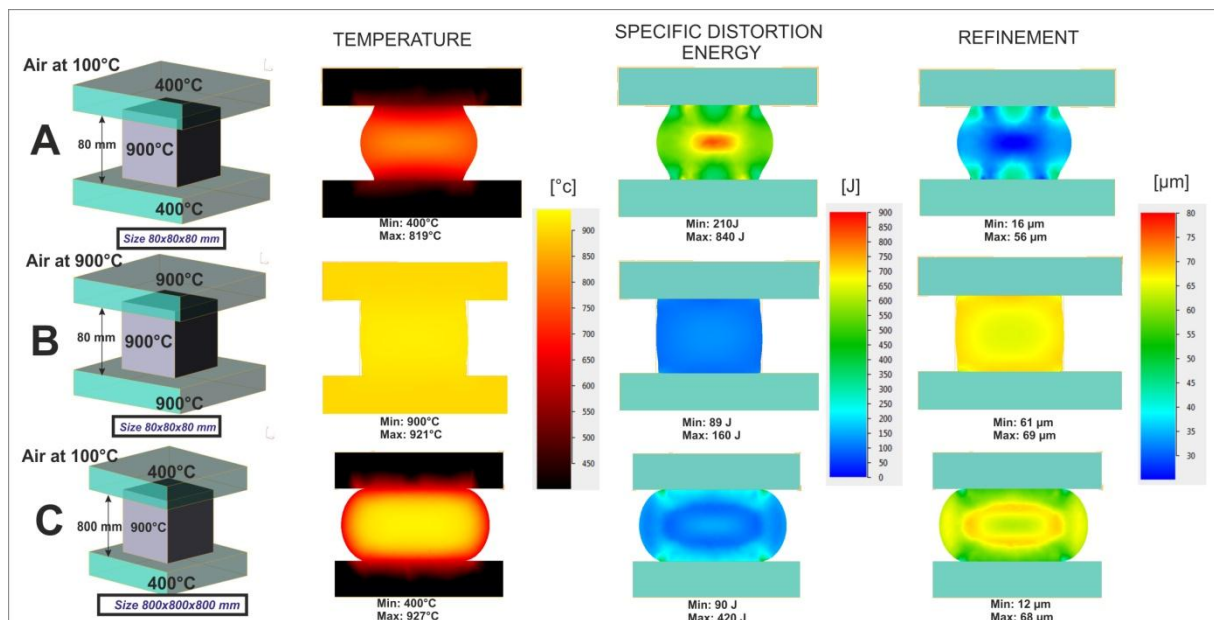


Fig. 5 The effect of the isothermal versus non-isothermal processing conditions and scale factor on the uniformity of the microstructure refinement.

4. Results and discussion

4.1. Analysis of the uniformity of microstructure processing

Non-uniformity within the developed microstructure is an important problem not only for SPD but for all hot and warm working processes. Utilization of the proposed approach in the FEM simulation gives the ability not only to attempt to map the non-uniformity of structure, but also to access the dispersion of the average structural characteristics within the volume of the workpiece. It may help to decide whether such a level of non-uniformity is acceptable or not for different purposes, decide about required thermal treatment for possible improvement or to give ideas for possible optimization of the forging processes.

As the example, some role of the scale ratio on the non-uniformity of the microstructure refinement during triaxial forging was studied. Three cases were simulated (see Fig. 5) – a small cube of size 80 x 80 x 80mm for isothermal and non-isothermal forging was compared a cube 800 x 800 x 800mm of the same material and non-isothermal forging. It can be seen, that the large scale workpiece is getting more uniform refinement than the small one, which at the same time is more efficient than the isothermal one. This may be the direction for finding the optimal regime for the forging of large scale parts. Instead of attempting to achieve the uniformity of temperature, the uniformity of the distortion energy field can be targeted. In this way the lower temperature at the contact surfaces with relatively low deformations can increase the rate of refinement in these regions due to the higher stresses.

4.2. Insufficiency of the chosen state variable.

Establishing the relation between the trajectories of deformation and microstructure development can be very promising from the viewpoint of the optimization of the SPD processes. However, current variants of the model do not contain any state variables which are sensitive to changes in the direction of loading. As can be seen from the results of the simulations, the refinement depends mainly on the accumulated strain energy but not much on the strain path. There are a few structural parameters which can be examined for the modification of the model for the second and third approach and used for coupling with the deformation trajectories. The following parameters can be proposed for this: damage accumulation parameter, percentage of high angle boundaries (HAB), metallographic and crystallographic textures. The first two parameters are mainly used as extra microstructure characterizations and can perhaps be as addressed during post-processing in FEM (their effect to the flow stress can be to some extent neglected). The metallographic and crystallographic texture may affect the anisotropy of the material and have to be related to the tensor part of the constitutive model which is not discussed in this paper.

There is another internal parameter, the shortage of which could be observed in this analysis and this is the effect of the spheroidisation of the alpha phase. On heating a lamellar structure to forging temperature the lamellae will seek to spheroidise to minimize surface energy. Mechanical deformation will tend to accelerate this process and this can cause flow softening. This is not presently incorporated into the model. A further factor is the influence of phase equilibrium [21]; the dissolution of alpha at higher temperatures is time dependent and may also be influenced by mechanical work. This latter factor can be taken into account by including the variable related to the phase balance into equation (1).

5. Conclusion

A model with a single internal variable (level of microstructure refinement) was proposed and used for the simulation of a few SPD processes in FEM software. The results of the simulations have shown that the developed approach can be useful for tracing basic microstructure refinement during these types of processes and to analyze the non-uniformity of this process due to various loading conditions. It was also proposed that trajectories of the deformation can be used for taking into account the complexity of the loading process.

However, it is unlikely that a single variable is sufficient for following the effects related to the complex loading as well as for accurate description of the changes in mechanical behavior of material. More parameters such as the damage accumulation, percentage of HAB's, metallographic and crystallographic textures and phase balance can be included in the model for its improvement. In general this approach can be useful for optimization of hot and warm working processes. Further work is being carried out to develop this approach.

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