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POSSIBILITIES OF THE MECHANICAL BEHAVIOUR MODELLING OF STRUCTURES AFTER SEVERE PLASTIC DEFORMATION

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Abstract

Modelling of the mechanical response of the materials using computer simulation is very useful tool to optimize their mechanical properties. It is especially important for ultrafine-grained (UFG) materials obtained using severe plastic deformation (SPD) techniques. Those materials are characterized by high strength however their application on an industrial scale is limited, first of all because of poor ductility. Proper understanding of the deformation and strengthening mechanisms that govern the mechanical response of UFG materials can be the way to propose the guidelines to improve their ductility. Application of the Finite Element Method (FEM) for calculations and modelling of the mechanical response of UFG materials needs properly built rheological models. In the case of heavily deformed microstructures that are mostly characterized by high inhomogeneity of microstructure and mechanical properties, existing flow stress models need to be modified and justified to the new conditions.

The present study shows some modelling results of the mechanical behaviour of specimens subjected to severe plastic deformation using MaxStrain system. Different grades of steels were examined and their mechanical response was simulated using modified Khan-Huang-Liang (KHL) flow stress model that was implemented into Abaqus Explicit code via user subroutine VUMAT. An effect of various deformation conditions was discussed with respect to the microstructure evolution and its influence on final mechanical properties. The methodology, using Considére criterion to assess the plastic instability in a tensile test, was also implemented into FEM code. The comparison of the measured and calculated results shows that presented approach can be successfully applied to the evaluation of the ductility of various materials with different levels of microstructure refinement.

Key words: ultrafine-grained materials, mechanical response, ductility, Considére criterion

1. INTRODUCTION

A proper description of the constitutive laws governing the mechanical behaviour of UFG materials that is based on the actual physical phenomena occurring in these microstructures can significantly improve the accuracy of the computer modelling process. There are a number of well known constitutive laws that describe mechanical response of the "typical" structures (with the mean grain size range down to 1 μm). However, the situation becomes much more complicated in the case of ultrafine-grained and nanostructured materials. Such structures are mainly obtained by large cold deformation that is followed by annealing process. This processing route produces dislocation structure with a significant fraction of low angle boundaries (LABs), that finally transform into more stable high angle boundaries (HABs). It has been already proven that physical phenomena governing the deformation and strengthening mechanisms of UFG and nanostructured materials are different comparing to their

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"typical" counterparts and still poorly understood [6, 9,11]. Therefore, proper prediction of the mechanical response of UFG materials using computer modelling requires that new constitutive laws will be established or existing description will be modified.

It is also well known that UFG materials are characterized by excellent mechanical strength [9, 11]. However, their production on an industrial scale is still restrained by poor ductility, as necking usually occurs at low plastic strains [8,12]. Different ways to improve plastic properties in UFG and nanostructured materials have been already proposed such as: creating bimodal structures, increasing the work hardening or the strain rate sensitivity, providing the dispersion strengthening, etc [6,9-12]. One of the fundamental sources of loss of ductility is decreasing rate of work hardening. The loss of ductility corresponds to the plastic instability, which is observed on a true stress-true strain curve in the tensile test as the end of uniform elongation. The plastic instability leads to the localized deformation and formation of a neck [8,12]. It should be also mentioned, that from the point of view of the continuum mechanics the usefulness of constructional materials is determined by mechanical properties, which material represents under the most demanding conditions i.e. tensile stresses.

In the present work, UFG microstructures were produced in two grades of low carbon steels using MaxStrain system [5]. Subsequently, their mechanical responses were studied and data from experimental results were used to calibrate flow stress model that was subsequently implemented into FEM code. Flow stress model used in the preset study has been recently modified by the Authors in order to take into consideration the microstructural effects of heavily deformed UFG structures [7]. Simulations of the tensile tests were performed using Abaqus Explicit [1] and the results were compared with experimental data.

The second aim of present work was to propose an approach of ductility assessment in studied UFG materials that can be easily implemented into FEM code. There is a possibility to determine the point where necking begins, providing that a true stress-true strain curve is obtained directly from a tensile test. The point of necking corresponds to the point of tensile instability. The plastic deformation begins in a tensile test when the stress in the sample reaches the critical value. The plastic strain causes local reduction of a cross sectional area, thus the deformation of the material will be continued when stress increases. The necking begins with some value of the effective strain, which can be obtained from a true stress-true strain curve by finding the point, where the rate of work hardening equals to the stress or to the point on the curve of a subtangent of unity (figure 1). This method is known as Considére criterion (necking criterion) and it is expressed by the following equation [2]:

$$\frac{d\sigma}{d\varepsilon} = \sigma \tag{1}$$

Proposed methodology due to its simplicity, can be easily implemented into computer modelling and, as a part of a designing chain, can be used to modify the manufacturing process towards improvement of final properties of UFG materials [8,10].

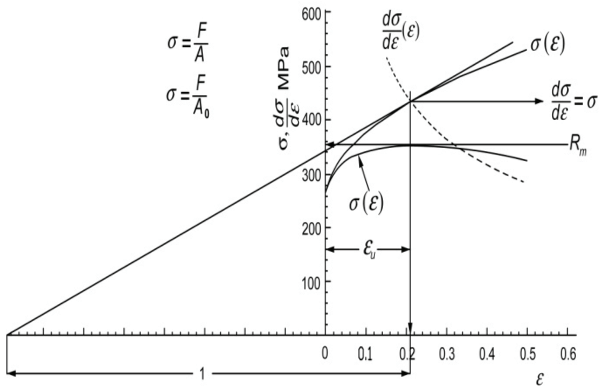

Fig. 1. Determination of the tensile instability point from a strain-stress curve.

In the present work, the above mentioned approach has been also implemented into Abaqus Explicit code (via user subroutine-VUMAT) and utilized for the determination of the uniform elongation in the tensile tests simulations.

2. EXPERIMENTAL PROCEDURES

In order to test the presented approach of ductility assessment, two types of structures were developed: typical coarse-grained structure – with the mean grain size in the micrometer range, and ultrafine-grained structure, with the grain size below 1 µm. To assess the correlation between mechanical response and microstructure evolution in structures, where the solid-solution and the precipitation strengthening play a significant role, two grades of steels were studied: high strength low alloy steel (Y) and, as a more ductile material, interstitial-free steel (IF). The basic chemical compositions of the investigated steels are summarized in table 1.

Table 1. *Basic chemical composition of investigated steels.*

Steel	C	Mn	Si	Ti	Nb	B
IF	0.0022	0.11	0.009	0.073	-	-
Y	0.07	1.36	0.27	0.031	0.067	0.002

The typical coarse-grained structures were produced in hot rolling process. The mean grain size was estimated (using linear mean intercept method) to be 15 μm for Y steel, and 80 μm for IF steel.

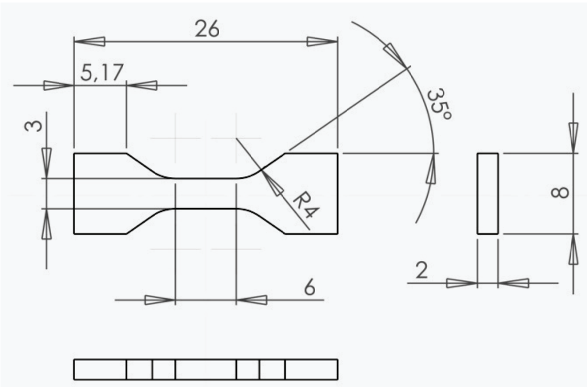

Fig. 2. *Dimensions of tensile specimens used in the present work.*

Ultrafine-grained structures were obtained using MaxStrain system, that is one of the severe plastic deformation methods. A total strain of 20 at room temperature was applied with subsequent annealing at 500ºC (for 1200s). The mean grain size in this case was 600nm for Y steel, and about 1000 nm for IF steel, respectively. Mechanical properties were measured in the tensile test using flat specimens (see figure 2), that were cut parallel to the rolling direction. More details concerning this methodology can be found in Authors' recent work [5,7].

3. RESULTS

Results of the tensile test for both investigated steels are presented in figure 2. It is clearly confirmed that the strong grain refinement causes significant increase in strength. Also the decrease in ductility can be easily observed. The uniform elongation significantly decreased with grain refinement in both deformed materials and reached value below 10% after deformation in case of IF steel, and below 12% in case of Y UFG steel. Hence, it is very interesting observation that the high strength steel (Y), in this case, represents better ductility than IF steel. In the initially more ductile IF steel, the drop in the uniform elongation after MaxStrain deformation is more pronounced than in the high strength Y steel.

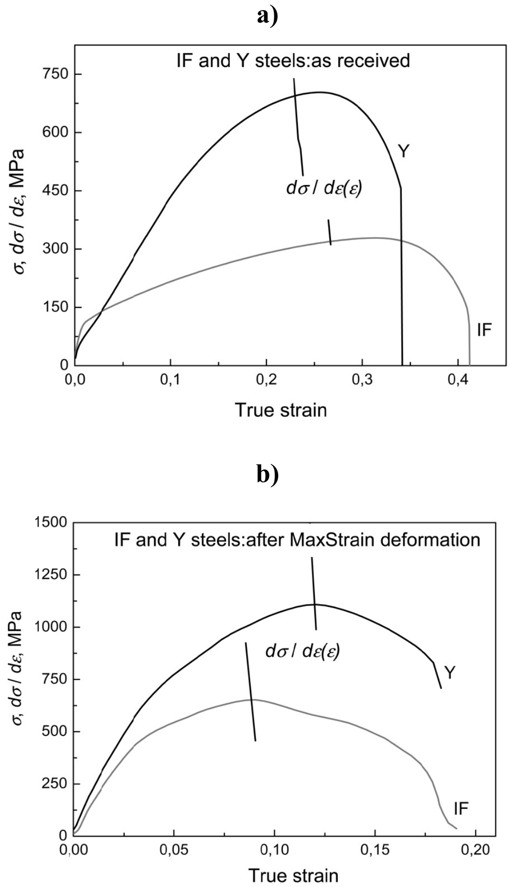

Fig. 2. *Determination of the uniform elongation in: coarse-grained (a), and ultrafine-grained materials (after MaxStrain deformation) (b).*

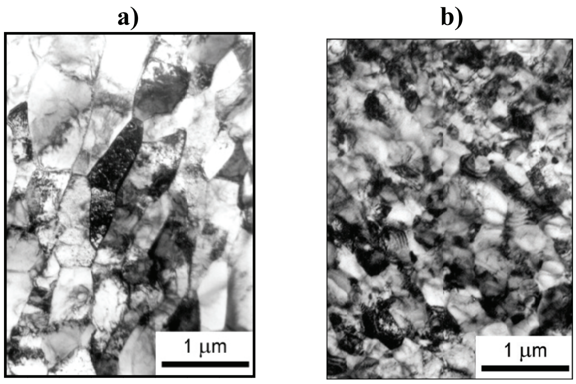

Fig. 3. *TEM microstructures observed in IF steel (a), and Y steel (b), after MaxStrain deformation.*

TEM microstructures observed for the ultrafine-grained materials are shown in figure 3. It can be noticed that application of severe plastic deformation (total strain = 20) had enabled to obtain strong grain subdivision into cells and subgrains that subsequently were transformed into the stable microstructure (with the aid of annealing applied at 500°C). The volume fraction of grains with high angle boundaries measured using electron back scattered diffraction (EBSD) was about 50% in the case of IF steel, and 70% in the case of Y steel. It can be stated that more stable high angle grain boundaries and higher level of precipitation strengthening have led to higher strength observed in this steel. However, we can also expect that the presence of precipitates and higher volume fraction of grains with high angle boundaries (70% vs. 50%) are the main sources of the increased ductility in Y steel i.e. its ability to keep the increasing of work hardening (Considére criterion).

Strain-stress data from the experimental work were subsequently used to calibrate the model of the flow stress that will be introduced in the following chapter.

4. MODELLING

In order to simulate the real mechanical response of UFG materials there is a need to use a proper flow stress model that is able to reflect the phenomena occurring in such structures. In the present work, the Khan-Huang-Liang (KHL) flow stress model [4] was used in the simulations of tensile test. This model has been recently modified in order to take into consideration contribution in strength from LABs and HABs separately [7]. The final form of the model is presented below:

$$\sigma = \left(a + M\alpha Gb\sqrt{1.5bS_V\theta_{LAB}(1-f)} + k\sqrt{\frac{S_V}{2}f} \right) \left[1 + B^*\left(1 - \frac{\ln\dot{\varepsilon}}{\ln D_0^p}\right)^{n_1} \left(\varepsilon^p\right)^{n_0} \right] \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}^*}\right)^C \left(\frac{T_m - T}{T_m - T_r}\right)^m \quad (2)$$

where: σ - flow stress; a - friction stress; M - Taylor factor; α=0.24; G - shear modulus; b - Burgers vector; S_v - the area of boundary per unit volume ($S_v = 2/D_B$) where D_B is the distance between HABs measured along random lines; f - the density of HABs, θ_{LAB} - the average misorientation angle of LABs; ε^p - plastic strain; $D_0^p = 10^6 s^{-1}$, $\dot{\varepsilon}^*$ - reference strain rate; $\dot{\varepsilon}$ - the current strain rate; T, T_m, T_r, k, B^*, n_0, n_1, C, m - constants. At this stage of the study, the temperature effect was not considered.

Following the experimental mechanical testing, 2D finite element models were created for analysis in Abaqus Explicit [1]. Shell elements (S4R) were used to mesh the models. Material behaviour was described using linear elasticity, with isotropic plasticity. A von Mises yield surface was used. Material model together with modified KHL flow stress model, and Considére criterion were implemented using user subroutine (VUMAT). Calculated values of logarithmic strain, von Mises stress, and rate of work hardening were stored as state variables (SDV).

In order to determine the set of material constants, results from the experimental part were utilized and a combination of the simplex method (Nelder-Mead algorithm) as well as optimization procedure were used to minimize the error between predicted and actual data. The core procedures were commercial programs in MATLAB software. The set of equation coefficients obtained is summarized in table 2. The values of average misorientation angle, average boundary spacing and HABs volume fraction were calculated on the basis of the EBSD analysis and are summarized in table 3.

Table 2. *Material constants of modified KHL model (Eq.2) for investigated steels.*

Steel	M	α	G, MPa	b, nm	a, MPa	k, MPa/nm$^{-0.5}$	B^*	n_1	n_0	C
IF	2.75	0.24	81700	0.248	230	5458	2165	0.14	0.57	0.98
Y					460	5950	2165	0.16	0.57	0.97

Table 3. *The values of θ_{LAB}, D_B and f for studied UFG specimens.*

	θ_{LAB}, deg	D_B, nm	f
IF	6.85	1000	0.55
Y	7.15	600	0.716

Since, the criterion of plastic instability does not take into consideration the fracture mechanisms, in the present work, the Johnson-Cook damage model was employed [3]. The Johnson-Cook constitutive model is one of the models used in the numerical simulations of processes with a high strain rate and a heavy plastic deformation and is expressed as:

$$\varepsilon^f = \left[D_1 + D_2 \exp D_3\sigma^*\right]\left[1 + D_4 \ln\dot{\varepsilon}^*\right]\left[1 + D_5 T^*\right] \quad (3)$$

where: ε^f - equivalent strain to fracture; $\sigma^* = \frac{\sigma_m}{\bar{\sigma}}$ - the dimensionless pressure-stress ratio; σ_m - the average of the three normal stresses; $\bar{\sigma}$ - von Mises equivalent stress; $\dot{\varepsilon}^* = \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}$ - dimensionless strain rate $\dot{\varepsilon}_0 = 1{,}0 s^{-1}$ - reference strain rate $T^* = \frac{T - T_{ROOM}}{T_{MELT} - T_{ROOM}}$ - homologous temperature

D_1, D_2, D_3, D_4, D_5 - material constants taken from [3]. Equation (3) takes into consideration the strain to fracture dependence of stress state, strain rate and temperature. The strain to fracture decreases as the mean stress, σ_m, increases. However, at this stage of the work, fracture criteria and its parameters were not analysed and its usage was only limited to terminate the simulation when fracture occurs.

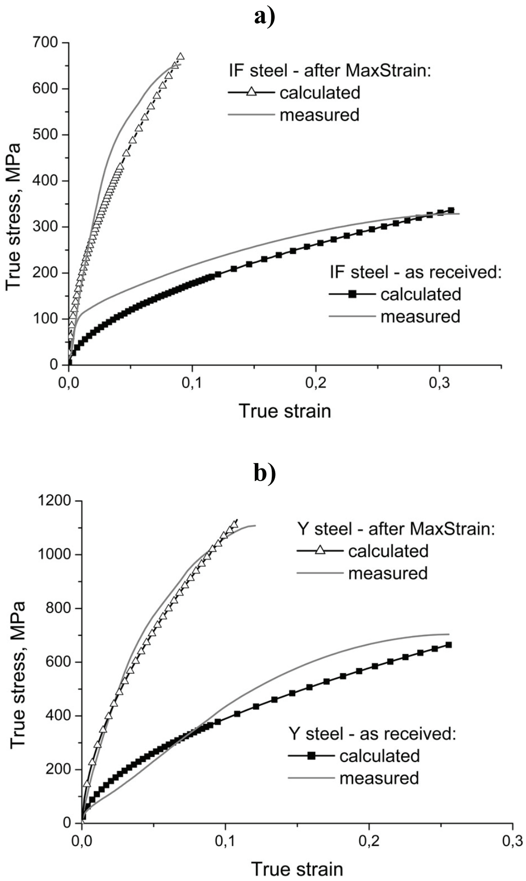

Fig. 4. Comparison of calculated and measured tensile curves for IF steel (a), and Y steel (b).

Figure 4 summarizes the results of the strain-stress curves calculation using the modified KHL model (equation (2)) compared with the experimental results. The good convergence of the model can be observed for both materials. In figure 5, values of the rate of work hardening vs. true strain calculated in Abaqus Explicit were plotted and compared with experimental data. As it was already mentioned, basing on a true stress-true strain curve and using criteria of plastic instability, there is an opportunity to determine, in unequivocal way, the field of the uniform elongation by Considére criterion.

Uniform plastic deformation occurs as long as the true stress is below the value of work hardening rate ($\frac{d\sigma}{d\varepsilon} < \sigma$). When these quantities are equal, the

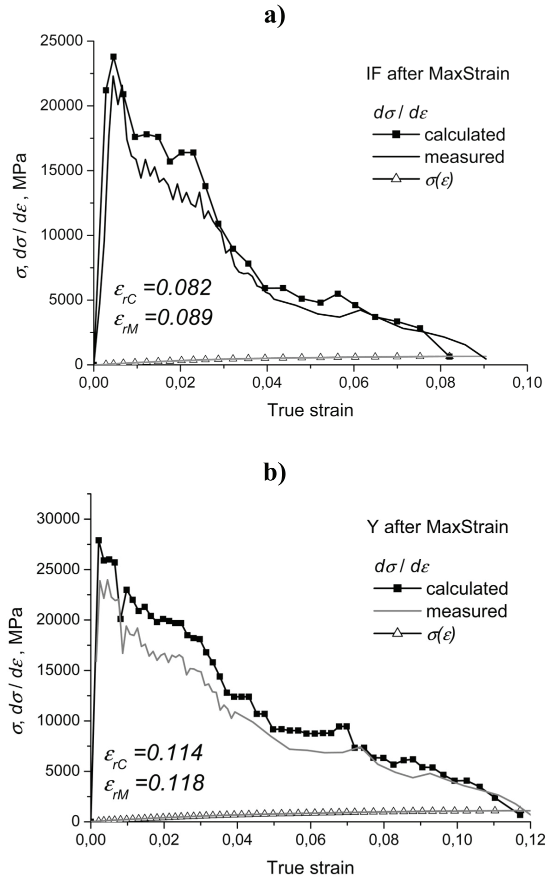

Fig. 5. Comparison of calculated and measured uniform elongations after MaxStrain deformation; IF steel (a), and Y steel (b). ε_{rC} - calculated uniform elongation, ε_{rM} - measured.

uniform deformation stops and necking begins. Comparing measured and calculated values of the uniform elongation it can be noticed that values calculated in Abaqus are slightly lower from those, calculated from the tensile tests. In VUMAT, necking criterion calculations are based on the maximum principal values of stress and strain, $\sigma(1)$ and $\varepsilon(1)$, respectively. However, the corresponding curves, calculated from the real tensile tests are based on equivalent stress and equivalent stress (note: the cross sections of the specimens were rectangular).

Figure 6 shows the onset of necking in tensile test simulations for Y steel. Dark elements of the mesh represent the values of the rate of work hardening (that are below actual values of stress). These elements are related to the places in the material where onset of necking has just occurred. As it can be visible in the subsequent time steps, these regions are moving into the middle part of the specimen and concentrating there, what reflects the strain localization in the real tensile test.

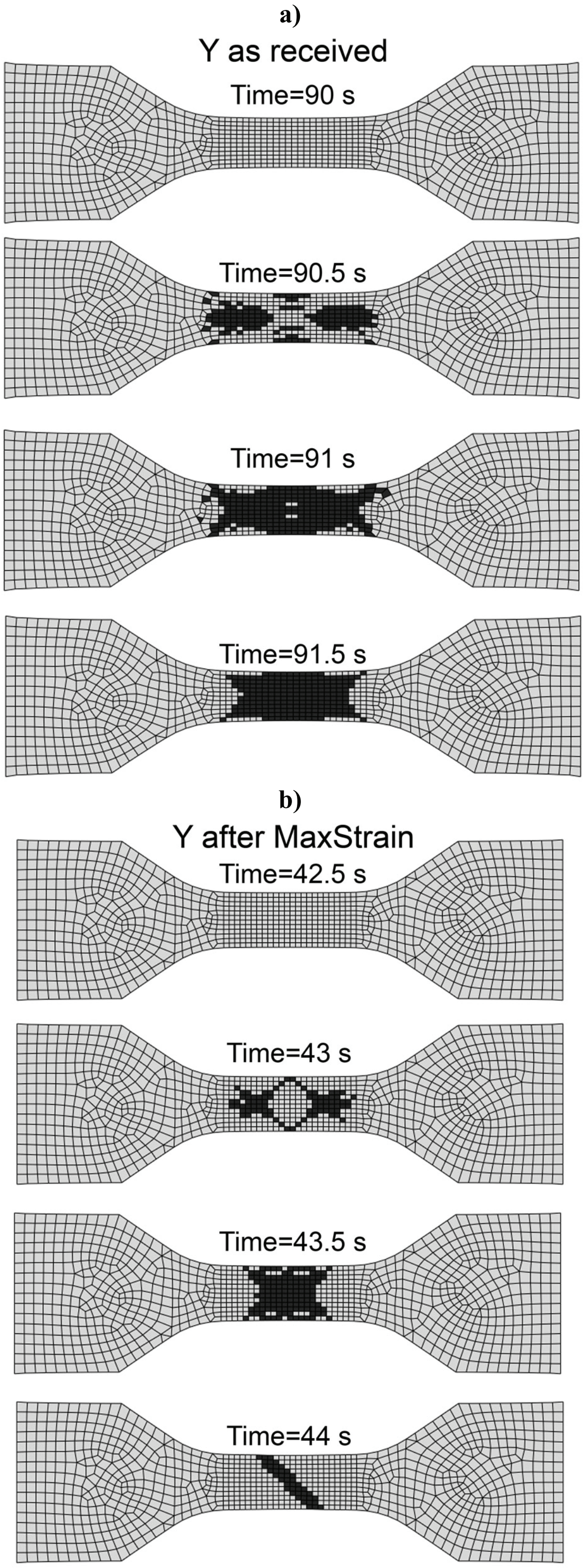

Fig. 6. *Fig. 6. An example of calculations showing onset of necking in subsequent simulation time steps (dark elements represent values of* $\frac{d\sigma}{d\varepsilon} < \sigma$ *) in Y steel: as received (a), and after MaxStrain deformation (b).*

5. CONCLUSIONS

It the present study, modified form of the KHL flow stress model was used together with plastic instability criterion in the computer modelling process of the mechanical response of UFG structures. Results of calculations show very good accuracy with data obtained from experiments. Therefore, it can be concluded that presented approach can be successfully used for the prediction of the mechanical response of the materials subjected to deformation process by the means of SPD, with high microstructural and mechanical inhomogeneity, where dislocation and substructure strengthening is significant. In the future work, our focus will be made on improvement and proper calibration of the Johnson-Cook damage model. This will give us a complex tool that will be able to model correctly both strength and ductility of UFG structures. Taking into account that ductility, strain rate and deformation mechanisms are strictly connected to each other, there is a possibility to improve the ductility in UFG materials by the proper use of their synergetic effect.

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WŁASNOŚCI MECHANICZNE MATERIAŁÓW ULTRADROBNOZIARNISTYCH WYTWORZONYCH TECHNIKĄ SPD – MOŻLIWOŚCI MODELOWANIA

Streszczenie

Modelowanie własności mechanicznych materiałów z wykorzystaniem symulacji komputerowej stwarza bardzo dobre narzędzie do ich optymalizacji. Wydaje się to być szczególnie istotne dla materiałów o strukturach silnie rozdrobnionych uzyskanych na drodze silnej akumulacji odkształcenia plastycznego (SPD). Materiały te charakteryzują się bardzo wysoką wytrzymałością. Ograniczeniem ich zastosowania w skali przemysłowej są jednak ich niskie własności plastyczne. Zrozumienie mechanizmów odkształcenia i umocnienia, działających w tych materiałach jest kluczowe dla poprawy ich własności plastycznych. Wykorzystanie w tym celu metody elementów skończonych wymaga poprawnie zdefiniowanego modelu reologicznego. W przypadku struktur silnie rozdrobnionych charakteryzujących się głównie dużą niejednorodnością mikrostruktury i własności mechanicznych, konieczne jest zaproponowanie nowych, bądź zmodyfikowanych modeli naprężenia uplastyczniającego.

Przedstawione badania dotyczą modelowania własności mechanicznych materiałów poddanych silnemu odkształceniu plastycznemu z wykorzystaniem systemu MaxStrain. Analizie poddano różne gatunki stali, a do reprezentacji ich własności mechanicznych wykorzystano zmodyfikowany model naprężenia uplastyczniającego Khan-Huang-Liang (KHL). Model ten został zaimplementowany do programu Abaqus Explicit (za pomocą procedury użytkownika VUMAT). Poddano dyskusji wpływ różnych warunków odkształcania na rozwój mikrostruktury oraz na końcowe własności mechaniczne materiału. Do oceny własności plastycznych w próbie rozciągania wykorzystano model oparty o kryterium niestabilności plastycznej (Considére). Porównanie wyników symulacji z wynikami z rzeczywistej próby rozciągania dało dobrą zgodność, co wskazuje, iż zaprezentowane rozwiązania mogą być z powodzeniem wykorzystane do oceny własności plastycznych materiałów ultradrobnoziarnistych wytworzonych techniką SPD.

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