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APPLICATION OF CRYSTAL PLASTICITY MODEL FOR SIMULATION OF POLYCRYSTALLINE ALUMINUM SAMPLE BEHAVIOR DURING PLAIN STRAIN COMPRESSION TEST

ZASTOSOWANIE MODELU PLASTYCZNOŚCI KRYSZTAŁU DO SYMULACJI ZACHOWANIA UMOCNIENIOWEGO POLIKRYSTALICZNEJ PRÓBKI ALUMINIOWEJ W PŁASKIM STANIE ODKSZTAŁCENIA

Capabilities of crystal plasticity finite element (CPFE) model in application to modeling polycrystalline aluminum sample behavior during plain strain compression test are discussed within the present work. To simplify analysis of material behavior during plain strain compression the aluminum specimen is composed of only three grains, both in experiment and numerical simulation. To reconstruct appropriate grains morphology a digital material representation (DMR) technique is used. The predicted/calculated values of loads and pole figures are compared with the experimental data. Calculated results remain in good agreement with experimental data what highlight predictive capabilities of the proposed approach in modeling material behavior under loading conditions. The conclusions regarding model capabilities and possible improvements during further work are also drawn in the paper.

Keywords: crystal plasticity, texture, microstructure, digital material representation

W artykule przedstawiono możliwości opisu zachowania umocnieniowego, polikrystalicznej próbki aluminiowej ściskanej w płaskim stanie odkształcenia, z wykorzystaniem modelu plastyczności kryształu i Metody Elementów Skończonych. Ściskana próbka składała się z trzech ziaren, co ułatwiło analizę jej zachowania umocnieniowego oraz weryfikację wyników numerycznych. Zastosowanie modelu plastyczności kryształów do symulacji zachowania odkształceniowego próbek polikrystalicznych wymaga odwzorowania rzeczywistej (mikro)struktury próbki, do czego wykorzystano koncepcję Cyfrowej Reprezentacji Materiału (DMR – ang. Digital Material Representation). Metoda DMR umożliwia rekonstrukcję morfologii oraz określenie początkowej orientacji ziaren w symulacji. Wyniki obliczeń w postaci figur biegunowych oraz naprężenia w funkcji odkształcenia zostały porównane z wynikami doświadczalnymi. Obliczone wyniki wykazują dobrą zgodność z doświadczeniem. W artykule omówiono wyniki porównania oraz przedstawiono wnioski głównie dotyczące kierunku udoskonalenia modelu w dalszej pracy.

1. Introduction

The influence of texture on material hardening and its anisotropic behavior in a wide range of deformation routes is a well known phenomenon [1-3]. Precise control of the texture development of formed polycrystalline metals allows obtaining desired mechanical properties and behavior of the final product. The Finite Element (FE) simulation of the crystallographic aspects of deformation gives the possibility to evaluate the influence of texture on mechanical behavior; however it requires proper material description, which takes into account texture development with incising deformation. Common approach to simulate texture development of polycrystalline materials by the FE method is to separately use model of material hardening and texture development. However, this method requires identification of parameters for two models and does not include direct influence of crystallites orientation on mechanical behavior.

That is why in this paper, to simulate texture development a fully coupled finite element crystal plasticity (CP) model was used. The model allows taking directly into account the influence of crystallite orientation on mechanical properties. However, precise simulation of polycrystalline material deformation with CP model requires explicit description of microstructure. That is why to create microstructure for the CPFE simulation purposes the digital material representation (DMR) method was used.

To analyze basic crystallographic relationships the investigated specimen was composed only from three grains. This simplifies the analysis of deformational behaviour of the polycrystalline material and allows for detailed evaluation of each grain behaviour and its mutual interactions. Such investigation would be impossible for the specimen composed from large number of grains.

The specimen was plain strain compressed at liquid nitrogen temperature. Initial and deformed orientation of crystal-

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lites was measured. During compression test the force and displacement data were recorded. These experimental data allow evaluating capability of the model to describe the microstructure influence on hardening behavior.

2. Experimental setup

In order to obtain the data for validation of numerical simulation, the plain strain compression test was carried out. As mentioned, the 99.998% pure aluminum was compressed at liquid nitrogen temperature. The specimen was cut from carefully chosen location and as a result it is composed of only three large grains. The specimen was cut from semi – continuous cast aluminum ingot. In the first step the long bars with rectangular cross-section (10 mm ×10 mm) were cut out. In subsequent steps the bars were preliminarily polished in order to reveal grain boundaries and finally location for final sample extraction was selected.

Prior the compression test the specimen was grinded on sand papers (grade from P800 to P2000) and polished on diamond paste (3, 6, 1 and 1/4 μm). Finally the sample was electrolytically polished with Struers A2 electrolite at 25V for 10 sec. After theses operations the specimen size was reduced by ca. 0.3 mm for each dimension.

Obtained specimen is presented in Figure 1a. The specimen is shown with visible grain boundary and marked orientation with respect to channel die directions (which corresponds to rolling directions: ED – elongation direction, TD – transverse direction, ND – normal direction). The sample co-ordinate system for channel-die test is presented in Fig. 1a. The grain boundaries on each side of the specimen were approximated by polynomial curves for further DMR microstructure reconstruction (Figure 1b).

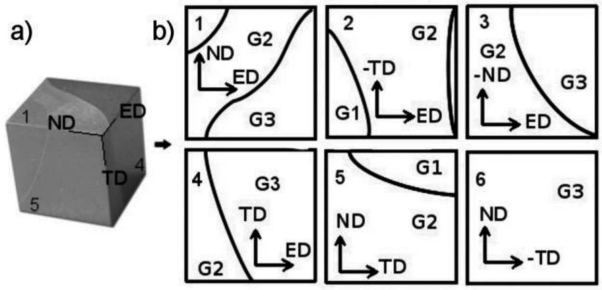

Fig. 1. a) The specimen composed of three grains prepared for compression test, b) grain boundaries schematically depicted for each side of the specimen

Initial orientation of each grain was measured by high resolution Scanning Electron Microscope (SEM) equipped with the electron backscattered diffraction (EBSD) detector. The local SEM/EBSD measurements allowed to verify if the grains are free from any kind of imperfections e.g. subgrains or domains. Examples of typically measured initial orientation of each grain are presented in Figure 2a. The measurements does not reveal sub-grains or domains in the grains.

The analyzed specimen was then compressed under plane strain condition at the Accredited Laboratory of Strength of Materials of Polish Academy of Sciences up to 20% of initial height. Magnitude of deformation rate was equal to 10^{-4} s^{-1}. During subsequent compression stages the force as function of displacement was measured (Figure 2b).

The analysis of deformed specimen was particularly focused on the local lattice rotations in order to obtain data for validation of model prediction. The pole figures that were measured by SEM/EBSD, provided data for analysis of local lattice rotation tendencies in each grain (Figure 2c).

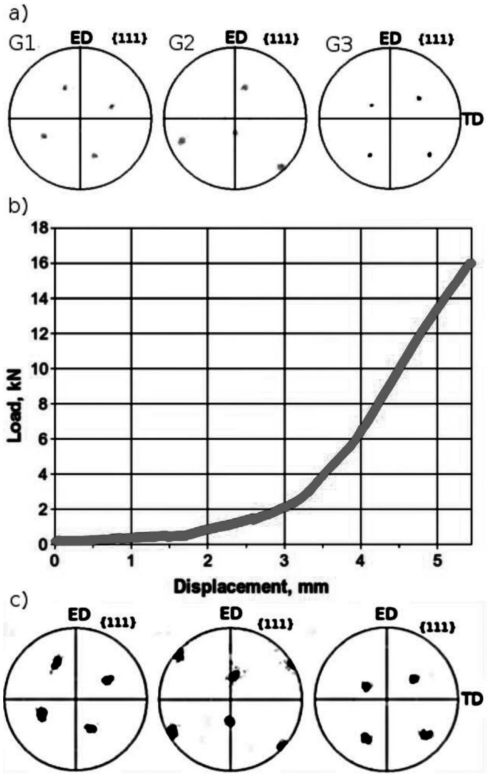

Fig. 2. a) Force vs. displacement as received during plain strain compression of the specimen. b) Measured by SEM/EBSD initial orientation of each grain. c) The orientation of each grain measured after the specimen deformation up to 20%

As seen after 20% of deformation in plain strain conditions the orientations remain stable with only minor scattering. Obtained grain morphology as well as initial crystallographic orientations were used as input data during creation of the 3d digital material representation. As DMR sample exactly replicates sample morphology numerically obtained pole figures can be directly validated with experimental results.

3. Numerical simulation – Digital Material Representation and Crystal Plasticity model

As mentioned in order to simulate behavior of the specimen composed of three grains its microstructure has to be accurately reconstructed. For microstructure reconstruction the concept of DMR was used. The main objective of this methodology is creation of the digital representation of microstructure with its features (e.g. grains, grain boundaries, etc.) explicitly visible during calculations.

The generation of material microstructure with specific properties is always one of the most important algorithmic parts of systems based on the DMR. Authors of this paper developed numerical grain growth algorithms for single and

two-phase microstructures with and without inclusions based on the cellular automata (CA) method [4]. The algorithm allows to recreate microstructures statistically as well as exactly – to precisely reflect specimen microstructure on the basis of experimental observations. A detailed review on the state of the art as well as authors contribution in this field can be found in earlier works [4,5].

Due to different crystallographic orientations of the grains in the investigated microstructure, stress or strain gradients can occur along grain boundaries as well as close to triple point junctions. To properly capture this behavior a non-uniform FE mesh that is refined along boundaries of mentioned microstructure features and coarse in the interior of these features have to be created. However, such meshes cannot be created automatically in available commercial FE codes. That is the reason why authors developed an in-house code for finite element non-uniform mesh generation called DMRmesh [6]. The FE mesh, reflecting morphology of the specimen presented in figure 1a, is shown in Figure 3. It has to be pointed out, that the grains morphology was recreated based only on information about grains boundary shape visible on sides of the specimen. The inverse cellular automata grain growth algorithm was applied in this case [7]. Unfortunately, due to lack of information about microstructure morphology from inside the sample this reconstruction approach may lead to inaccurate grains boundary approximation in the volume of specimen. Nevertheless, this was only non-destructive method of microstructure reconstruction, which provided a possibility of further sample deformation and investigation of its behavior during loading.

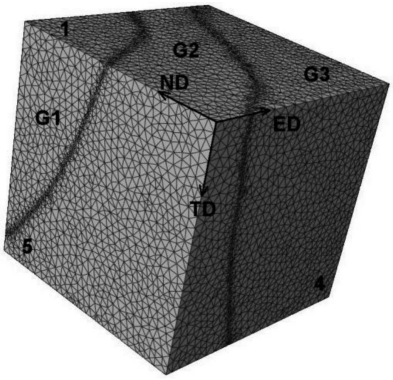

Fig. 3. The FE mesh reflecting morphology of grains of the real specimen. The mesh is finer on grain boundaries and coarser in bulk material

Based on the obtained morphology a FE mesh was generated and used for simulation of aluminum sample behavior during compression in plain strain conditions. The mesh was prepared to be compatible with commercial FE software Abaqus. To describe material behavior the CP model developed by Huang [8] was used. In order to reflect different hardening behavior of differently oriented grains appropriate initial orientations were assigned to each mesh element on the basis of experimental measurement (Figure 2a). Exactly the same orientations were assigned to the elements belonging to the same grain. Initial orientations used for the simulation purposes were as follows: grain G1 – (13 1 1) [-1 4 9], grain G2 – (5 6 -2)[0 1 3] and grain G3 – (1 3 1)[13 -4 -1].

Application of the CP model for material behavior description allows taking into consideration the contribution of each slip system to the global deformation and lattice rotation. In the model, the plastic deformation occurs due to crystallographic dislocation slip. Deformation by diffusion, twinning and grain boundary sliding is not taken into account in the present model. The slip phenomenon on a slip system occurs solely due to acting of the resolved shear stress on this particular system.

The crystalline slip in the model is assumed to follow the Schmid's law. This implies the slip rate $\dot{\gamma}^{(\alpha)}$ on any slip system depends only on the Schmid stress ($\tau^{(\alpha)}$). The Schmid stress depends on the current stress state (σ) and the current lattice orientation ($\boldsymbol{s}^{*(\alpha)}$, $\boldsymbol{m}^{*(\alpha)}$):

$$\tau^{(\alpha)} = m^{*(\alpha)} \cdot \sigma \cdot s^{*(\alpha)} \tag{1}$$

The amount of shear on a slip system $\dot{\gamma}^{(\alpha)}$ is calculated based on the Schmid's law. For rate-dependent crystallite, it is determined by means of the following equation (2):

$$\dot{\gamma} = \dot{a}^{(\alpha)} \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right|^{n-1} \tag{2}$$

where: $\dot{a}^{(\alpha)}$ is the reference strain rate on slip system α, is the current strength for slip system α and it is described by equation (3),

$$\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^{(\beta)} \tag{3}$$

where: is the matrix of hardening modules. It describes the self-hardening and latent hardening of slip systems. The self-hardening module is given by equation (4):

$$h_{\alpha\alpha} = h(\gamma) = h_0 \sec h^2 \left| \frac{h_o \gamma}{\tau_s - \tau_o} \right| \tag{4}$$

The latent module is related to the self-hardening module by coefficient q:

$$h_{\alpha\beta} = q h(\gamma), \quad \alpha \neq \beta \tag{5}$$

The hardening calculated by equations (4)-(5), decreases with progressive deformation. This kind of hardening description does not take into account first stage of crystallite deformation (easy glide). In case of aluminum specimen, where the easy glide is observed during compression this may lead to some discrepancies in the flow stress prediction and experimental results at early stages of deformation. The 'easy glide' stage is observed for displacement between 1.5 and 3 mm in Figure 2b.

The models parameters were obtained using an inverse technique were goal function was defined as an error of obtained force in simulation with reference to force obtained from single crystal plain strain compression test [9]. A set of single crystals with various initial orientations were used during the identification procedure. Obtained major model parameters are shown in Table 1.

TABLE 1
Major CP model parameters identified by an inverse approach (the parameters description is commonly used and can be found in literature e.g. [1])

h_0	τ_s	τ_0	N	$\dot{a}$
45.5 Mpa	104.9 Mpa	12.1 Mpa	9.7	0.01 s^{-1}

It has to be pointed out that over one million finite elements were used in the model to properly reflect grain morphology. As a result the model required large quantities of computer memory and disk space to store the results. To run calculation a cluster of computers SGI Altix 3700 (baribal) located at Academic Computer Centre CYFRONET AGH was used.

4. Numerical simulation results

The main advantage of CP model combined with DMR approach is possibility of evaluation of local orientation changes, which directly influence the hardening behavior. This allows calculating flow curves for the material with specific microstructure. In this work for evaluation of the CP DMR model capabilities the calculated flow curves and pole figures were compared to experimental data. In Figure 4a comparison of strain-stress curves is presented. Larger discrepancies

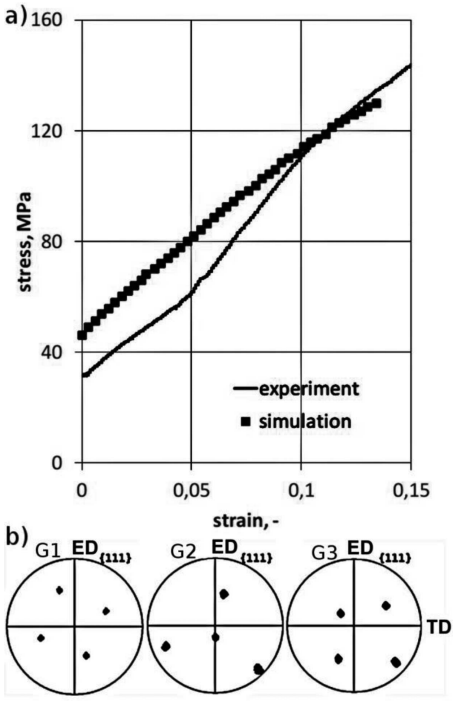

Fig. 4. Numerical calculation results: a) Calculated strain – stress curve reffered to experimental data; b) Calculated pole figures for grains G1, G2 and G3

between experimental and calculated stresses are observed at the beginning of the flow curves. The discrepancies decrease with progressing deformation. Most probably, the discrepancies arise due to lack of 'easy glide' stage in hardening mechanism description. Inaccuracy of grain boundaries description in bulk material, may also contribute to these differences. However, the comparison of pole figures (Figure 4b and 4c) shows good correlation. This suggests that grain boundary and mechanism of lattice rotation is properly described and its contribution to the error is less then hardening mechanism description. This approach will be extended to modeling microstructure containing larger amount of grains within future research.

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5. Conclusions

The simulation results obtained from the proposed CP DMR model are in good agreement with experimental measurements, considering complexity of the mechanical behavior of the aluminum specimen. The digital material representation approach proved to be useful and efficient for simulation of microstructure deformation and texture development. The lattice rotation described by CP model is in good agreement with experimental data what proves that the model parameters were identified accurately and the model itself takes most important mechanisms of deformation into account. To improve stress curve prediction hardening model should be more elaborate. It should take into consideration 'easy glide' stage of deformation. This will be the subject of future research.

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