A simple dislocation model of the influence of high-angle boundaries on the deformation behavior of ultrafine-grained materials

W Blum\textsuperscript{1} and P Eisenlohr\textsuperscript{2}

\textsuperscript{1} Department of Materials Science and Engineering, Institute I: General Materials Properties, Martensstraße 5, 91058 Erlangen, Germany
\textsuperscript{2} Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Wolfgang.Blum@ww.uni-erlangen.de, p.eisenlohr@mpie.de

Abstract. The deformation resistance of ultrafine-grained (UFG) materials is modelled on the basis of the evolution of the average dislocation density with strain in the course of glide and recovery of dislocations. In contrast to materials with conventional grain size (CG), dislocations are stored and annihilated solely at the high-angle boundaries, where screw dislocations glide and edge dislocations climb towards annihilation sites. The high-angle boundaries enhance both the rates at which dislocations are stored and recovered. Depending on the spacing of high-angle boundaries, temperature and strain rate, UFG materials are softer or harder than their CG counterparts.

1. Introduction

In [1] a simple dislocation model was presented which describes the maximum deformation resistance of UFG and nanostructured materials. The model adapts classical dislocation theories of steady-state creep of CG materials at elevated temperatures to the case of UFG materials. UFG materials are defined here not on an absolute grain size scale, but on a microstructural basis as materials where the spacing $d$ of high-angle boundaries is so small that new low-angle boundaries do not form, implying that dislocations are no longer stored in the grain interior in the form of a subgrain structure, but at the high-angle boundaries limiting the mean free dislocation path. This means that the stored edge dislocations find a relatively easy exit from the material by grain boundary diffusion. Screw dislocations are relatively easily absorbed by gliding parallel to the boundaries to sinks (like triple junctions of grains); consequently steady-state deformation of UFG materials is directly linked with grain boundary sliding.

The steady-state deformation resistance was determined analytically in [1] by solving the condition of dynamic equilibrium, $\dot{\rho}^+ = \dot{\rho}^-$, for the average dislocation density $\rho$ and neglecting the thermal activation of glide by relating the flow stress $\sigma$ at given temperature $T$ and strain rate $\dot{\varepsilon}$ to the inverse of the average dislocation spacing $\delta \approx \rho^{-0.5}$ in the form $\sigma = \alpha' G b \sqrt{\rho}$ where $G$ is the shear modulus, $b$ is the Burgers vector length and $\alpha'$ is the dislocation interaction constant [1] for UFG materials.

In the present work, the model presented in [1] is extended by including the evolution of the dislocation structure during straining and the thermal activation of glide. The results are
compared to experimental data for UFG Cu produced by equal channel angular pressing (ECAP) [2] and nanocrystalline Ni produced by pulsed electro deposition (PED) [3].

2. The model

2.1. UFG materials

Most of the model equations for the UFG case have appeared in [1]. Here we describe their physical meaning.

The microstructural definition of UFG materials given above can be expressed as $\Lambda = 0.6d$ where $\Lambda$ is the mean free path of dislocations, in other words, $1/\Lambda$ is the dislocation length which is stored at the high-angle boundaries per slipped area. The rate at which dislocation length is stored per volume of UFG material with resolved shear strain $\gamma$ follows as $d\rho^{+}/d\gamma = 1/(b\Lambda)$.

Edge dislocations generate single-sided steps at the high-angle boundaries which are addressed in the literature as extrinsic grain boundary dislocations. They are annihilated by extrinsic grain boundary dislocations (steps) of opposite sign. The annihilation occurs either spontaneously when the spacing $d_{dip}$ of the dipole partners is less than a certain value $d_{spon,b}$ or, else, by climb along the high-angle boundaries with the aid of grain boundary diffusion, which is assumed to be driven by the self stresses of edge dipoles. Spontaneous annihilation simply reduces the rate of dislocation storage by the factor $1 - d_{spon,b}/d_{dip}$ and thereby sets a low-temperature limit to the dislocation density which can be stored in the material. Climb yields the rate of loss of edge dislocations with time, $\dot{\rho}_{\text{climb}}$.

The net rate of change of $\rho$ in UFG materials results as the difference of storage and recovery rates, $\dot{\rho} = (d\rho^{+}/d\gamma) (1 - d_{spon,b}/d_{dip}) \dot{\gamma} - \dot{\rho}_{\text{climb}}$, where $\dot{\gamma}$ is the resolved shear.

Several numerical parameters were introduced [1] which quantify the relative contribution of a given slip system to the total strain, the fractions of dislocations which are stored directly at the boundaries and in front of them inside the grain, the relative factor of relaxation of the stress field when an edge dislocation reaches a high-angle boundary and the fraction of dislocations at the boundaries which find a dipole partner there. These factors were used to fit the model to the experimental results [1].

The generation and glide of dislocations are supported by thermal activation. The rate $\dot{\gamma}$ of thermally activated glide is expressed as the density of gliding dislocations, set to be a fraction $f_{\text{mob}} \approx 10^{-3}$ of the dislocations inside the grains, and the velocity of glide formulated according to [4]. The parameters of the thermal obstacles were chosen such that the flow stress is diminished by less than 20% compared to the maximum shear stress $\dot{\tau}$ which the dislocation obstacles can withstand. This means that the dependence of the flow stress on temperature $T$ and strain rate $\dot{\gamma}$ is mainly controlled by recovery, not by glide of dislocations as proposed for instance in [1].

With these expressions the evolution of the deformation resistance from yielding to the steady state can be modelled by integrating the set of ordinary differential equations for $\rho$ (structure evolution) and $\dot{\gamma}$ (glide).

2.2. CG materials

For the sake of comparison with the UFG case a simple model of deformation of CG materials was also set up. It uses expressions for thermally activated glide and for dipole capture and spontaneous as well as climb-controlled annihilation of edge dislocations similar to the ones in [5]. The model parameters were adjusted with the only aim to bring the model into reasonable agreement with the behavior of CG Cu which, in the temperature and stress range considered, is characterized by an exponential stress dependence of the steady-state deformation rate (so-called power law breakdown behavior), but is not well documented by experimental results.
3. Results and discussion

Fig. 1 shows examples of the modelled evolution of the deformation resistance of pure UFG Cu produced by severe plastic deformation (i.e., with initial high-angle boundary spacing $d = 0.35 \, \mu m$). It is postulated that $d$ increases in the course of coarsening of the subgrain structure towards the stress-dependent steady-state value (see [2]). The deformation resistance quickly attains a maximum and declines with further straining. The agreement with experimental curves (grey) is good.

The steady-state deformation resistance of UFG Cu is given in Fig. 2 for constant $d$; this corresponds to the maximum of the deformation resistance where the effect of subgrain coarsening is still negligible. When the stress becomes higher than indicated by the vertical dashed line, the steady-state subgrain size $14 b G / \sigma$ becomes smaller than $d$. This means that subgrains can form in the grains so that the UFG behavior is expected to break down. For the nanostructured Cu with $d$ of 0.1 $\mu m$ no such breakdown is predicted implying that the UFG behavior should prevail. It is seen that for the lower two temperatures the UFG Cu is stronger than the CG material. In the UFG Cu with $d = 1 \, \mu m$ a transition to CG behavior is predicted.

**Figure 1.** Evolution of flow stress $\sigma$ and high-angle boundary spacing $d$ with strain $\epsilon$ for UFG Cu (black lines: model, grey lines: experiment).

**Figure 2.** Steady-state deformation resistance at 600, 500, 400, and 300 K (in sequence from light grey to black, i.e., left to right) for $d = 0.1$ and $1.0 \, \mu m$ for UFG (lines with symbols) and CG Cu.
as indicated by the heavy S-shaped connecting line for 400 K. The UFG material is softer than the CG material due to the faster recovery at high-angle boundaries compared to recovery in the grain interior.

![Comparison of modelled steady-state deformation resistance with experimental data from [2, 3]; left: UFG Cu with initial $d = 0.35 \mu m$ without (blue) and with (red) $d$-evolution during subgrain coarsening, right: nanocrystalline PED Ni with $d = 90$ (red) and 50 nm (blue). Note difference in $T$-normalization; $k_B$ and $R$ are Boltzmann constant and gas constant, respectively.](image)

**Figure 3.** Comparison of modelled steady-state deformation resistance with experimental data from [2, 3]; left: UFG Cu with initial $d = 0.35 \mu m$ without (blue) and with (red) $d$-evolution during subgrain coarsening, right: nanocrystalline PED Ni with $d = 90$ (red) and 50 nm (blue). Note difference in $T$-normalization; $k_B$ and $R$ are Boltzmann constant and gas constant, respectively.

Fig. 3 shows the steady-state deformation resistance of UFG Cu prepared by ECAP and nanostructured Ni prepared by pulsed electro deposition. At constant $d$ the modelled curves for UFG Cu (blue lines, left) are in reasonable agreement with the data for the measured maximum deformation resistance (open circles). When subgrain coarsening is included, the model results (red lines, left) are consistent with the experimentally observed softening during strain-induced subgrain coarsening up to the steady state (black symbols). For nanostructured Ni the maxima of the modelled deformation resistance are consistent with the experimental data, at least up to the point where the spacing $s_b$ of extrinsic edge dislocations at high-angle boundaries is less than the boundary spacing $d$. The influence of $d$ is captured by the model.

4. Concluding remark

The present work confirms that the simple dislocation model proposed in [1] is capable of describing the behavior of UFG metals. This means that the deformation resistance and its strain rate sensitivity can be understood in terms of dislocation recovery at high-angle boundaries occurring after thermally activated glide through the grain interiors.

References

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