Experiments and Simulations on the micromechanics of single- and polycrystalline metals

A. Ma, F. Roters, D. Raabe

Abstract. Crystallographic slip, i.e. movement of dislocations on distinct slip planes, is the main source of plastic deformation of most metals. The Crystal Plasticity FEM combines this basic process with the Finite Element Method by assuming that the plastic velocity gradient is composed out of the shear contributions of all slip systems. To apply the method to forming simulation of “real” parts suffered from the fact, that a huge number of single orientations is needed to approximate the crystallographic texture of such parts. This problem was recently solved by the introduction of the Texture Component Crystal Plasticity FEM (TCCP-FEM), which uses orientation distributions (texture components) for the texture approximation instead of single orientations. Excellent agreement of experiments and numerical simulations for different forming operations has shown the feasibility of this idea. Most crystal plasticity codes use simple empirical constitutive equations. However, as crystal plasticity is build on dislocation movement it was an obvious idea to introduce a constitutive model based on dislocation densities (internal state variables) instead of strain (external variable) into the crystal plasticity.

The dislocation model used is based on five main ingredients: 1) For every slip system mobile and immobile dislocations are distinguished. 2) A scaling relation between mobile and immobile dislocations is derived. 3) The immobile dislocations are divided into parallel and forest dislocations for every slip system. 4) The Orowan equation is used as kinetic equation. 5) Rate equations for the immobile dislocation densities are formulated based on distinct dislocation processes, e.g. lock formation or annihilation by dislocation climb.

For a wide range of temperature and strain rate the constitutive behavior of single and polycrystals is studied and simulation results are checked by comparison with experiments.

Keywords: texture components, dislocation density, crystal plasticity, anisotropy

INTRODUCTION

Crystalline engineering materials mostly occur in polycrystalline form, where each grain has a different crystallographic orientation, shape, and volume fraction. The distribution of the grain orientations is referred to as the crystallographic texture. The discrete nature of crystallographic slips along certain lattice directions on preferred crystallographic planes together with the occurrence of pronounced textures with certain preferred orientations entail an overall highly anisotropic plastic response of such polycrystalline samples under mechanical loads.

In order to simulate the mechanical property of crystalline aggregates, on the one hand the initial crystallographic information should be mapped into the finite element mesh by some way such as defining certain proper internal variables, on the other hand the constitutive laws for single crystals should be understood well.

Recently the so called Texture Component Crystal Plasticity Finite Element Method has been introduced by Raabe and Roters [1] which is basically a combination of a crystal plasticity FEM with a texture component method for the representation of initial statistical texture. In general the initial texture information is derived through analysis of huge discrete orientation data measured by tools such as the EBSD in one or two dimensions using a small lateral resolution, alternatively one can get the orientation distribution function in Euler space by X-ray diffraction. In a first step the experimental texture information is fitted by texture components which represent spherical Gaussian distributions specified by mean orientations with a scatter and volume fractions or intensities. Secondly the spherical Gaussian texture components are mapped onto the integration points of a finite element mesh to give initial orientations for every Gauss point [2].

Most crystal plasticity codes use simple empirical constitutive equations. However, as crystal plasticity is build on dislocation movement it was an obvious idea to introduce a constitutive model based on dislocation densities into the crystal plasticity.

On the one hand, since plastic deformation of metals and alloys at room temperature is mainly the result of dislocation slip on certain slip system, based on the Orowan equation the deformation mechanism of the single crystal has been well constructed, although in the majority of
The plastic flow is described by a simple power law. On the other hand it is the complex structure of the dislocations that causes it to be very difficult to describe the hardening rule. In many models the hardening behavior of commercial alloys is represented in terms of another power law of strain and strain rate empirically. Optimized hardening laws should depend on microstructural state variables such as dislocation densities rather than the macroscopic quantities such as the accumulated plastic deformation.

The evolution law for a dislocation density is governed by balance equations involving production and annihilation rate terms, which are all determined by dislocation interactions in a basically anisotropic way. The production rate for immobile dislocations is connected with the lock and dipole forming mechanisms, while the annihilation rate is always based on the thermal activated cross slip of the screw dislocation and climb of the edge dislocation [3, 4]. This means the hardening law based on the dislocation evolution has a clear physical background and strain rate can be introduced more naturally as compared with phenomenological hardening models.

The dislocation structures are much more complex than a scalar dislocation density for every slip system [5]. Similar as in the concept of Roters [3] the interaction of dislocations with the microstructure can be expressed as: dislocation sources inside the single crystal generate mobile dislocations, at the same time a certain part of mobile dislocations change to immobile ones and certain parts annihilate; those immobile dislocations are stored in the cell blocks (CBs) and dense dislocation walls (DDWs) according to different manners: that is the dislocation locks are stored in CBs and DDWs, while the dislocation dipoles are stored only in DDWs; the applied stresses cause the mobile dislocations to run across the CBs and DDWs to accommodate the plastic deformation.

In this paper the crystal plasticity is studied based on the dislocation density and the following notations are used to describe the dislocation microstructure:

- $M$ — the mobile dislocation density
- $I$ — the immobile dislocation density
- $F$ — the forest dislocation density
- $P$ — the parallel dislocation density
- $\alpha, \beta$ — different slip systems

**THE CONSTITUTIVE EQUATIONS**

**The kinematics**

The velocity gradient tensor $L = F F^{-1}$ is used to express the loading process. For large deformation we have the multiplicative decomposition of the deformation gradient $F$ tensor

$$F = F_e F_p$$

where $F_e$ is the elastic part comprising the stretch and rotation of the lattice, and $F_p$ corresponds to the plastic deformation caused by the slip of dislocations. Two rate equations can be derived for the two different mechanisms

$$\dot{F}_e = L F_e - F_e L_p$$

$$\dot{F}_p = L_p F_p$$

where $L_p$ is the plastic velocity gradient defined in the stress free intermediate configuration.

**The elastic law**

The Cauchy stress $T$ is the stress measure in the current configuration

$$T = \frac{1}{J} F_e \tilde{K} \left[ \frac{1}{2} (F^T_e F_e - I) \right] F_e^T$$

with

$$\tilde{J} = \text{det}(F) = \text{det}(F_e)$$

where the fourth order tensor $\tilde{K}$ is the elasticity tensor with respect to the undistorted configuration, and isochoric deformations are assumed.

**The flow rule**

In the case of crystal plasticity the dislocation can only slide on certain slip systems and the following constitutive assumption is often used to connect the phenomenological variable and the physical phenomena

$$L_p = \sum_{\alpha=1}^{N} \gamma_\alpha \bar{M}_\alpha$$

where $\bar{M}_\alpha = \bar{d}_\alpha \otimes \bar{n}_\alpha$ is the Schmid tensor for the slip system $\alpha$ where $\bar{d}_\alpha$ expresses the slip direction and $\bar{n}_\alpha$ the slip plane normal with respect to the undistorted configuration. $N$ is the total number of slip systems, for the FCC crystal, there are 12 octahedral slip systems, so $N = 12$.

From the Orowan equation the plastic shear rate $\gamma_\alpha$ of one slip system $\alpha$ is a function of the mobile dislocation density and the average slip velocity of dislocation lines

$$\gamma_\alpha = \rho_{Ma} a v_\alpha.$$
and the forest dislocation density $\rho_{Fa}$ for slip system $\alpha$ as [6]

$$\rho_{Fa} = \sum_{\beta=1}^{N} \rho_{\beta} \left| \cos(\bar{n}_{\alpha} \cdot \tilde{n}_{\beta} \times \tilde{d}_{\beta}) \right|$$

(8)

$$\rho_{Fa} = \sum_{\beta=1}^{N} \rho_{\beta} \left| \sin(\bar{n}_{\alpha} \cdot \tilde{n}_{\beta} \times \tilde{d}_{\beta}) \right|.$$  

(9)

Based on the framework of thermally activated dislocation motion and for the reason of simplicity neglecting the backward jumps of the dislocation, the average velocity $v_{\alpha}$ reads

$$v_{\alpha} = \frac{1}{2} \lambda_{\alpha} \nu_{0} \exp \left( -\frac{Q_{\text{slip}}}{K_{B} T} \right) \exp \left( \frac{|\tau_{\alpha}| - \tau_{\text{pass}}^{\alpha}}{K_{B} T} V_{\alpha}^{C} \right).$$

(10)

with

$$\tau_{\alpha} \equiv \bar{K} \left[ \frac{1}{2} (F_{c}^{C} F_{c} - 1) \right] \cdot \tilde{M}_{\alpha}$$

(11)

and

$$\tau_{\text{pass}}^{\alpha} = c_{1} G b \sqrt{\rho_{Fa} + \rho_{Ma}}$$

(12)

where $c_{1}$ is a constant, $G$ the shear modulus, $b$ the magnitude of the Burges vector, $\theta$ the temperature, $K_{B}$ the Boltzmann constant, $\nu_{0}$ the attack frequency and $Q_{\text{slip}}$ the effective activation energy. $\tau_{\alpha}$ and $\tau_{\text{pass}}^{\alpha}$ are the external driving force and the athermal resistance or the passing stress for the mobile dislocations. The jump width $\lambda_{\alpha}$ and the activation volume $V_{\alpha}^{C}$ can be calculated as functions of $\rho_{Fa}$ as

$$\lambda_{\alpha} = \frac{c_{2}}{\sqrt{\rho_{Fa}}}$$

(13)

and

$$V_{\alpha}^{C} = c_{3} b^{2} \lambda_{\alpha}$$

(14)

where $c_{2}$ and $c_{3}$ are constants.

### THE REDUCTION OF THE DISLOCATION STRUCTURE

For the mobile dislocation density there is no simple model to describe its evolution. This difficulty arises from the fact that both the number of the mobile dislocation and the sliding velocity effect the plastic deformation. Fixing one one can accommodate the external plastic deformation by changing the other, but in general both quantities will change at the same time. This makes it very difficult to get a proper production term for the evolution law without any additional assumption. An new idea has been presented in [7] to circumvent those above mentioned difficulties. In this concept it is assumed, that although there are many ways for the dislocation structure to evolve, the proper one should satisfy that the given external stress generates the maximum plastic deformation or the given plastic deformation rate causes minimum external stress. This is fulfilled if

$$\frac{\partial \tau_{a}}{\partial \rho_{Ma}} d \rho_{Ma} + \frac{\partial \tau_{a}}{\partial \rho_{Pa}} d \rho_{Pa} + \frac{\partial \tau_{a}}{\partial \rho_{Fa}} d \rho_{Fa} = 0.$$  

(15)

As the parallel dislocation density $\rho_{Pa}$ and the forest dislocation density $\rho_{Fa}$ have their independent evolution laws, the criteria changes to

$$\frac{\partial \tau_{a}}{\partial \rho_{Ma}} \rho_{Ma} \rho_{Fa} = 0.$$  

(16)

This constraint condition gives the control equation for the mobile dislocation

$$\rho_{Ma}^{2} - 4A^{2} \rho_{Fa} \rho_{Ma} - 4A^{2} \rho_{Fa} \rho_{Pa} = 0.$$  

(17)

with the parameter

$$A = \frac{K_{B} \theta}{c_{1} c_{2} c_{3} G b \Gamma}.$$  

(18)

Solving (17) and knowing that $\rho_{Ma} > 0$ we get

$$\rho_{Ma} = 2A^{2} \rho_{Fa} + 2A \sqrt{A^{2} \rho_{Fa}^{2} + \rho_{Pa} \rho_{Fa}}.$$  

(19)

If we take the the parameters $K_{B} = 1.38 \times 10^{-23}$ J K$^{-1}$, $0.1 \leq c_{1} \leq 0.5$, $20 \leq c_{2} \leq 100$, $3 \leq c_{3} \leq 10$ and material data $(b, G)$ for aluminium, the parameter $A$ is in the range of $[10^{-5}, 10^{-3}]$ for temperatures between room temperature and 723K. So it is convenient to simplify equation (19) as

$$\rho_{Ma} \approx B \sqrt{\rho_{Pa} \rho_{Fa}}.$$  

(20)

with another constant

$$B = \frac{2K_{B}}{c_{1} c_{2} c_{3} G b \Gamma}.$$  

(21)

This means the mobile dislocation density is proportional to the geometric mean of the parallel one and the forest one, and has a linear relationship with the temperature. So it is an intrinsic constraint equation for the dislocation structure. One can easily see that the dislocation structure with two kinds of internal variable ($\rho_{Ma}, \rho_{Pa}, \alpha = 1, N$) has been reduced to one with only one kind of internal variable ($\rho_{Pa}, \alpha = 1, N$). Using the same principle for a composite dislocation structure one can get

$$\rho_{Ma} \approx B \theta \sqrt{f_{W} \rho_{Pa} \rho_{Fa}^{W} + f_{W} \rho_{Pa}^{W} \rho_{Fa}^{W}}.$$  

(22)

where the volume fractions $f_{a}$ and $f_{w}$ satisfy $f_{b} + f_{w} = 1$. An important proerty of equation (22) is that for either $f_{b} = 0$ or $f_{w} = 0$ equation (20) is recovered.

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1. In fact they are functions of $\rho_{i}$, see equation (8).
2. Remember once again that $\rho_{F}$ and $\rho_{P}$ are functions of $\rho_{i}$ (eq. (8)).
DISLOCATION DENSITY EVOLUTIONS

The immobile dislocation density for CBs

There are three processes influencing the change of the immobile dislocation density for CBs. The first one is the formation of dislocation locks which are mainly caused by the interaction of mobile dislocations and forest dislocations. For the quasi-stationary load case the mobile dislocation density can be treated as a constant for every time step during the loading history and a mobile dislocation is immobilized after moving an average distance. This means, the lock forming rate will be approximated by the immobilization rate of mobile dislocations. At last the increasing rate for the immobile dislocation density reads

$$\dot{\rho}_{I_{1a}}^{B} = c_4 \sqrt{\rho_{F\alpha}^B \gamma_a}. \quad (23)$$

with a constant $c_4$. The second process is the interaction of mobile dislocations and immobile dislocations. We assume this interaction mechanism will cause a decrease of the immobile dislocation density. This mechanism is very important for low temperature when the probabilities of thermal activated cross slip of screw dislocations and climb of edge dislocations are very small. The non thermal pair annihilation rate reads

$$\dot{\rho}_{I_{1a}}^{B} = -c_5 \rho_{I_{1a}}^B \gamma_a. \quad (24)$$

with a fitting constant $c_5$. The last process is the thermally activated pair annihilation mechanism. For elevated temperatures the pair annihilation caused by the climb of edge dislocations becomes most important. The climb of edge dislocation is controlled mainly through the lattice diffusion and the core diffusion mechanisms. In general the climb motion of edge dislocation is based on the viscous motion of vacancies

$$v_{\text{climb}} = \frac{DS}{K_B \theta} \tau. \quad (25)$$

with $D$ the diffusion coefficient and $S$ the activation area. The direct result of this assumption for the description of time dependent deformations such as the creep is $\dot{\gamma} \propto \tau^3$. For pure materials such as single crystals of Al and LiF this linear rule gives a big deviation from the experimental results, and a relation around $\dot{\gamma} \propto \tau^5$ is always observed [8]. Till now there is no generally accepted theory to naturally account for exponents larger than 3 according to [9]. This implies we should modify equation (25) to a nonlinear shape for the dislocation motion

$$v_{\text{climb}} \propto \frac{DS}{K_B \theta} \tau \gamma_a^8. \quad (26)$$

Finally we can get the new pair annihilation equation for edge dislocations

$$\dot{\rho}_{I_{1a}}^{B^-} = -c_6 \exp \left( \frac{Q_{\text{bulk}}}{K_B \theta} \right) \left| \frac{\tau_a^B}{\gamma_a} \right| \left( \rho_{I_{1a}}^B \right)^2 \gamma^s. \quad (27)$$

where $Q_{\text{bulk}}$ is the effective activation energy for dislocation climb and $\tau_a^B$ the external driving force acting on CBs, and $c_6$ and $c_8$ are two fitting parameters. Finally the complete rate equation for the immobile dislocations in CBs reads

$$\dot{\rho}_{I_{1a}}^B = \dot{\rho}_{I_{1a}}^{B^+} + \dot{\rho}_{I_{1a}}^{B^-} + \dot{\rho}_{I_{1a}}^{B^\omega}. \quad (28)$$

The immobile dislocation density for DDWs

The immobile dislocations in the DDWs will also undergo the three evolution processes for the CBs. Meanwhile one additional mechanism should be considered for DDWs. According to [3] dislocation dipoles are formed in the whole crystal but stored in the DDWs only, this is another increasing mechanism for the immobile dislocation density. So we find the rate equation

$$\dot{\rho}_{I_{2a}}^W = \dot{\rho}_{I_{2a}}^{W^+} + \dot{\rho}_{I_{1a}2}^{W^-} + \rho_{I_{1a}}^{W^-} + \dot{\rho}_{I_{1a}2}^{W^-}. \quad (29)$$

with

$$\dot{\rho}_{I_{1a}}^{W^+} = c_{7W} \rho_{I_{1a}}^W \gamma_a \quad (30)$$

$$\dot{\rho}_{I_{1a}}^{W^-} = -c_{5W} \rho_{I_{1a}}^W \gamma_a \quad (31)$$

$$\dot{\rho}_{I_{2a}}^{W^-} = -c_6 \left( \gamma_a \right) \exp \left( -\frac{Q_{\text{bulk}}}{R \theta} \right) \left| \frac{\tau_a^W}{\gamma_a} \right| \left( \rho_{I_{1a}}^W \right)^2 \gamma^s \quad (32)$$

where $c_7$ is another fitting parameter, $\tau_a^W$ the external driving force acting on the DDWs. The parameter $d_{\text{dipole}}$ is the critical distance for the formation of dipoles, which can be calculated as [3]

$$d_{\text{dipole}} = \frac{\sqrt{3Gb}}{16\pi(1-v)} \left( f_B |\tau_a^B| + f_W |\tau_a^W| \right)^{-1}. \quad (34)$$

CONSTRAINT FOR THE COMPOSITE DISLOCATION STRUCTURE

Indeed in our model the relation of CBs and DDWs looks like two parallel connected Maxwell models [9]. The constraint equations for the composite dislocation structure are

$$v_{\text{elastic}}^B + v_{\text{plastic}}^B = v_{\text{elastic}}^W + v_{\text{plastic}}^W \quad (35)$$

$$f_B \tau_B + f_W \tau_W = \tau \quad (36)$$
which should be satisfied for every slip system. Here we discuss the deformation load case, and consider that the elastic deformation is very small compared with the plastic one, therefore in this work equation (35) has been changed to

\[ \dot{\gamma}^B = \dot{\gamma}^W = \dot{\gamma} \] (37)

APPLICATION TO UNIAXIAL COMPRESSION OF ALUMINUM SINGLE CRYSTALS

Force controlled uniaxial compression experiments of 99.99% pure Al single crystals were performed. The compression axis was parallel to the \( \langle 110 \rangle \) direction of the single crystals. Tests where performed at three different force rates, e.g. 0.2 N/s, 2 N/s and 10 N/s, and at three different temperatures, e.g. 623K, 673K and 723K to obtain a total of nine stress strain curves [10]. For the force controlled uniaxial compression experiments, the resolved shear strain rate is not fixed. Nevertheless the simulations where performed at an average strain rate. The two volume fractions are set to \( f_C = 1 - f_W = 0.9 \).

Figures 1, 2 and 3 show the comparison of numerical results of our dislocation model and experimental stress strain curves for different strain rates and temperatures, and figure 4 shows a comparison of hardening rates for different loading cases. One can see, that both the strain rate and temperature dependencies have been catched by the dislocation model and the stage IV of the hardening rate has also been successfully simulated.

Figures 5, 6 show the evolution of different dislocation densities and stresses inside the CBs and DDWs. One can see, that the dislocation density in the DDWs saturates faster compared with the CBs, this is because all of the dislocation dipoles are stored in DDWs. At smaller stresses the hardening is controlled by the DDWs. This process will continue to the end of stage III. For larger
stresses the dislocation density of DDWs almost saturates, while that of CBs still increases, so the hardening is controlled by the CBs and stage IV appears. Furthermore the saturation of the dislocation density of the CBs implies the end of stage IV.

In Table 1 the fitting parameters used are listed. As the aluminum single crystals are well annealed before the experiments a very low initial dislocation density of $1 \times 10^8 \text{m}^{-2}$ is assumed for the immobile dislocation density of every slip system.

**REFERENCES**