FROM DISLOCATION JUNCTIONS TO THE THREE STAGES CURVE

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Summary The strain hardening matrix of fcc crystals can be obtained from crystallographic continuum models deriving from the Kocks-Mecking framework. DD simulations were used to compute the coefficients of the interaction matrix between slip systems. The resulting constitutive formulation is inserted into a numerical crystalline model using a FE code, which is used here to test single crystal behavior. As a result, parameter-free deformation curves can be obtained.

The strain hardening properties of fcc metals, from elementary intersection events between dislocations to the definition of a continuum constitutive formulation, have been investigated with the help of a mesoscopic simulation of Dislocation Dynamics (DD), the "Mixed" model. In this work, all the elementary mechanisms that contribute to strain hardening have been treated within an elastic framework. Indeed, contact reactions between dislocations are essentially governed by the minimization of elastic energy, as was recently confirmed by atomistic simulations.

In a first step, DD simulations were used for studying in detail the properties of individual junctions between dislocations. In a second step, the connection between elementary mechanisms and the hardening properties of bulk single crystals was achieved for the first time, and in a parameter-free manner [1]. To model plastic deformation, it is necessary to account for the activation of various slip systems and for their mutual interactions. In formal terms, these pair interactions are described by an interaction matrix, which, owing to the symmetries of the fcc lattice, contains only six independent coefficients. In continuum constitutive formulations, this matrix serves as a base for the definition of the hardening matrix. The computed values extracted from DD simulations are in good agreement with experimental measurements for five out of the six coefficients of the interaction matrix.

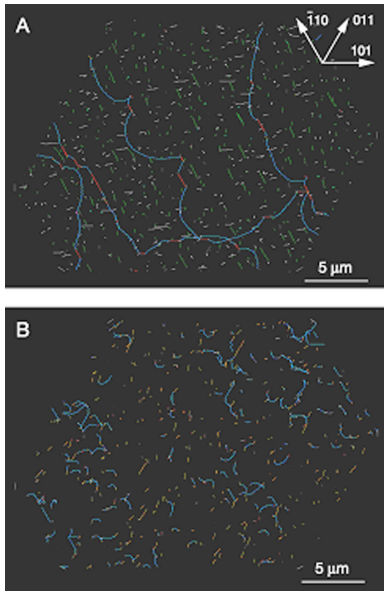

Figure 2 Non-coplanar interactions between slip systems. Dislocations (blue lines) of Burgers vector 1/2[011] glide in (11-1) slip planes and interact with randomly distributed forest segments 2 µm in length. The figures show (11-1) thin films of thickness 0.1 µm extracted from the simulations. (**A**) Formation of Lomer locks (straight red segments) through the interaction with a forest of 1/2[110](1-11) and1/2[-101](111) dislocations. (**B**) Collinear interaction with a forest of 1/2[011] dislocations gliding in the (11-1) cross-slip plane of the mobile dislocation.

The sixth coefficient, which has never been investigated theoretically, was considered up to now as leading to a weak or medium contribution to the flow stress. It is related to the so-called "collinear" interaction between dislocations of same Burgers vector gliding in two slip planes, each of thembeing the cross-slip plane of the other. Actually, our computations show that the collinear interaction is by far the strongest of all interactions [2]. Indeed, it results in an annihilation of the density of mobile dislocations and in the production of many debris characterized by a high remobilisation stress (Figure 1). This result has now been confirmed using different methods, including atomistic simulations that were carried out by D. Rodney (GPM2, Grenoble). It applies quite generally to all crystallographic structures, leading to the conclusion that all traditional models for strain hardening in single and polycrystals, as well as for the analysis of latent hardening tests, have to be revisited.

The strain hardening matrix of fcc crystals obtained by DD simulation is introduced in a continuum models deriving from the Kocks-Mecking framework. In this type of modeling, the internal variables are average dislocation densities per slip system $\rho^{(s)}$. The critical resolved shear stress on system (s) is related to the dislocation densities by:

$$\tau_c^{(s)} = \mu b \sqrt{\sum_u a^{(s)(u)} \rho^{(u)}}$$

The evolution of the dislocation density, based on Orowan's relation and an annihilation process of dislocation dipoles, is given by

$$\dot{\rho}^{(s)} = \frac{1}{b}\left(\frac{1}{L^{(s)}} - y_c \rho^{(s)}\right)\left|\dot{\gamma}^{(s)}\right|$$

where b is the magnitude of the Burgers vector, y_c a parameter proportional to the characteristic length associated with the annihilation process of dislocation dipoles and $L^{(s)}$ the mean free path of system (s). The mean-free path of the dislocations and their critical annihilation distance by cross-slip, can be estimated from various sources.

The resulting constitutive formulation is inserted into a numerical crystalline model using a FE code, which is used here to test single crystal behavior. The kinetics of large transformations, based upon the multiplicative decomposition of the deformation gradient into its elastic and plastic parts, is used. As a result, parameter-free deformation curves can be obtained for fcc crystals, which depend in a known manner on the nature of the material, the orientation of the crystal and temperature. This is illustrated by a comparison between aluminum and copper crystals initially oriented for easy glide at room temperature (Figure 2).

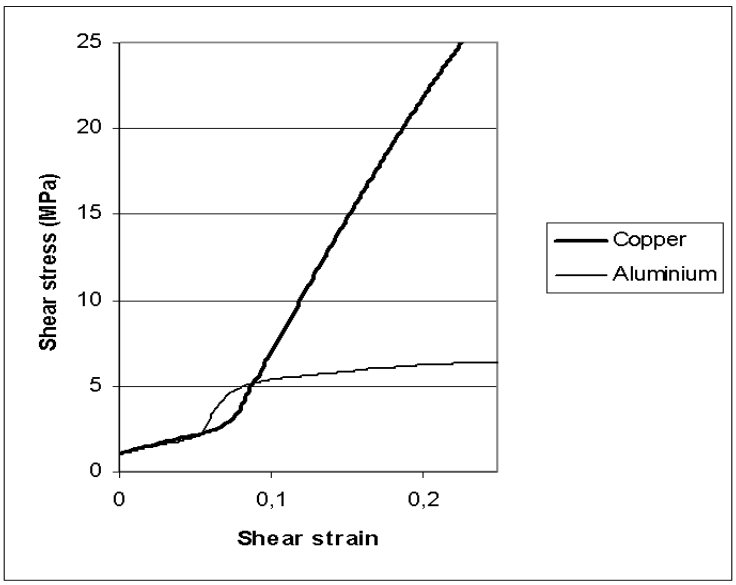

Figure 2 : Three stage curve obtained by finite element computation for aluminum and copper crystals initially oriented for easy glide at room temperature

Thus, although dislocation patterning is not accounted for, the traditional three-stage stress vs. strain behavior is fully recovered. The present results seem to indicate or confirm that, as long as there is no change in strain path, there is no need to account for dislocation patterning when modeling strain hardening properties up to the end of stage III. This statement raises a few interesting questions.

[1] R. Madec, B. Devincre and L.P. Kubin, Phys. Rev. Lett. ,. 89: 255508, 2002
[2] R. Madec, B. Devincre, L. Kubin, T. Hoc, and D. Rodney Science 301: 1879-1882