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Prediction of intergranular strains using a modified self-consistent elastoplastic approach

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A novel approach is adopted to describe the plasticity evolution and determine the active deformation systems with an elastoplastic self-consistent approach. A modified formulation of the crystal behaviour is proposed. This model is tested by simulating the development of intergranular strains during

uniaxial tension of MONEL-400 as well as commercial purity aluminium. Neutron diffraction measurements of the elastic strains are used as a reference. The results show the relevance of the model for fcc polycrystals.

1 Introduction Metal forming processes require knowledge of the evolution of the anisotropic elasto-plastic behaviour of the material during the deformation. Actually, the scale transition approach based on homogenisation techniques is currently used to predict the mechanical behaviour of metallic materials at the macro- and microscopic levels [1, 2].

For example, the rate independent incremental elastoplastic self-consistent model (EPSC) [3] has been successfully tested for texture development, monotonic loading and internal or residual stress predictions [4]. This approach considers the elastoplastic interaction between the grains which are regarded as ellipsoidal inclusions in an infinite homogeneous matrix with the overall effective polycrystal moduli. The crystallographic slip in fcc metals is the main mechanism for plastic deformation ($\{111\}\langle 110 \rangle$ slip system). For more details, refer to [3]. The main problem of this model is to determine which combination of slip systems will be really activated at each step of the plastic deformation path. In this case, all possible combinations of potentially active systems must be scanned. Running time considerations become the main task of the model. Moreover, this method can give several equivalent solutions for some hardening matrix [5]. Recently, Ben Zineb et al. [6] have proposed a new formulation to resolve the problem of ambiguous selection of slip systems and reduce

the running time computation. Their numerical results in the case of bcc single crystals present a good agreement with the ‘classic’ crystal plasticity. This approach seems promising but they were not, to the present authors’ knowledge, correlated with experimental results or implemented to a EPSC code. This work proposes to extend this formulation in the polycrystalline model framework and compare with the EPSC model. The accuracy of the simulations is evaluated by referring to mechanical experiments (tensile tests, neutron diffraction) [7, 8]. Even though a model can describe correctly the macroscopic behaviour, this does not provide verification of the model at a mesoscopic level. So the neutron diffraction has been used to validate the model at the grain level.

2 Model description The plastic flow can take place when the Schmid criterion is verified, i.e. slip occurs if the resolved shear stress τ^g on a system g is equal to the critical value τ_c^g depending on the hardening state of the slip system. A complementary condition which states that the increment of the resolved shear stress must be equal to the incremental rate of the critical resolved shear stress (CRSS) has to be verified simultaneously. In small strain formulation, one has

$$\tau^g = \mathbf{R}^g \cdot \boldsymbol{\sigma} = \tau_c^g \quad \text{and} \quad \dot{\tau}^g = \mathbf{R}^g \cdot \dot{\boldsymbol{\sigma}} = \dot{\tau}_c^g, \quad (1)$$

where $\mathbf{R}^g$ is the Schmid tensor on a system g . $\dots$ is the double scalar product. If $\dot{\gamma}^g$ denotes the slip rate on a system g , the Schmid criterion is thus given by

$$\tau^g < \tau_c^g \Rightarrow \dot{\gamma}^g = 0, \quad (2a)$$

$$\tau^g = \tau_c^g \quad \text{and} \quad \dot{\tau}^g < \dot{\tau}_c^g \Rightarrow \dot{\gamma}^g = 0, \quad (2b)$$

$$\tau^g = \tau_c^g \quad \text{and} \quad \dot{\tau}^g = \dot{\tau}_c^g \Rightarrow \dot{\gamma}^g > 0. \quad (2c)$$

The relations (2a), (2b) and (2c) can be expressed by the following equation:

$$\dot{\gamma}^g = M^g \dot{\tau}^g. \quad (3)$$

The slip rate is linked to the resolved shear stress through a function M^g . This formulation is based on the crystalline rate-dependent flow rule. On the other hand, the temporal variable does not play any role in this approach. The selection of active and non-active deformation systems is established with M^g . This function depends on the ratio τ^g/τ_c^g and can describe the hardening behaviour during the plastic regime. The hardening parameter M^g is given by

$$M^g = \beta \left[\frac{1}{2} \left(1 + \text{th} \left(k_0 \left(\frac{\tau^g}{\tau_c^g} - 1 \right) \right) \right) \right] \times \left[\frac{1}{2} (1 + \text{th}(k_0 \dot{\tau}^g)) \right] \left[\frac{1}{2} (1 + \text{th}(k_0 \dot{\tau}^g)) \right]. \quad (4)$$

Hyperbolic tangent function has been tested and used because it permits to reproduce the mechanical and the hardening behaviour, where β and k_0 are material constants. With Eq. (4) and after some algebraic calculations, the constitutive relation which links the overall stress rate and strain rate in the grain is then given by

$$\dot{\epsilon} = \left[s + \sum_g (\mathbf{R}^g \dots M^g \dots \mathbf{R}^g) \right] \dots \dot{\sigma} = \ell^{-1} \dots \dot{\sigma}, \quad (5)$$

ℓ is the elastoplastic consistent tangent moduli tensor. This tensor depends on active systems, elastic properties, stress rate and deformation history of the material. The other mechanical variables are determined by the usual relations given by the EPSC model [3], taking into account the Eqs. (3) and (5).

3 Simulation results and discussion The modified model has been used to predict the development of elastic lattice strains during uniaxial loading. Clausen and Lorentzen [7] have measured lattice strains in commercial purity aluminium loaded up to 3% strain with in-situ neutron diffraction measurements. Holden et al. [8] have made a similar study on MONEL-400 (Cu–Ni alloy) samples during uniaxial tension up to 5% strain. Lattice strains have been determined in the tension direction for the (111) and (220) reflections. The elastic single crystal stiffness (GPa) for aluminium (respectively MONEL-400) are: $C_{11}=107.3$ (220.8), $C_{12}=60.9$ (148), $C_{44}=28.3$ (107.4). The development of elastic lattice strains has been simulated using

Figure 1 (online colour at: www.pss.rapid.com) Simulated and experimental tensile curves for aluminium (a) and MONEL-400 (b).

the EPSC and the modified models. The input texture was the same in all simulations: 2000 equally-weighted lattice orientations representing a random texture (the initial experimental texture was very weak). A linear hardening matrix containing only two terms H_1 and H_2 corresponding to weak and strong interactions between the slip systems has been chosen. H_1 , H_2 , β , k_0 and τ_c^0 (initial value of CRSS) have been determined by fitting the experimental macroscopic tensile curves plotted in Fig. 1.

The parameter values are listed in Table 1. The lattice strains predicted by applying the different schemes are plotted in Fig. 2. The experimental data are also shown in these plots. The accuracy on the experimental strains is of the order of 10^{-4} .

The two approaches enable a very accurate representation of the measured macroscopic stress–strain curves using the fitting parameters shown in Table 1. The modified model gives similar results as the SC model. It should be noticed that the running time computation is considerably

Table 1 Values of material parameters.

	H_1 (MPa)	H_2 (MPa)	τ_c^0 (MPa)	β	k_0
Aluminium	55	$H_1 \times 1.1$	10.2	3.4×10^4	5
Monel-400	331	$H_1 \times 1.1$	66.5	9.4×10^3	7.5

Figure 2 (online colour at: www.pss.rapid.com) Calculated and experimental elastic lattice strain for the (111) and (220) reflections for aluminium (a) and MONEL-400 (b).

reduced with this novel approach. The development of lattice strains is non-linear once the specimen reaches the plastic regime. The SC model provides a good agreement with the experimental observations on a mesoscopic scale. This model predicts the elastic lattice strain evolution for

the (111) and the (220) reflections and the numerical level of elastic strains is correctly described. The linear hardening law is sufficient to reproduce the different experimental data. On the other hand, the modified model reflects the elastic lattice strain evolution for the two crystallographic planes in the elastic and plastic regimes. For the (220) reflection, the numerical predictions show a better agreement with experimental results beyond a macroscopic strain of 1.5%. After this strain value, the model underestimates the lattice strain evolution. At 3% macroscopic strain for aluminium, the standard deviation is 4%. For Monel-400, this deviation is 7% at 5% total strain. Nevertheless, this discrepancy, owing to different experimental uncertainties, is weak. For the (111) reflection, predictions with the modified model are especially accurate and similar with the SC model and experimental results.

4 Conclusions A modified algorithm has been proposed for computing the mechanical response of a single crystal. The new formulation of the crystal plasticity has been validated at the meso- and macroscopic levels with published experimental results and a good agreement between theory and experiment was found. Numerical results, obtained at the different scales, show the relevance of this approach.

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