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On the role of local grain interactions on twin nucleation and texture evolution in hexagonal materials

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Abstract: Texture evolution in plastically deformed HCP metals is strongly influenced by the nucleation and growth of deformation twins and twin variant selection. Statistically based EBSD analyses of deformed microstructures in HCP metals indicate that the nucleation of deformation twins depends on, among other factors, the local stress fields arising from neighboring grain interactions at grain boundaries [1]. Inspired by these findings a probability model for twin nucleation was developed [2,3], based on the activation of defect sources statistically occurring in grain boundaries. This nucleation model was implemented in a Visco-Plastic Self-Consistent (VPSC) code. Because the latter is based on an Effective Medium assumption and the inclusion formalism, it only provides average stress values in the grains, and the nature of local stress fields at grain boundaries had to be considered in a heuristic manner. In order to have better insight on the effect of local textures on twin nucleation, in this work we employ a viscoplastic full field Fast Fourier Transform (FFT) method as a numerical tool for conducting virtual experiments to study the role of crystal orientation and local neighbor grain interactions on stress localization close to the interfaces and, consequently, on twin nucleation in hexagonal materials, such as Zr and Mg.

Introduction: The model proposed in [2,3] assumes that twins nucleate at grain boundaries as a result of the dissociation of defects existing in them. These reactions are driven by the local stresses in the grain boundaries, presumably much higher in magnitude and dispersion than those in the grain interiors. To trigger twins from grain boundaries, a representative grain boundary stress (σ_{gb}) was used to calculate the resolved shear stress (RSS) on the possible twinning variants. The RSS is then compared to a probabilistic nucleation stress supplied by the model to determine when a stable twin nucleus forms and of which variant it is. Since the homogenization scheme does not provide local information on σ_{gb} and hence, the resulting RSS values on the variants, it was assumed that the RSS values at the grain boundaries can be estimated by adding a local fluctuation term to those obtained by projecting the grain average stress tensor on the variants i.e. $\tau^{\mathbf{gb}} = \tau^{\mathbf{g}} \pm \mathbf{r} \cdot \Delta\tau$ where $\tau^{\mathbf{g}}$ is the RSS on the variant using the grain average stress (obtained by VPSC), $\mathbf{r}$ is a random number between 0 and 1, $\Delta\tau$ is the fluctuation term and $\tau^{\mathbf{gb}}$ is the estimate of the RSS on the variant at the grain boundary. When the model was applied for pure Mg in compression [2], a value of 9 MPa for $\Delta\tau$, the fluctuation term, was used. The variant selection using σ_{gb} matched the experimentally observed variants better than that obtained using the grain average stress (σ_g). In this work, we use the viscoplastic version of the full field Fast Fourier transform (FFT) method to conduct a virtual experiment on a model microstructure [4]. Since the FFT method provides spatially- resolved micromechanical fields in 3-D polycrystals, it is well suited to study the local stress fields close to grain boundaries. The overarching goal is to gain insight into the magnitude and nature of the stress fluctuations and their distributions in the vicinity of grain boundaries, and incorporate such knowledge to improve the existing model. Here, we report first observations about the dependency of the RSS values of the twin variants on the crystal orientation and their proximity to grain boundaries.

Simulation Details: The macroscopic texture of extruded+rolled pure Mg (see Figure1) is represented by 512 distinct cube-shaped orientations (grains). A numerical grid of 64 x 64 x 64 Fourier points was used, where each grain consists of 512 (8 x 8 x 8) voxels. In each grain, the inner 6 x 6 x 6 block of voxels was considered as part of the grain interior and the layer of voxels close to the grain boundary as the grain boundary zone (Figure 1c). The applied boundary condition was one small strain step of 0.5% in compression along axis 2 (TD, Figure 1a). Standard rate-sensitive crystal plasticity formulation with an exponent n = 10 is employed. Basal, pyramidal <c+a>, prismatic slip modes and the tensile $\{10\bar{1}2\}$ twin mode were assumed to be active, with initial critical resolved shear stresses 3.3, 35.7, 86.2 and 11.0 MPa respectively. Since twinning is unidirectional, a large CRSS was used to prevent deformation along the 'opposite' twinning direction.

Results: At each voxel, the six possible twin variants are ranked according to their RSS values, obtained by projecting the stress tensor calculated by FFT on the Schmid tensors corresponding to each twin system. Variant 1 is the system with the highest and variant 6 correspond to the system with the lowest RSS value. The highest and the lowest values of all the six variants are shown in Table 2. The maximum value is found to steadily decrease as one goes to less favored variants. Nevertheless the maximum values are close to the CRSS (11 MPa) even in these less favored variants.

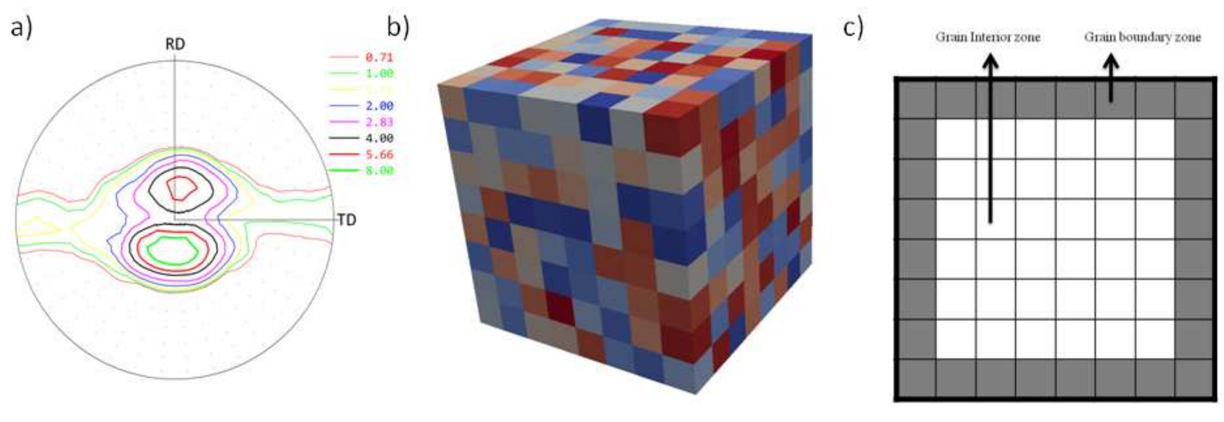

Figure 1: a) (0001)basal pole figure of the initial texture of pure Mg; b) 3D polycrystal with cuboidal grains used in the FFT calculations; c) 2D schematic showing the "grain interior" and the "grain boundary" zone in one grain.

Table 2: Maximum and minimum values of the RSS (in MPa) on all twin systems at each voxel in the entire polycrystal.

Variant	V1	V2	V3	V4	V5	V6
Maximum	13.13	12.76	12.05	11.9	10.85	10.52
Minimum	-41.78	-42.1	-44.38	-44.76	-47.63	-47.87

In each grain, two distinct distributions of the RSS values are studied depending on whether a voxel belongs to the “grain boundary zone” or “grain interior zone”. The average value of the RSS on the highest and the second highest variants (V1 and V2) on all the voxels in 5° bins are plotted against the inclination of the c-axis with respect to ND (axis 3) in 5° bins (Figure 2a). The standard deviations of the RSS values are plotted in Figure 2b. Under the prescribed loading, the smaller the c-axis inclination, the higher is the propensity for twinning, and closer the average values of the RSS to the twin CRSS. The results show that the average RSS is basically the same for interior and grain boundary zones and, as expected, the dispersion in the grain boundary zone is generally higher compared to the grain interior zone. There is, however, a strong dependence of the mean and variation in RSS on the orientation (Schmid factor) of the voxel (shown here as the c-axis inclination). The average values and the standard deviations of the RSS values of all the variants in the “grain boundary zone” voxels are shown in Figure 3a & 3b. If one were to average over all orientations of the crystals and all the variants of twin systems, a value of 9 MPa appears to be appropriate. This is in fact the limit value that was used for random local fluctuations in the probabilistic twin nucleation model [2].

Summary: A full field viscoplastic FFT simulation was performed on a model polycrystal microstructure to study the distributions of the RSS values on the six possible tensile twin variants in pure Mg. Both the average and the standard deviation of the RSS values on highest variant were found to be highly dependent on the inclination of the c-axis. It is observed that for grains well suited for tensile $\{10\bar{1}2\}$ twinning, the average value of the RSS is close to the corresponding CRSS with relatively lower dispersion.

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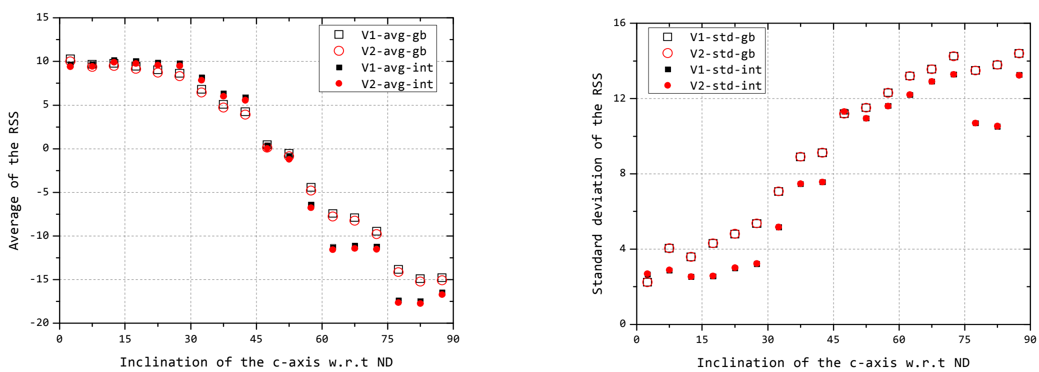

Figure 2a (Left): The average and 2b (Right) standard deviation of the RSS distribution on the highest and second highest variants as a function of c-axis inclination.

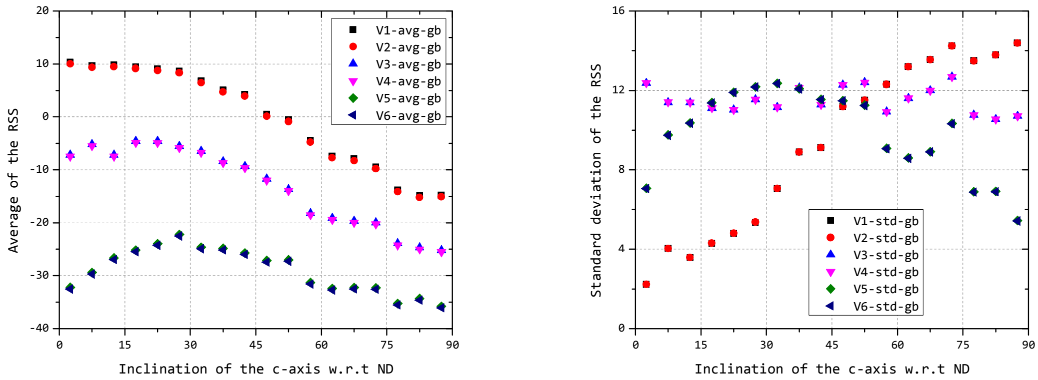

Figure 3(Left): The average and 3b (Right) standard deviation of the RSS distribution on all variants as a function of c-axis inclination for grain boundary zone voxels.

References:

[1] I.J. Beyerlein, L. Capolungo, P.E. Marshall, R.J. McCabe and C.N. Tomé, Statistical analyses of deformation twinning in magnesium, Phil. Mag. 90 (2010) 2161–2190.

[2] I.J. Beyerlein, R.J. McCabe and C.N. Tomé, Effect of microstructure on the nucleation of deformation twins in polycrystalline high-purity magnesium: A multi-scale modeling study, J. Mech. Phys. Solids. 59 (2011) 988-1003.

[3] I.J. Beyerlein and C.N. Tomé, A probabilistic twin nucleation model for HCP polycrystalline metals, Proc. R Soc. London A. 466 (2010) 2517-2544.

[4] R.A. Lebensohn, N-site modeling of a 3D viscoplastic polycrystal using fast Fourier transform, Acta Mater. 49 (2001) 2723–2737.