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COMPARISON OF A SELF-CONSISTENT APPROACH AND A PURE KINEMATICAL MODEL FOR PLASTIC DEFORMATION AND TEXTURE DEVELOPMENT

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ABSTRACT

The present work is concerned with the comparison of a visco-plastic self-consistent (VPSC) approach and a new purely kinematical scheme called Grain Axes Coincidence Model (GACM). Both formulations are conceived for modeling plastic deformation and texture development of polycrystals and lead to spin equations for each grain that make evident the interaction between grain strain and a homogeneous effective medium strain. The interaction term is linear in the difference between both strains with a coefficient that is, for the VPSC model, an integral function of the anisotropic visco-plastic compliances and some form factors related with the current degree of deformation. Meanwhile, the coefficients of the GACM are, as expected, only function of the principal axes of the ellipsoid representative of the grain shape. The comparison of both kinds of interaction terms will be presented for rolling and torsion tests in cubic and hexagonal materials.

INTRODUCTION

In the field of texture development the influence of the grain shape has been recognized and modeled by many authors [1-3]. Each grain must keep compatibility with the matrix guaranteeing coincidence of shape and size with the hole lodging the grain. It means that the principal axes of the ellipsoid representative of the grain must be collinear with the principal axes of the ellipsoid representative of the hole. The models based in the Taylor hypothesis, assuming equal deformation for each grain and equal to the macroscopic strain, do not follow the shape and orientation of such ellipsoids. The Relaxed Constraints (RC) models approach the problem allowing some of the strain components to be different from the average when the grain is far from the initial spherical shape. The self-consistent models approach the problem right from the beginning and they will be briefly discussed in the second section. In the present work we compare a VPSC model with a pure kinematical model named Grain Axes Coincidence Model (GACM) for modeling both the plastic deformation and texture development in polycrystals. The GACM model has the Taylor model as a limit for spherical grains and it is related with the RC model in ways that will be discussed.

THE GRAIN AXES COINCIDENCE MODEL

In this model the grain is considered as part of a continuum media subject to finite deformations [4]. The deformation gradient **F** can be decomposed in two components: a) Proper plastic deformation reached by activation of crystal slip systems $\mathbf{F^P}$. b) Elastic deformation and "any other cause" for extra reorientations $\mathbf{F^*}$. They can be decomposed, by the polar decomposition, in the product of a pure rotation matrix **R** and a pure stretching **V**.

$$\mathbf{F} = \mathbf{F^*F^P} = \mathbf{R^*V^*R^PV^P} \tag{1}$$

The elastic deformation is regarded negligible compared with the plastic one and it does not appreciably reorient crystal or grain axes. **R** can be differentiated by the chain rule and transposed:

$$\dot{\mathbf{R}} = \dot{\mathbf{R}}^* \cdot \mathbf{R}^P + \mathbf{R}^* \cdot \dot{\mathbf{R}}^P \tag{2}$$
$$\mathbf{R}^T = \mathbf{R}^{PT} \cdot \mathbf{R}^{*T}$$

that leads to

$$\boldsymbol{\Omega} = \dot{\mathbf{R}} \cdot \mathbf{R}^T = \dot{\mathbf{R}}^* \cdot \mathbf{R}^{*T} + \mathbf{R}^* \cdot \dot{\mathbf{R}}^P \cdot \mathbf{R}^{PT} \cdot \mathbf{R}^{*T} = \boldsymbol{\Omega}^* + \mathbf{R}^* \cdot \boldsymbol{\Omega}^P \cdot \mathbf{R}^{*T} \tag{3}$$

where $\boldsymbol{\Omega}$ is the time derivative of the orientation called "spin". The magnitudes representing $\boldsymbol{\Omega}$-spins can be written in terms of the antisymmetrical component of its velocity gradient and certain functions α_{ij} of the eigenvalues λ_i , representative of the ellipsoid axes, multiplying the component of the strain rate tensor. Rearranging we can obtain an expression slightly different from the usual in Taylor models. The extra term depends on the grain deformation and the difference between the average strain rate and the grain strain rate.

$$\Omega^*_{ij} = \Omega_{ij} - \Omega^P_{ij} = w_{ij} - w^P_{ij} - \frac{\lambda_i - \lambda_j}{\lambda_i + \lambda_j}(D_{ij} - d^P_{ij}) = w_{ij} - w^P_{ij} - \alpha_{ij}(D_{ij} - d^P_{ij}) \tag{4}$$

The α_{ij} coefficients are identically null for spherical grains, no matter how large the differences between the strain rates are. They grow asymptotically from zero to one for large deformations. This is the expected behavior in RC models for some components. The anisotropy of the matrix is not taken in account but only the grain anisotropy, through the slip systems activated. A similar equation is obtained for the SC models.

THE VISCO-PLASTIC SELF-CONSISTENT MODEL

The viscoplastic equation relating the plastic velocity gradient with the deviatoric stress applied to each crystal (grain) can be written:

$$d^P_i = \dot{\gamma}^0 \sum^s m^s_i (m^s_j \sigma'_j / \tau^s_c)^n \tag{5}$$

summing over all the slip systems. m_i^s is the Schmid tensor, σ_k' is the deviatoric stress in each grain, τ_c is the critical stress, $\dot{\gamma}^0$ is a normalization factor and n is the inverse of the strain rate sensitivity of the material (n>>1). The single index magnitudes d_i^P , σ_j' and m_j^s are the vectorized form of d_{ij}^P, σ_{ij}' and m_{ij}^s. Equation (5) can be rewritten as:

$$d_i = [\dot{\gamma}^0 \sum^s (m_i^s m_j^s / \tau_c^s)(m_j^s \sigma_j' / \tau_c^s)^{n-1}]\sigma_j' = M_{ij}^c(\sigma')\sigma_j' \tag{6}$$

where M^c is the grain viscoplastic compliance modulus. An analogous pseudo linear relation can be written at the polycrystal level:

$$D_i = M_{ij}(\Sigma')\Sigma_j' \tag{7}$$

where Σ_i' and D_i are the deviatoric stress and the velocity gradient in the polycrystal in the vectorized form and M_{ij} is the polycrystal viscoplastic compliance modulus. The equations (6) and (7) are the constitutive equations of an inclusion and a viscoplastic matrix. Applying the Eshelby formalism for the resolution of the inclusion problem we obtain the interaction equation:

$$D_i - d_i^P = \tilde{d}_i = -\tilde{M}_{ij}\tilde{\sigma}_j = -\tilde{M}_{ij}(\Sigma_i - \sigma_i^P) \tag{8}$$

where $\tilde{\sigma}$ and $\tilde{d}$ are the deviations in stress and velocity gradient of the grain with respect to the macroscopic magnitudes and $\tilde{M}$ is the interaction tensor defined as $n(I-S)^{-1}SM$. The viscoplastic Eshelby tensor S is function of the macroscopic modulus M and of the grain shape. The self-consistent equation is:

$$M = < M^c(M^c + \tilde{M})^{-1}(M + \tilde{M}) > \tag{9}$$

The SC formulation can be used for texture development modeling [5]. An incremental step of deformation is imposed to a polycrystal composed of a discrete number of ellipsoidal grains, fixing a velocity gradient D in a time interval Δt. A first try guess is proposed for the stresses in each grain and iteratively the solution of equation (9) can be obtained. Each grain can be reoriented by:

$$\Omega_{ij}^* = w_{ij} - w_{ij}^P - \Pi_{ijkl} S_{klmn}^{-1}(D_{mn} - d_{mn}^P) \tag{10}$$

where we have gone back to the tensorial notation and w_{ij} is the antisymmetrical part of the macroscopic velocity gradient, W_{ij}^P is the antisymmetrical part of the distortion due to plastic slip and the third term is the local spin. The tensor Π is the antisymmetrical complementary component of the symmetric Eshelby tensor **S**. Its product by $\mathbf{S^{-1}}$ is a tensor that linearly combines the differences in strain rates. They are a set of interaction coefficients evaluated numerically in each deformation step.

RESULTS

Fig. 1 shows the evolution of the α_{ij} parameters proposed by the GACM for rolling up to a Von Mises equivalent deformation of 2.00. The rolling, normal and transversal directions are assumed to be along the axis 3, 1 and 2 respectively. This model, being purely kinematical, cannot be used to calculate the grain reorientation without an additional constitutive equation connecting the spin with the stresses or, alternatively, allowing the calculation of the strain rate differences. The asymptotic evolution of the coefficients becomes evident as the accumulated deformation increases.

The SC simulations were performed starting from a polycrystal with equiaxed grains and random distribution of orientations. Rolling deformation was simulated for copper polycrystal up to a Von Mises equivalent strain of 2.00. Equation (10) shows that the coefficients potentially significant are more than one for each spin component. Nevertheless, it is numerically observed that the coefficients presented in Fig. 2, which correspond one to one to the kinematically calculated coefficients, are at least two orders of magnitude higher than the others. Their behavior is also similar to the behavior of the α_{ij} coefficients except because they approach faster to the asymptotic value. Fig. 3 shows the evolution of the standard deviations (SD) of the respective strain rates. They represent the average differences between the strain rates of the grains and the polycrystal strain rates. The component $SD(d_{13})$ grows with the deformation stage and it is the most important one.

The kinematical coefficients for torsion are shown in Fig. 4. They evolve slower than in rolling because the shape does not change at the same pace. A similar VPSC simulation was performed for torsion in copper and the coefficients are shown in Fig. 5. They evolve similarly to the rolling coefficients but closer to the kinematical ones.

A VPSC simulation was performed for rolled zirconium (hexagonal symmetry) at high temperature (no twinning has been considered) and the coefficients are shown in Fig. 6. They behave similarly to the kinematical ones keeping the other coefficients close to zero.

The VPSC model also takes into account the anisotropy of the matrix. The coefficients include the influence of such anisotropy simultaneously with the shape influence. The shape evolution can be turned off in the code like if the grains were kept spherical during the deformation process and allowing just for crystal reorientation and consequent texture evolution. The anisotropy influence can be extracted and it should be complementary of the kinematical shape influence. Fig. 7 shows the calculated coefficients for rolled copper without grain shape evolution. At low deformation they show the right evolution to be complementary of the kinematical coefficients. The disagreements at higher deformations with the simple subtraction of Fig. 1 and 2 can be attributed to the fact that the grains, deprived of shape evolution, reorient differently from the shape evolving case and the consequent anisotropy is different. The evolution of anisotropy can also explain the differences between copper in rolling and torsion. The anisotropy evolves not only different but also slowly in torsion tests than in rolling because the texture reaches lower strength for the same deformation. For hexagonal crystal symmetry the coefficients are also strongly influenced by the anisotropy.

CONCLUSIONS

It has been shown that a pure kinematical model can give a better insight about the reorientation mechanisms in texture development. It does not provide the kinetics of crystal reorientation and an extra constitutive relationship has to be used in order to calculate the grain strain deviation. Self-consistent models are suitable for that purpose and simultaneously they provide the values of the interaction coefficients, which also include the anisotropy influence. The machine time consumption could be reduced by using the kinematical coefficients but further tests are necessary to check its influence in the final texture. For RC approaches the GACM model provides the value of the coefficients, at any deformation step, with no divergence problems for spherical grains.

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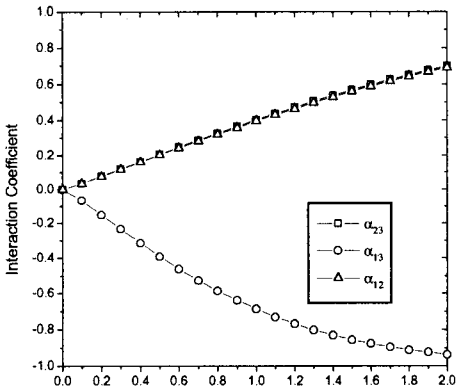

Fig. 1: Interaction coefficients calculated by the GACM for rolling.

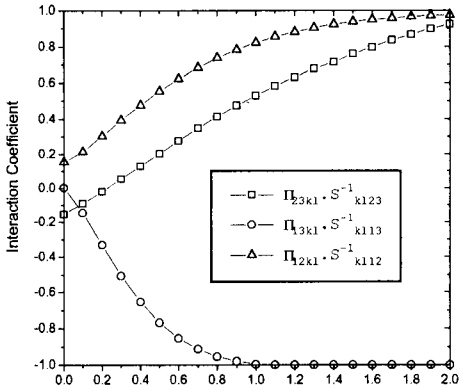

Fig. 2: Interaction Coefficients calculated by the VPSC model for copper. Rolling with shape and anisotropy evolution. Starting from randomly distributted spherical grains.

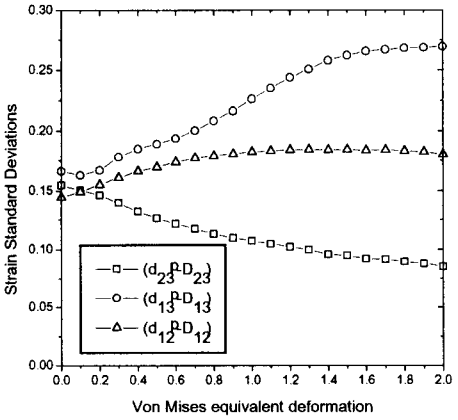

Fig. 3: Standard deviations for the three components significantly different from the average. Rolling in copper by VPSC simulation.

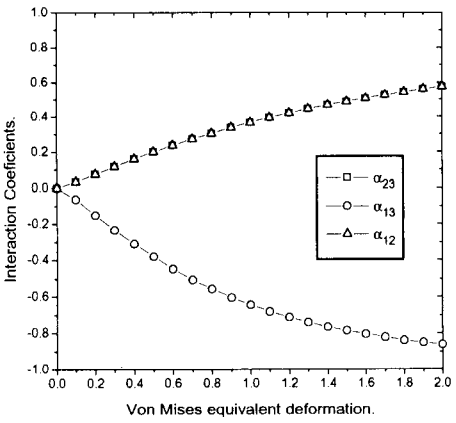

Fig. 4: Interaction coefficients calculated by GACM for torsion.

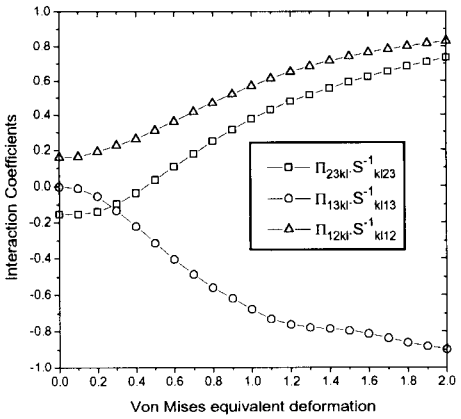

Fig. 5: Interaction coefficients calculated by VPSC model. Torsion in copper with initially spherical grains.

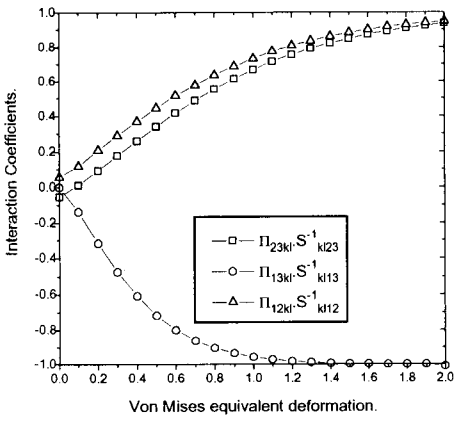

Fig. 6: Interaction Coefficients for initially spherical grains. VPSC calculation for zirconium rolled at high temperature.

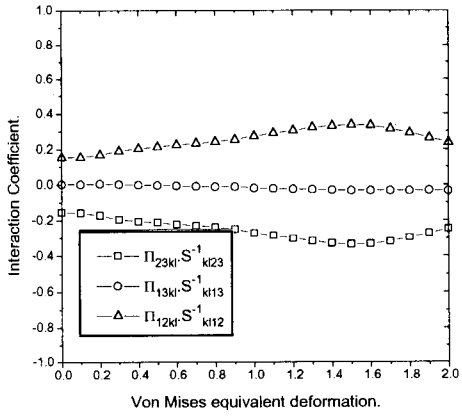

Fig. 7: Interaction Coefficients for rolling without shape updating. VPSC model for spherical copper grains.