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THE SELF-CONSISTENT SEQUENTIAL AVERAGING SCHEME FOR MODELLING ELASTIC-VISCOPLASTIC POLYCRYSTALS: VALIDATION BY FINITE ELEMENT CALCULATIONS

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Introduction

The assessment of the overall properties of heterogeneous material with use of the micromechanical approaches based on the Eshelby solution is difficult if both elastic and viscous properties are to be simultaneously taken into account. For linear viscoelasticity the problem can be solved in an elegant way by using the Laplace-type transform technique. Extensions of that formalism to cases when elasticity is accompanied by non-linear viscous properties, as in elastic-viscoplastic materials, lead to rather complex formulations [4]. Therefore the approximate linearization schemes are of interest. One of such proposals for the Maxwell-type materials is a sequential linearization that has been proposed in [2]. In the case of Mori-Tanaka averaging scheme, used for composites, the method coincides with the additive approach due to Molinari [5]. For the self-consistent scheme, used for polycrystals, in some cases an additional accommodation step must be added to obtain satisfactory predictions. The model is formulated within the small strain framework.

Objectives and Methodology

Within the sequential scheme the response of the Maxwell-type elastic-viscoplastic polycrystal is found by using elastic and viscous properties sequentially within one incremental step. Consequently, two subproblems with different interaction rules between homogenized equivalent medium (HEM) and single crystal are solved separately: an instantaneous purely elastic one and a creep-type viscous one. In the simplest version of the sequential self-consistent scheme, when the additional accommodation step is not necessary and the grains are of the spherical shape, these two interaction equations take the form:

a creep-type viscous problem

$$\dot{\boldsymbol{\varepsilon}}_{g}^{v} - \dot{\boldsymbol{\varepsilon}}_{0}^{\text{Vg}} = -\bar{\mathbf{M}}_{*}^{v} \cdot (\boldsymbol{\sigma}_{g} - \boldsymbol{\sigma}), \qquad (1)$$

where $\dot{\varepsilon}_g^v$ and σ_g are local viscoplastic strain rate and stress in the grain g, respectively. $\dot{\varepsilon}_0^{Vg}$ and σ are auxiliary external viscous strain rate for grain g and the overall macroscopic stress in the polycrystal, respectively. The tensor \overline{M}_*^v is the inverse Hill tensor for a purely viscous problem obtained with use of the overall viscous stiffness. In the case of non-linear viscoplastic polycrystals, tangent or secant linearization of the local response is performed in order to use the Eshelby result;

an instantaneous purely elastic problem

$$\dot{\boldsymbol{\varepsilon}}_{g}^{e} - \dot{\boldsymbol{\varepsilon}} + \dot{\boldsymbol{\varepsilon}}_{0}^{Vg} = -\bar{\mathbf{M}}_{*}^{e} \cdot (\dot{\boldsymbol{\sigma}}_{g} - \dot{\boldsymbol{\sigma}}), \quad \dot{\boldsymbol{\varepsilon}}_{g}^{e} + \dot{\boldsymbol{\varepsilon}}_{g}^{v} = \dot{\boldsymbol{\varepsilon}}_{g} \tag{2}$$

where $\dot{\varepsilon}_g^e$ and $\dot{\sigma}_g$ are local elastic strain rate and stress rate in the grain g, respectively. $\dot{\varepsilon}$ and $\bar{\sigma}$ are an overall strain rate and an overall stress rate in the polycrystal, respectively. The tensor M_*^e is the inverse Hill tensor for a purely elastic problem obtained with use of the overall elastic stiffness.

The main objective of the present paper is to validate proposed averaging scheme by comparison of its predictions with the result of the finite element (FE) calculations. FE calculations are performed for the volume element of polycrystal of checkerboard distribution of randomly selected 125 grain orientations (see Fig. 1(a)). The macroscopic uniaxial tension is imposed and microperiodic boundary conditions are applied.

Classical rate-dependent crystal plasticity formulation is used for a constitutive description at the level of single grain. Viscous flow takes place by slip on the crystallographic slip systems. The relation between the slip rate and the resolved shear stress follows the rate dependent power law without hardening. The linear anisotropic elasticity is assumed. More details can be found in [1].

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Multiscale modelling

Results and analysis

Micromechanical and FE calculations are performed for two polycrystals: a fcc Cu aggregate (12 slip systems $\{111\}\langle 1\overline{10}\rangle$ with the critical shear stress $\tau_c = 10$ [MPa]) and a tetragonal γ -TiAl aggregate (L1 lattice geometry, 4 ordinary dislocations: $\{111\}\langle 1\overline{10}\rangle$, 8 super-dislocations $\{111\}\langle 10\overline{1}\rangle$, with $\tau_c^{sup}/\tau_c^{ord} = 5$ - strong viscous anisotropy due to only 3 independent easy slip systems). Components of the elasticity tensors are assumed as reported in [1]. The results of FE calculations (the average response for 5 distinct orientation distributions) are compared in Fig. 1 b-d with the predictions of the sequential approach combined with three different linearization schemes most often used for the purely viscoplastic polycrystals [4]: secant (Sec.), tangent (Tan.) and affine (Aff.). It is seen that satisfactory agreement between both predictions of the overall stress-strain behaviour is obtained for polycrystals of low viscous anisotropy (Cu) and the tangent linearization of viscous response. For polycrystals of strong viscous anisotropy (TiAl) satisfactory agreement has been obtained for n = 1. For higher non-linearity FE predictions lie between the results of sequential method combined with the tangent and affine linearization of viscous response.



Figure 1: (a) 3D checkerboard subdivision of FE polycrystal model into 125 grains (AceGen/AceFEM environment has been used); macroscopic response in uniaxial tension of (b) Cu polycrystal (n = 10 in the power law, FFT - after [3]), (c) TiAl polycrystal (n = 1), (d) TiAl polycrystal (n = 8)

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