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Deformation Mechanisms

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AN ELASTO-PLASTIC MICROMECHANICAL METHOD FOR TWIN DRIVEN PLASTICITY

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Abstract

In this work, a mean-field self-consistent approach based on a generalization of the Tanaka-Mori method is introduced to predict the mechanical response of polycrystalline Mg. The key idea is to homogenize the response of grains containing twin domains such that a direct coupling between the twin and parent domain is introduced. The work is particularly suited to study Mg as it allows for a direct coupling of the mechanical response of twin and parent domains. Such coupling accounts, for the first time, for relative size and shape effects on the development of internal strains in twin domains.

Introduction

Due to its low symmetry, plasticity in Mg is typically conveyed by the activation of different types of deformation modes: twinning and slip[1]. While the motion of dislocations mediates both mechanisms, their effects on the development of internal strains are different. Indeed, the motion of twinning dislocations engenders substantial lattice rotation.

The role of twinning to plasticity is complex. On the one hand the motion of the twinning dislocations provides for a strain/stress relaxation. On the other hand, the new orientation of the lattice in twin domains can allow for the activation of secondary slip and twin, which can either lead to hardening or softening. The accuracy of the prediction of the activity of secondary slip and twinning is conditional on that of the predictions of the stress state in the twin domains.

Recent high-energy X-ray measurements have revealed that at the onset of twinning, the stress state within the twin and parent domains can be significantly different [2]. Precisely, it was found that the resolved shear stress of the activated tensile twin is of opposite sign in the parent and twin phases. These "backstresses" can be rationalized by the following two considerations. First, at a fine length scale, it is conceivable that, upon penetrating the grain boundary opposite to their emission site, the twinning partial dislocations lead to a distortion of the grain boundary. Such distortion can be the source of long-range (back)stresses. However, adopting a reasoning based on the conservation of Burgers vector to estimate the energy associated with the distortion, it appears unlikely that the dissociation of twinning partial dislocations can lead to such effect.

Second, the lattice rotation associated with twinning and the elastic anisotropy of hexagonal crystals yields an elastic constant mismatch across the twin interface. The mismatch in elastic constants can constrain the twin domain and be the primary source of back-stresses. Essentially, the process is similar to the volume constraint during corrosion- and described with the Pilling Bedworth ratio- or during phase transformation.

While substantial effort is dedicated to the development of full-field methods -both finite element and fast Fourier transform based- to model plasticity, mean-field methods remain widely used. Indeed mean-field Eshelbian micromechanics models allow for a numerically efficient way to model plasticity and texture evolutions in high and low symmetry polycrystals [3, 4]. Currently, the formation of twin domains is treated in two different ways whether coupling between the twin and parent phases is taken into account or not. In the decoupled approach, the mean stress and strain fields within the twin domains are simply obtained by solving the elementary inclusion problem of Eshelby –after linearization of the constitutive response- whereby the twin domain is embedded in a homogeneously equivalent medium. Effects arising from elastic mismatches between the twin and parent domains are thus not accounted for. In the coupled approach, traction continuity conditions between the twin and parent domains are imposed on the averaged fields in each phase. Therefore this coupling method is more appropriate when the twin domains remain relatively thin. In any case, the direct effect of elastic mismatches between the twin and parent phases is not accounted for.

In recent work by the authors [5], a third method was introduced to solve rigorously a double inclusion problem. This topology corresponds to that of a twin domain embedded in a parent phase (see Figure 1). The proposed approach, basically extending the Tanaka-Mori method [6], and was limited to a purely elastic approach and to a double inclusion topology. Nonetheless, it was shown that large effects arising from elastic mismatches are to be expected.

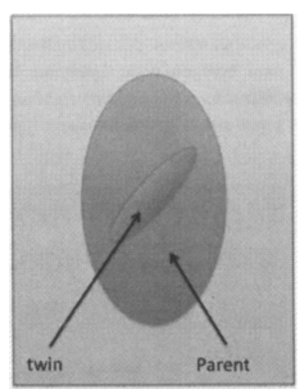

Figure 1: Schematic of the topological representation of grains containing twins. The red domain denotes the twin volume while the blue domain refers to the grain without twin volume or parent volume.

In the proposed work an extension of previous work is proposed such as to introduce the generalized Tanaka-Mori method in an elasto-plastic self consistent frameowork (EPSC).

Generalized elasto-plastic Tanaka Mori method in Elasto plasticity

Let us consider first the topology described in Figure 1 whereby a grain embedded in a medium contains a twin domain – appearing in red-. Denoting $\boldsymbol{r}$ the position vector, in an incremental theory the constitutive response of the material is written as:

$$\dot{\sigma}(r) = L(r)\dot{\varepsilon}(r) \tag{1}$$

Here σ and ε denote the Cauchy stress and small strain tensors, respectively. L denotes the tangent modulus of the material. In what follows, t and g used either as subscripts or superscripts will refer to the twin domain and grain phase – including the twinning domain-. 'gt' is used to denote quantities associated to the parent phase –i.e. grain without the twin domain-.At any point within the medium, the tangent modulus can be written as the sum of a homogensous modulus, corresponding to that of an effective medium and of a spatial variation:

$$L(r) = L^{eff} + \delta L(r) \tag{2}$$

Where,

$$\boldsymbol{\delta L(r') = (L^g - L^{eff})\delta v_g(r') + (L^t - L^g)\delta v_t(r')} \tag{3}$$

Here δv_i with i=t,g denote characteristic function taken the value 1 within volume i and zero outside. Applying both equilibrium and compatibility conditions on (1) yields the Navier equation. A solution of Navier equation is given by the Lippman-Schwinger equation:

$$\boldsymbol{\dot{\varepsilon}(r) = \dot{E} - \int_V \Gamma^{s,\infty}(r - r') : \delta L(r') : \dot{\varepsilon}(r')dV_{r'}} \tag{4}$$

here V denotes the entire volume. $\Gamma^{\infty,s}$ denote the modified Green functions As δL is null outside the grain, equation 4 reduces to a sum of two integrals:

$$\boldsymbol{\dot{\varepsilon}(r) = \dot{E} - \int_{V_g} \Gamma^{s,\infty}(r - r')dV_{r'} : (L^g - L^{eff}) : \dot{\varepsilon}^g}$$
$$\boldsymbol{- \int_{V_t} \Gamma^{s,\infty}(r - r')dV_{r'} : (L^t - L^g) : \dot{\varepsilon}^t} \tag{5}$$

Here V_t and V_g denote the twin and grain domains –with the twin-, respectively. From (5), one can compute the average strain rate in the twin and parent domains including the twin and in the parent domain without the twin:

$$\dot{\varepsilon}^t = \frac{1}{V_t}\int_{V_t} \dot{\varepsilon}(r)dV_r \tag{6}$$

and

$$\dot{\varepsilon}^g = \frac{1}{V_g}\int_{V_g} \dot{\varepsilon}(r)dV_r \tag{7}$$

and

$$\boldsymbol{\dot{\varepsilon}^{gt} = \frac{1}{V_g - V_t}\int_{V_g - V_t} \dot{\varepsilon}(r)dV_r}$$

In order to proceed with analytical derivations, it is assumed here that the strain rates within the twin and grain (with twin) domains are equal to their average within their respective volumes.

Twin domain

From (5) and (7), the average strain in the twin domain can thus be written as:

$$\boldsymbol{\dot{\varepsilon}^t = \dot{E} - \frac{1}{V_t}\int_{V_t}\int_{V_g} \Gamma^{s,\infty}(r - r')dV_{r'}dV_r : (L^g - L^{eff}) : \dot{\varepsilon}^g}$$
$$\boldsymbol{- \frac{1}{V_t}\int_{V_t}\int_{V_t} \Gamma^{s,\infty}(r - r')dV_{r'}dV_r : (L^t - L^g) : \dot{\varepsilon}^t} \tag{8}$$

If $\boldsymbol{r \in V_t \subset V_g}$, then $\boldsymbol{\int_{V_g} \Gamma^{s,\infty}(r - r')dV_{r'}}$ and $\boldsymbol{\int_{V_t} \Gamma^{s,\infty}(r - r')dV_{r'}}$ are uniform and one obtains the following expression of the average strain rate within the twin domain:

$$\boldsymbol{\dot{\varepsilon}^t = \dot{E} - P^{V_g} : (L^g - L^{eff}) : \dot{\varepsilon}^g - P^{V_t} : (L^t - L^g) : \dot{\varepsilon}^t} \tag{9}$$

With:

$$P^{V_g} = \int_{V_g} \boldsymbol{\Gamma}^{s,\infty}(\boldsymbol{r}-\boldsymbol{r}')dV_{r'} \tag{10}$$

$$P^{V_t} = \int_{V_t} \boldsymbol{\Gamma}^{s,\infty}(\boldsymbol{r}-\boldsymbol{r}')dV_{r'} \tag{11}$$

Grain domain

In the domain associated to the grain (including the twin) (5) reduces to:

$$\dot{\boldsymbol{\varepsilon}}^g = \dot{\boldsymbol{E}} - \frac{1}{V_g}\int_{V_t}\int_{V_g} \boldsymbol{\Gamma}^{s,\infty}(\boldsymbol{r}-\boldsymbol{r}')dV_{r'}dV_r : (\boldsymbol{L}^g - \boldsymbol{L}^{eff}) : \dot{\boldsymbol{\varepsilon}}^g$$
$$-\frac{1}{V_g}\int_{V_g}\int_{V_t} \boldsymbol{\Gamma}^{s,\infty}(\boldsymbol{r}-\boldsymbol{r}')dV_{r'}dV_r : (\boldsymbol{L}^t - \boldsymbol{L}^g) : \dot{\boldsymbol{\varepsilon}}^t \tag{12}$$

However here because $\boldsymbol{r} \in V_g - V_t$, only $\int_{V_g} \boldsymbol{\Gamma}^{s,\infty}(\boldsymbol{r}-\boldsymbol{r}')dV_{r'}$ is uniform such that the second integral needs to be computed by switching the order of the integration signs.

This is done by applying the Tanaka Mori theorem to (12) can be written as:

$$\dot{\boldsymbol{\varepsilon}}^g = \dot{\boldsymbol{E}} - \frac{1}{V_g}\int_{V_g}\int_{V_g} \boldsymbol{\Gamma}^{s,\infty}(\boldsymbol{r}-\boldsymbol{r}')dV_{r'}dV_r : (\boldsymbol{L}^g - \boldsymbol{L}^{eff}) : \dot{\boldsymbol{\varepsilon}}^g$$
$$-\frac{1}{V_g}\int_{V_t}\int_{V_t} \boldsymbol{\Gamma}^{s,\infty}(\boldsymbol{r}-\boldsymbol{r}')dV_{r'}dV_r : (\boldsymbol{L}^t - \boldsymbol{L}^g) : \dot{\boldsymbol{\varepsilon}}^t \tag{13}$$

Finally the average strain within the grain domain –i.e. containing the twin domain- can be written as:

$$\dot{\boldsymbol{\varepsilon}}^g = \dot{\boldsymbol{E}} - \boldsymbol{P}^{V_g} : (\boldsymbol{L}^g - \boldsymbol{L}^{eff}) : \dot{\boldsymbol{\varepsilon}}^g - \frac{V_t}{V_g}\boldsymbol{P}^{V_g} : (\boldsymbol{L}^t - \boldsymbol{L}^g) : \dot{\boldsymbol{\varepsilon}}^t \tag{14}$$

With,

$$\boldsymbol{P}^{V_g} = \int_{V_g}\int_{V_g} \boldsymbol{\Gamma}^{s,\infty}(\boldsymbol{r}-\boldsymbol{r}')dV_{r'}dV_r \tag{15}$$

From equations (12) to (13) one can introduce localization and concentrations relations between the strain rate imposed on the boundary and that on each volume. One has:

$$\dot{\boldsymbol{\varepsilon}}^g = \boldsymbol{A}^g : \dot{\boldsymbol{E}}$$
$$\dot{\boldsymbol{\varepsilon}}^t = \boldsymbol{A}^t : \dot{\boldsymbol{E}}$$
$$\dot{\boldsymbol{\varepsilon}}^{gt} = \frac{1}{V_g - V_t}\left[V_g\boldsymbol{A}^g - V_t\boldsymbol{A}^t\right] : \dot{\boldsymbol{E}} \tag{16}$$

The localization tensors are given by:

$$\boldsymbol{A}^g = \begin{bmatrix} \frac{V_t}{V_g}(\boldsymbol{S}^g(V_g) - \boldsymbol{S}^{eff}(V_g)) - \\ \left(\boldsymbol{I} + (\boldsymbol{S}^t(V_t) - \boldsymbol{S}^g(V_t))\right) : \left(\boldsymbol{I} + (\boldsymbol{S}^g(V_g) - \boldsymbol{S}^{eff}(V_g))\right) \end{bmatrix}^{-1} :$$
$$\left[\frac{V_t}{V_g}\boldsymbol{I} - \left(\boldsymbol{I} + (\boldsymbol{S}^t(V_t) - \boldsymbol{S}^g(V_t))\right)\right] \tag{17}$$

and

$$\boldsymbol{A}^t = \left(\boldsymbol{I} + (\boldsymbol{S}^t(V_t) - \boldsymbol{S}^g(V_t))\right)^{-1} :$$
$$\begin{bmatrix} \boldsymbol{I} - (\boldsymbol{S}^g(V_g) - \boldsymbol{S}^{eff}(V_g)) : \\ \begin{pmatrix} \frac{V_t}{V_g}(\boldsymbol{S}^g(V_g) - \boldsymbol{S}^{eff}(V_g)) - \left(\boldsymbol{I} + (\boldsymbol{S}^t(V_t) - \boldsymbol{S}^g(V_t))\right) \\ : \left(\boldsymbol{I} + (\boldsymbol{S}^g(V_g) - \boldsymbol{S}^{eff}(V_g))\right) \end{pmatrix} \end{bmatrix}^{1} : \tag{18}$$
$$\left[\frac{V_t}{V_g}\boldsymbol{I} - \left(\boldsymbol{I} + (\boldsymbol{S}^t(V_t) - \boldsymbol{S}^g(V_t))\right)\right]$$

$\boldsymbol{I}$ is the fourth order identity tensor. In (17) and (18), the following tensors were introduced:

$$\mathbf{S}^j(V_i) = \mathbf{P}^{V_i} : \mathbf{C}^j \quad \text{with j =t,g} \tag{19}$$

Finally, by identification one obtains an expression of the localization tensor associated with the grain without twin volume:

$$\boldsymbol{A}^{\bar{g}} = \frac{1}{V_g - V_t}\left[V_g\boldsymbol{A}^g - V_t\boldsymbol{A}^t\right] \tag{22}$$

Extension to polycrystals

In the previous section localization relations were obtained in the case of a double inclusion embedded in an effective medium. These relationships can be used in an elasto-plastic self-consistent method as that derived by Hill and implemented in EPSC [7].

Consider now a different topology whereby it is desired to homogenize the elasto-plastic response of a polycrystal. The effective response of the polycrystal is given by:

$$\dot{\boldsymbol{\Sigma}} = \boldsymbol{L}^{eff} : \dot{\boldsymbol{E}} \tag{23}$$

Here $\dot{\Sigma}$ denotes the macroscopic Cauchy stress rate. Using the same tangent/ incremental approach, the local constitutive response of each crystal is written as:

$$\dot{\sigma}^c = L^c \dot{\varepsilon}^c \tag{24}$$

The superscript c refers to a crystal. Note that, with the linearization adopted here the grain modulus is dependent on the grain shape and on its plastic history. In the self-consistent approach it is assumed that each crystal is embedded in an infinite medium with properties and behavior equal to that of the polycrystal.

From this point two cases are to be identified: either a twin domain has formed within a grain or not. Therefore two different types of localization relations have to be used.

Twin free grains

Following similar steps as that of Hill [8], the equivalent inclusion method leads to the following relationship between the

$$(\dot{\sigma}^c - \dot{\Sigma}) = -L^{eff} : \left(S^{-1} - I\right) : \left(\dot{\varepsilon}^c - \dot{E}\right) \tag{25}$$

From (25), the effective stiffness L^* tensor can be defined as:

$$L^* = L^{eff} : \left(S^{-1} - I\right) \tag{26}$$

S denotes the elasto-plastic Eshelby tensor. Using the local and global constitutive responses, the following localization relationship can be obtained:

$$\dot{\varepsilon}^c = A^c : \dot{E} \tag{27}$$

where

$$A^c = \left(L^c + L^*\right)^{-1} : \left(L^{eff} + L^*\right). \tag{28}$$

Grains containing a twin domain

In existing approaches whether a grain contains a twin or not, equation (28) is used to quantify the localization tensor of the crystal. In the present approach, it is acknowledged that when a grain contains a twin, the topology of the problem has changed and becomes equivalent to that treated in equations. Therefore, in grains containing twins, it is necessary to separate the twin and parent phases and use:

$$A^c = A^t \text{ for the twin phase} \tag{29}$$

and

$$A^c = A^{gt} \text{ for the parent phase} \tag{30}$$

With this, a direct micromechanical coupling between the different phases is introduced.

Self consistency

Finally, the effective response of the material is obtained by considering macro-homogeneity conditions. Focusing on the strain increment one has:

$$\dot{E} = \left\langle \dot{\varepsilon}^c \right\rangle \tag{30}$$

Here terms in brackets denote volume averages. In addition, if one introduces the localization relations into the macro-homogeneity condition on stress, the effective tangent modulus of the polycrystal can be uniquely determined self-consistently with:

$$L^{eff} = \left\langle L^c A^c \right\rangle \left\langle A^c \right\rangle^{-1} \tag{31}$$

Conclusion

In this work, a new self-consistent homogenization scheme is introduced in order to accurately predict the development of internal strains during twinning in polycrystals. The model is based on the introduction of new localization functions introducing a direct coupling between parent and twin domains. These are obtained by extending a generalized Tanaka Mori method to an elasto-plastic medium. While this has not been done yet, the model is well suited to be applied to the case of pure polycrystalline Mg. Among others it would be necessary to study the effect of these new localization relations on the predictions of internal stress in twins.

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