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ON ACCOUNTING FOR DEFORMATION BY TWINNING IN THE THEORY OF MICROSTRAINS

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ABSTRACT

In a variety of known plasticity models it is assumed that inelastic deformation occurs by plastic slip in crystals with different orientations which is true for many common polycrystalline metals. However, another mechanism of inelastic deformation, known as mechanical twinning, is dominant for a wide range of magnesium, aluminum, titanium, nickel, copper and other alloys. For modeling materials which exhibit twining the generalized variant of the theory of microstrains is developed. Heterogeneity of a representative volume element is modeled by introducing a domain of micro particles with different yield limits and orientations. At the scale of micro particles both twinning and slip deformation laws, which account for particle interaction, are introduced. Connection between mechanical behavior of particles and entire representative volume element is accomplished by introducing averaging rule and Kroner-type relation.Proposed variant of the theory can be used for predicting material`s response to complex unproportional and cyclic loading.

INTRODUCTION

Modern industry demands the development of new experimentally verified constitutive models. The simplicity of the created theories was the demand of last few decades, but it is not true anymore. Accurate description of material's response in the most complex situations is a first priority now. Such direction is supported by modern experimental and computational equipment. Irreversible deformation in real polycrystalline and multiphase materials develops on multiple size scales simultaneously [1].

One of the microstructural models, which gives good results for a wide range of polycrystalline materials is the theory of plasticity which accounts the microstrains [2]. This theory does not emphasize individual microscopic features, but approximately reproduces material's micro structure, grain interaction laws, response of a single crystal and tends to capture only statistical laws of inelastic deformation. To account of the heterogeneity of plastic deformation which presents the consequence of grained structure and various lattice defects, a representative volume element (RVE) is used as the domain of micro particles of an arbitrary nature. Plastic strain of the RVE is formed by local plastic strains of all micro particles. So the core assumption of the theory is that overall statistical response of anisotropic crystals can be approximated by isotropic particles with different orientations and yield limits.

Experimental verification showed that the proposed approach allowed the modeling of material's response to non-proportional loading with good accuracy. It was also shown that the theory can handle nontrivial unsymmetrical cyclic behavior.

However in the theory of microstrains and in many other well-known plasticity models it is assumed that inelastic deformation occurs only by plastic slip. This assumption is true for many commonly used metals. However, recent researches showed that another mechanism of inelastic deformation, known as mechanical twinning, plays a dominant role in a wide range of metallic alloys, which are used in modern branches of industry due to their special and even unusual mechanical properties [1, 3]. Twinning plays the important role in the inelastic deformation of some magnesium,

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aluminum, titanium, nickel, copper and other metallic alloys. Furthermore, inelastic deformation of metals known as shape memory alloys is connected with so-called martensitic transformation, which is a special case of twinning [4, 5].

In the present work, for the purpose of modeling the response of materials which deform by both twining and plastic slip, the generalized variant of the theory of microstrains is developed.

1. GOVERNING EQUATIONS

In the theory of microstrains a RVE is modelled as a domain of micro particles with distinct initial yield limits τ and orientations $\hat{\mu}_0$. Except direct physical meaning, these values serve as a particle's labels. We assume that yield limits are distributed with certain density $\Phi(\tau)$. The domain of all initial orientations we denote as Ω and define it as follows [6]:

$$\Omega = \left\{ \hat{\mu}_0 = \sin\varphi \hat{e} / \sqrt{3} + \cos\varphi \hat{\alpha}, tr\hat{\alpha}_0 = 0, \hat{\alpha} : \hat{\alpha} = w(\xi_\alpha) \right\},$$

where "*tr*" stands for trace, ":" denotes double contraction of tensors, $\hat{e}$ is the second order identity tensor, φ and $w(\xi)$ are material constant and function which govern the influence of hydrostatic pressure and stress state type on the inelastic response, ξ_α is the Lode angle for $\hat{\alpha}$ tensor and it is defined by the following equation:

$$\xi_\alpha = \frac{1}{3}\arctan\frac{(9/2tr(dev\,\hat{\alpha})^3)^{1/3}}{\sqrt{3/2dev\,\hat{\alpha} : dev\,\hat{\alpha}}} \quad ,$$

where "*dev*" is the tensor's deviator.

The constant φ and function $w(\xi)$ allow accounting for the influence of stress state type on the inelastic deformation. It was shown that simple choice $w(\xi) = \delta(\xi - \xi_0)$, where $\xi_0 \in [0..\pi/3]$ is material constant, leads to a wide 2-parametric family of initial yield surfaces which allow accounting for strength differential effect:

$$-\sqrt{3}\sin\varphi p + \sqrt{2/3}\cos\varphi\cos\left(\xi_0 - \theta\right)q - \tau_{min} = 0,$$

where p is hydrostatic pressure, q is von Mises equivalent stress, θ is Lode angle and τ_{min} is the minimum yield limit of all particles.

Also by assuming $w = 1$ and $\varphi = 0$ we can obtain the original variant of the theory [2] which leads to von Misses initial yield condition.

Orientation of a micro particle may change from original in the course of inelastic deformation, so we denote current orientation as $\hat{\mu}$. The current orientation defines the direction for development of inelastic deformation. Generally both plastic and twinning deformation can occur in a micro particle:

$$\dot{\hat{\varepsilon}}_p(\hat{\mu}_0,\tau) = \dot{\lambda}(\hat{\mu}_0,\tau)\hat{\mu} \;, \quad \dot{\hat{\varepsilon}}_{tw}(\hat{\mu}_0,\tau) = \dot{\eta}(\hat{\mu}_0,\tau)\hat{\mu},$$

where $\hat{\varepsilon}_p$ and $\hat{\varepsilon}_{tw}$ are plastic and twinning strain tensors, $\dot{\lambda}$ and $\dot{\eta}$ are plasticity and twinning parameters.

Like in a classical flow theories, the plasticity parameter $\dot{\lambda}$ is required to be positive during the process of active plastic straining: $\dot{\lambda}\left(\hat{\mu}_0,\tau\right) > 0$. The twinning parameter $\dot{\eta}$ is positive if the active twinning process takes place. However, unlike the plasticity parameter, it may also be negative during the detwinning. So, one of the following equations holds, depending on the direction of the process: $\dot{\eta}\left(\hat{\mu}_0,\tau\right) > 0$ or $\dot{\eta}\left(\hat{\mu}_0,\tau\right) < 0$. Another important feature of the twinning process is the boundedness of twinning strains. Therefore we assume that $0 \le \eta(\hat{\mu}_0,\tau) \le \eta_{max}$, where η_{max} is the maximum possible twinning strain, which is a material constant, and generally can vary from one particle to another. If the twinning parameter reaches one of the critical values, the twinning process stops and the particles can exhibit purely elastic or elastoplastic behaviour. Although a reverse process is possible in this case.

Microscopic inelastic deformation starts when the local yield or twinning condition is satisfied: $F(\hat{\tau}) = 0$, where $\hat{\tau}$ is defined separately for twinning, detwinning and plasticity:

$$\hat{\tau}(\hat{\mu}_0,\tau) = \begin{cases} \hat{\sigma}(\hat{\mu}_0,\tau) - \hat{\rho}_1(\hat{\mu}_0,\tau) \text{ for plasticity,} \\ \hat{\sigma}(\hat{\mu}_0,\tau) - \hat{\rho}_2(\hat{\mu}_0,\tau) \text{ for twinning,} \\ \hat{\sigma}(\hat{\mu}_0,\tau) - \hat{\rho}_3(\hat{\mu}_0,\tau) \text{ for detwinning.} \end{cases}$$

In the last equation tensors $\hat{\rho}_i, i = 1,2,3$ define internal stresses which appear in a micro particle due to interaction with other particles as a result of inelastic straining. Initial fields of internal stresses and their evolution laws are specified:

$$\hat{\rho}_i(\hat{\mu}_0,\tau)\big|_{t=0} = \hat{\rho}_{i0}(\hat{\mu}_0,\tau),\ i = 1,2,3,$$

$$\dot{\hat{\rho}}_i(\hat{\mu}_0,\tau) = \sum_{j=1}^{3}\int_0^{\infty}\Phi(\tau')d\tau'\int_{\Omega}\tilde{R}_{ij}(\hat{\mu}_0,\tau,\hat{\mu}'_0,\tau'):\dot{\hat{\varepsilon}}_j(\hat{\mu}'_0,\tau')d\Omega',$$

where $\tilde{R}_{ij}(\hat{\mu},\tau,\hat{\mu}',\tau')$ are the fourth rank tensor kernels which govern interaction between particles with different orientations and yield limits, $\hat{\varepsilon}_j$, $j = 1,2,3$ are plastic, twinning and detwinning strains correspondingly.

Let us examine the interaction law. Of course an interaction kernel of any complexity can be introduced however there are no experiments to verify such kernel directly and therefore it is reasonable [1,7] to use simple expressions accounting only for major macroscopic laws of deformation:

$$\tilde{R}(\hat{\mu},\tau,\hat{\mu}',\tau') = \begin{cases} R_1^*\delta_{\mu\mu'}\hat{\mu}\hat{\mu}' + R_2^*\tilde{\mathcal{I}} + R_3^*\hat{\mu}\hat{\mu}', (\hat{\mu},\tau)\in\Omega^*, \\ R_4^*\delta_{\mu\mu'}\hat{\mu}\hat{\mu}' + R_2^*\tilde{\mathcal{I}} + R_3^*\hat{\mu}\hat{\mu}', (-\hat{\mu},\tau)\in\Omega^*, \\ R_2^*\tilde{\mathcal{I}} + R_3^*\hat{\mu}\hat{\mu}', \text{otherwise,} \end{cases}$$

where $\delta_{\mu\mu'}$ is the Dirac's delta function which is nonzero if $\hat{\mu} = \hat{\mu}'$, $\tilde{\mathcal{I}}$ is the fourth rank isotropic identity tensor and R_k^* are scalar material functions, which are defined as follows:

$$R_k^* = \frac{R_k(\tau,\xi)}{w^2(\xi_\mu)}, k = 1,3,4,$$

$$R_2^* = G(\xi)\left(R_2(\tau,\xi) + R_{2\rho}(\tau,\xi)\sqrt{\hat{\rho}:\hat{\rho}}\right).$$

In the last expression the term with R_1^* describes the hardening which occurs in the actively deforming particles due to their own inelastic deformation and the $R_1(\tau,\xi_\mu)$ is the corresponding hardening modulus which may be different for particles with different yield limits and Lode angles. However good results can be often achieved by assuming all $R_k = const$. The term with R_2^* describes the hardening of all particles in the direction of macroscopic inelastic strain rate which is equivalent to well-known kinematic hardening mechanism, $R_2(\tau,\xi_\mu)$ is the kinematic hardening modulus and $R_{2\rho}(\tau,\xi_\mu)$ governs the relaxation of internal stresses which is important for modelling materials exhibiting ratcheting. The term with R_3^* as it can be easily observed is responsible for isotropic hardening. And the last term which contains R_4^* governs the behaviour of particles with directions opposite to the actively deforming particles which is important for modelling cyclically unstable materials.

The expression for the local yield function is defined as follows

$$F_{(\hat{\mu}_0,\tau)}(\hat{\tau}) = \cos(\kappa)\hat{\mu}_0:\hat{\tau} + \sin(\kappa) f\sqrt{dev\,\hat{\tau}:dev\,\hat{\tau}} = 0\ ,$$

where κ is the material constant which defines degree of a particle's anisotropy.

Particle's current orientation $\hat{\mu}$ is defined as the gradient of local yield function $F(\hat{\tau})$:

$$\hat{\mu} = \frac{\partial F(\hat{\tau})}{\partial \hat{\tau}}.$$

The macroscopic strain rate is decomposed into sum of elastic, plastic and twinning strains:

$$\langle \hat{\varepsilon} \rangle = \langle \hat{\varepsilon}_e \rangle + \langle \hat{\varepsilon}_p \rangle + \langle \hat{\varepsilon}_{tw} \rangle.$$

Elastic part of the strains is governed by the linear Hooke's law, and elastic constants are assumed to be independent of inelastic strains:

$$\langle \hat{\sigma} \rangle = \tilde{C}^e : \langle \hat{\varepsilon} \rangle, \tilde{C}^e = \frac{1}{E}\left((1+\nu)\tilde{\mathcal{I}} - \frac{\nu}{3}\hat{e}\hat{e} \right),$$

where E and ν are Young modulus and Poisson's ratio.

Macroscopic plastic and twinning strain rates are defined as the integrals over the corresponding domains of active particles:

$$\langle \hat{\varepsilon}_p \rangle = \int_{\Omega_p^*} \hat{\varepsilon}_p G_p(\xi_\mu) d\tau d\Omega, \langle \hat{\varepsilon}_{tw} \rangle = \int_{\Omega_{tw}^*} \hat{\varepsilon}_{tw} G_{tw}(\xi_\mu) d\tau d\Omega.$$

where ξ_μ is the Lode angle for $\hat{\mu}$, $G_p(\xi_\mu)$ and $G_{tw}(\xi_\mu)$ are the weight functions, Ω^* denotes the domain of actively deforming particles.

Additional expression which establishes connection between micro and macro variables is introduced in the form of Kroner's relation:

$$\langle \hat{\sigma} \rangle - \hat{\sigma}(\hat{\mu},\tau) = m\left(\hat{\varepsilon}_p(\hat{\mu},\tau) + \hat{\varepsilon}_{tw}(\hat{\mu},\tau) - \langle \hat{\varepsilon}_p \rangle - \langle \hat{\varepsilon}_{tw} \rangle \right).$$

where m is a material constant which defines the deviation of microscopic stresses and strains from corresponding macroscopic values.

Aforementioned equations form the basic set of the governing equations. Providing all material functions and constants are specified directly, these equations can be used to obtain a relation between stress and strain rates.

CONCLUSIONS

Nowadays available computational potential doesn't limit engineers and even very complex models can be used to simulate mechanical response of real structures. So the microstructural approach in constitutive modeling becomes even more important. This is especially actual for materials which exhibit twinning as they often have a variety of nontrivial physical and mechanical features like strength differential, strong temperature dependence, complex cyclic response, superelasticity and shape memory effect.The variant of the theory of microstrains which accounts for both twinning and plasticity is discussed in the paper. This theory accounts for the heterogeneity of the plastic deformation in a RVE by introducing a domain of interacting micro particles. Such approach allows obtaining well-known hardening mechanisms: isotropic, kinematic and vertex point thus allowing to simulate material`s response to non-proportional loading. Also theory gives good possibilities for modeling plastic strain accumulation in the non-ideal superelasticity, ratcheting and other mechanical effects which appear in complex cyclic processes.

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