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EXTENDING TAYLOR PLASTICITY THEORY FOR MICROSCOPIC SLIP TRANSFER CONDITIONS

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Abstract The main focus of the paper is an extension of the classical Taylor theory of plasticity to include the microscopic conditions for slip transfer at grain boundaries. It is demonstrated that such leads to consideration of the grain boundary character distribution function, in concert with the usual local state distribution function. The primary result is an expression for the generalized Taylor Factor that includes an inverse grain size dependence (Hall-Petch).

1. INTRODUCTION

Most studies in crystal plasticity are based upon Taylor's original 1938 work.[1] Within Taylor's framework the dependence of yield strength on microstructure, beyond lattice orientation, is carried within the critical resolved shear stress for slip. Thus, as the grain size decreases, the critical resolved shear stress is required to increase. This increase in critical resolved shear stress is applied, uniformly across the entire interior of the slipping grains according to the basic assumption of the model (uniform plastic strain or strain rate). It is well known that slip patterns are not uniform over the grain interior. (If they were there would be negligible development of geometrically necessary dislocation content in the grain interior.) It is known, from the evidence of transmission electron microscopy, that certain *microscopic conditions* must exist near grain boundaries and triple junctions within polycrystalline materials, leading to differences in the patterns of dislocation slip near the boundaries, as compared with the grain interior.[2-4]

The purpose of this paper is to introduce a framework in which these microscopic conditions can be incorporated within the classical Taylor model. It will be shown how these considerations lead to a grain-size and grain-boundary-character dependence in the initial yield stress. The results are expressed in the Fourier space of microstructures.

2. BRIEF REVIEW OF TAYLOR PLASTICITY

Let $\overline{F}$ denote the macroscopic plastic deformation gradient tensor. Our focus shall be on initial plastic yielding, and therefore $\overline{F}$ can be separated into $I+\overline{\varepsilon}+\overline{\varpi}$, where I is the second-order identity tensor, $\overline{\varepsilon}$ the infinitesimal strain and $\overline{\varpi}$ the infinitesimal rotation. Let F, ε and ω denote the local (crystallite) plastic deformation gradient, infinitesimal strain and infinitesimal rotation tensors, respectively. Taylor's theory assumes that all grains within the material will undergo the same shape change imposed upon a representative macroscopic sample of the material. Thus,

$$\varepsilon=\overline{\varepsilon}\,. \tag{1}$$

Crystal plastic strain can be accommodated by slip on any compatible set of slip systems, chosen from the set *S*. The deformation gradient associated with slip system $s \in S$ is defined by it associated deformation gradient, strain and rotation tensors: $F^{(s)}$, $\varepsilon^{(s)}$, and $\omega^{(s)}$, respectively. If $\hat{b}^{(s)}$represents the unit slip direction vector, and $\hat{n}^{(s)}$ the unit slip plane normal direction vector associated with slip system *s*, and if $\gamma^{(s)}$ is the scalar slip strength, then

$$F^{(s)}=I+\gamma^{(s)}\hat{b}^{(s)}\otimes\hat{n}^{(s)},\ \varepsilon^{(s)}=\frac{F^{(s)}+F^{(s)^T}}{2}-I,\ \omega^{(s)}=\frac{F^{(s)}-F^{(s)^T}}{2} \tag{2}$$

where superscript *T* denotes the transpose and $\otimes$ denotes the dyadic product. Whenever the slip strengths are sufficiently small ($\gamma^{(s)} << 1$ for all $s \in S$) then to a good approximation

$$F=I+\sum_{S'}(F^{(s)}-I),\ \varepsilon=\sum_{S'}\varepsilon^{(s)},\ \omega=\sum_{S'}\omega^{(s)}, \tag{3}$$

where $S'\subset S$ denotes the set of slip systems that have $\gamma^{(s)}>0$. If $\tau_c^{(s)}$ is taken to be the operative critical resolved shear stress associated with slip system *s*, then the plastic work done is *W*:

$$W=\sum_{s\in S'}\tau_c^{(s)}\gamma^{(s)}\,. \tag{4}$$

The question naturally arises as to what are the possible sets, S', that satisfy the basic compatibility relation embodied in (1). Given that, to first order, the plastic strain tensor ε is volume conservative, and therefore $tr(\varepsilon)$ is zero, it follows that there will generally be five independent components of ε. Therefore, five slip systems, selected from among the set *S*, will be required to satisfy relation (1). Define S to be the set of all possible combinations of slip systems such that the compatibility relation is satisfied; thus,

$$\mathrm{S}=\left\{S'\,|\,S'\subset S;\ \sum_{s\in S'}\varepsilon^{(s)}=\overline{\varepsilon}\right\}. \tag{5}$$

Taylor then postulates that the particular operative set of slip systems is the set S'' that minimizes the plastic work. In mathematical terms

$$S''=S'\subset \mathrm{S}\ni W=\min\,. \tag{6}$$

In cases where more than one set S'' satisfies the same minimum plastic work criterion, then the solution is ambiguous; such cases, however, will not be of further importance to that which follows. The so-called Taylor Factor (TF), $M(\varepsilon^o)$, is defined to be a function of the *unit strain*, ε^o, according to the relation

$$\sigma:\varepsilon=\eta\sigma:\varepsilon^o=\sum_{s\in S''}\tau_c^{(s)}\gamma^{(s)}=\tau_c^o\sum_{s\in S''}\alpha^{(s)}\gamma^{(s)}=\eta M(\varepsilon^o)\,\tau_c^o\,. \tag{7}$$

Here the parameter η scales the imposed strain to the unit strain: $\varepsilon=\eta\varepsilon^o$; the coefficients $\alpha^{(s)}$ scale the critical resolved shear stress to the reference critical resolved shear stress, τ_c^o: $\alpha^{(s)}=\tau_c^{(s)}\big/\tau_c^o$; and σ denotes the Cauchy stress tensor. It is evident that the TF is dependent, not only upon the character of the imposed unit strain, ε^o, but also upon the reference critical resolved shear stress, τ_c^o, the scaling coefficients, $\alpha^{(s)}$, and the slip strain tensors, $\varepsilon^{(s)}$. The latter are clearly dependent upon the orientation of the crystal lattice in which $\hat{b}^{(s)}\otimes\hat{n}^{(s)}$ is fixed; the former (scalar parameters) are dependent upon crystal phase, composition, and other local state parameters. Let $h=h(\phi,g,c,\ldots)$ denote the complete set of local state parameters, including lattice phase ϕ and orientation *g*, chemical composition *c*, and any other pertinent parameters. Then

$$M=M(h\,|\,\varepsilon^o)\,. \tag{8}$$

The macroscopic TF, $\overline{M}(\varepsilon^o)$, is obtained by averaging the local Taylor factors, $M(h\,|\,\varepsilon^o)$, over the representative volume of the sample. If the volume fraction distribution of the local state is defined by

$$dV/V=f(h)dh\,, \tag{9}$$

where *dh* is the appropriate invariant measure on local state space[5], then

$$\overline{M}(\varepsilon^o)=\int_H f(h)M(h\,|\,\varepsilon^o)dh\,, \tag{10}$$

where *H* denotes the complete local state space.

Let ${}^{\phi}T_{lr}^{\mu\nu}(h)$ represent the complete set of orthogonal basis functions for the set of real-valued, square-integrable functions of the form $F:H\rightarrow\Re$. Also, define the Fourier representation of the local state function be

$$f(h)=\sum_{all\ \phi,\mathrm{l},\mathrm{r},\mu,\nu}{}^{\phi}F_{lr}^{\mu\nu}\,{}^{\phi}T_{lr}^{\mu\nu}(h)\,, \tag{11}$$

and the local TF to be

$$M(h\,|\,\varepsilon^o)=\sum_{all\ \phi,\mathrm{l},\mathrm{r},\mu,\nu}{}^{\phi}m_{lr}^{\mu\nu}(\varepsilon^o)\,{}^{\phi}T_{lr}^{\mu\nu}(h)\,. \tag{12}$$

It follows that relation (10) can be expressed, in terms of the Fourier coefficients that define the local state distribution function, ${}^{\phi}F_{lr}^{\mu\nu}$, and the coefficients that define the local Taylor Factor, ${}^{\phi}m_{lr}^{\mu\nu}(\varepsilon^o)$, by the expression

$$\overline{M}(\varepsilon^o) = \sum_{all\ \phi,\mathrm{l},\mathrm{r},\mu,\nu} {}^{\phi}\tilde{m}_{lr}^{\mu\nu}(\varepsilon^o)\,{}^{\phi}F_{lr}^{\mu\nu}, \qquad (13)$$

where ${}^{\phi}\tilde{m}_{lr}^{\mu\nu}(\varepsilon^o) = \beta_l\,{}^{\phi}m_{lr}^{\mu\nu}(\varepsilon^o)$. Further details on the Fourier description are given in the works of Bunge.[5] It is known that relatively small numbers of the coefficients ${}^{\phi}m_{lr}^{\mu\nu}(\varepsilon^o)$ are required for convergence in relation (12), and hence the number of coefficients of the microstructure that are important in (13) is also similarly limited.[6]

3. EXTENSIONS OF TAYLOR PLASTICITY TO INCLUDE MICROSCOPIC CONDITIONS

3.1 Experimental Evidence

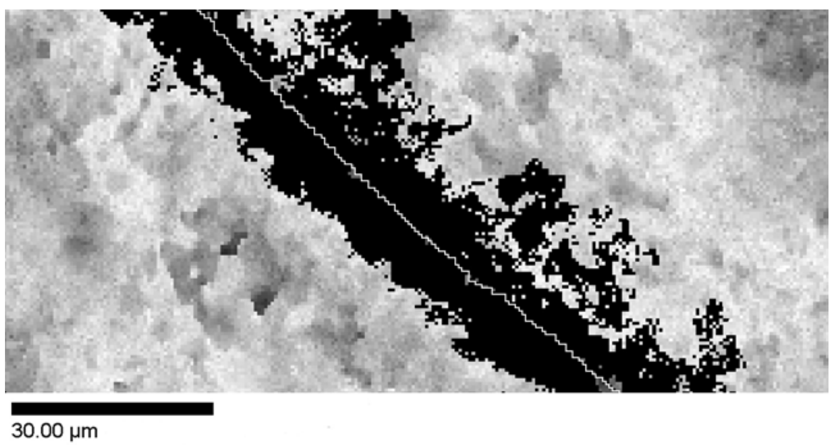

Figure 1. Typical orientation boundary layer in 30% plastically-deformed <001> aluminum.

Figure 1 illustrates the experimental evidence for the modifications to Taylor's fully constrained theory. The sample consists of <001> directionally solidified aluminum, deformed plastically in compression to ~0.30 height reduction. The starting grain size of the material is ~ 5 millimeters. Using fine-scale orientation imaging microscopy[7], the orientation field of material adjacent grain boundaries is observed. The step size of the scan is 0.5 microns. Lattice orientation is determined at each step point, to within $\pm 0.5^o$. In Figure 1 all scan points that lie with 2.5^o of the average orientation in the near boundary zone are shaded black. It is evident that a boundary layer develops adjacent the grain boundaries; and this boundary layer has a distinct orientation compared to that found in the grain interior. The two regions are separated by a system of geometrically necessary dislocations.

3.2 Modified Taylor Theory with Microscopic Conditions

Transmission electron microscopy suggests that certain microscopic conditions favor dislocation slip transmission across grain boundaries.[2-4] These include: a) a minimum of residual net burgers vector is left behind in the grain boundary, b) the shear stress ahead of a slip system pileup, resolved in the adjacent grain, is maximized, and c) the angle of intersection between two adjacent slip systems in the grain boundary plane is minimized.

Here we maintain the basic compatibility requirement that pertains to Taylor's theory, embodied in relation (1). We shall relax, in the vicinity of the grain boundary, however, the minimum plastic work hypothesis of Taylor, embodied in relation (6). In its place we postulate the existence of a microscopic condition that governs the slip patterns near the grain boundary.

Let a local element of the grain boundary have unit normal vector $\hat{n}$. Let it separate grain A and grain B. Let h_A and h_B denote the local state of grain A and B. We suppose that the nominal thickness of the grain boundary layer is *a* in grain A and *b* in grain B. We shall assume that it is only in these regions that Taylor's minimum plastic work criterion must be altered. Let S_A denote the set of all possible slip system combinations that satisfy relation (1) in grain A. Similarly, let S_B denote the set of all possible slip system combinations that satisfy relation (1) in grain B. Following the notational conventions of the previous section, let S_A'' and S_B'' represent the patterns of slip in grains A and B that satisfy the minimum plastic work criterion of Taylor. The associated TFs shall be $M(h_A\,|\,\varepsilon^o)$ and $M(h_B\,|\,\varepsilon^o)$.

Next, consider the boundary layers associated with grains A and B. It is evident from the experimental observations that the slip pattern in the boundary layer in grain A is dependent upon the slip pattern in the boundary layer in grain B, and vice-versa. Without being more specific as to the exact nature of this dependence, let S_A''' denote the correct slip pattern in grain A in the boundary layer of thickness *a*, after due consideration for the pertinent microscopic condition. Similarly, let S_B''' be the associated slip pattern in B within the boundary layer of thickness *b*. Also, let $M(h_A\,|\,\hat{n},h_B,\varepsilon^o)$ be the TF in the boundary layer of grain A, associated with slip pattern S_A'''; and let $M(h_B\,|\,\hat{n},h_A,\varepsilon^o)$ represent the TF in the boundary layer of grain B, associated with slip pattern S_B'''. Also, since it is known that

$$M(h_A\,|\,\hat{n},h_B,\varepsilon^o) \ge M(h_A\,|\,\varepsilon^o),\ M(h_B\,|\,\hat{n},h_A,\varepsilon^o) \ge M(h_B\,|\,\varepsilon^o), \quad (14)$$

it is useful to define the Excess TF, ΔM, in the following way:

$$\begin{aligned} \Delta M(h_A\,|\,\hat{n},h_B,\varepsilon^o) &= M(h_A\,|\,\hat{n},h_B,\varepsilon^o) - M(h_A\,|\,\varepsilon^o), \\ \Delta M(h_B\,|\,\hat{n},h_A,\varepsilon^o) &= M(h_B\,|\,\hat{n},h_A,\varepsilon^o) - M(h_B\,|\,\varepsilon^o) \end{aligned} \quad (15)$$

The new macroscopic TF, $\tilde{\bar{M}}(\varepsilon^o)$ now contains two terms:

$$\tilde{\overline{M}}(\varepsilon^o) = \overline{M}(\varepsilon^o) + \tilde{M}(\varepsilon^o), \tag{16}$$

where $\overline{M}(\varepsilon^o)$ is the original TF, defined via the local state distribution function through relation (10), and $\tilde{M}(\varepsilon^o)$ is defined by

$$\tilde{M}(\varepsilon^o) = \frac{1}{2} \int_{H \times S^2 \times H'} S_V(h_A, \hat{n}, h_B) \begin{bmatrix} a\Delta M(h_A \mid \hat{n}, h_B, \varepsilon^o) \\ +b\Delta M(h_B \mid \hat{n}, h_A, \varepsilon^o) \end{bmatrix} dh_A d\hat{n} dh_B, \tag{17}$$

where $S_V(h_A, \hat{n}, h_B)$ is the grain boundary character distribution function.[8] In relation (17) the integration is over the space of possible grain boundary characters, $H \times S^2 \times H'$, where character is defined by local state $h_A \in H$ on side A of the grain boundary, unit normal $\hat{n} \in S^2$ defining the inclination of the boundary plane when passing from side A to side B, and local state $h_B \in H'$ on side B. Only in homophase materials will $H = H'$. (Additional details about this product space have been reviewed in Adams and Olson.[9]) The reader should note that $S_V(h_A, \hat{n}, h_B) dh_A d\hat{n} dh_B$ is equal to the surface area per unit volume of grain boundary that has local state lying in the range dh_A of h_A on side A of the boundary, normal direction lying in the range $d\hat{n}$ of direction $\hat{n}$, and local state lying in the range dh_B of h_B on side B. When multiplied by the Excess TFs, weighted by their thicknesses, contained in the term […] in equation (17), we obtain an approximation for the additional plastic work done due to relaxation of Taylor's minimum plastic work criterion to accommodate a local microscopic criterion. The approximation is valid if $a, b << d$, where d is the grain size of the material.

Note that the dimension of the grain boundary character function is d^{-1}, and therefore the grain boundary term in the Excess TF, $\tilde{M}(\varepsilon^o)$, is also inversely proportional to the grain size of the microstructure. The remainder of its functional dependence is found in the distribution of grain boundary character types within the microstructure.

Constructing a complete orthogonal system of basis functions on $H \times S^2 \times H'$ is achieved with products of the eigenfunctions defined on each separate space.[9] Thus, the Excess TF accepts a Fourier representation of the form

$$M(h_A \mid \hat{n}, h_B, \varepsilon^o) = \sum_{\substack{all\ \phi,\phi',\mathrm{l},\mathrm{l}',\mathrm{r}, \\ \mathrm{r}',\mu,\mu',\nu,\nu'}} {}^{\phi\phi'\mathrm{q}}_{\mathrm{p}} m^{\mu\mu'\nu\nu'}_{ll'rr'}(\varepsilon^o) \, {}^{\phi}T^{\mu\nu}_{lr}(h_A) k^q_p(\hat{n}) \, {}^{\phi'}T^{\mu'\nu'}_{l'r'}(h_B) \tag{18}$$

where $k^q_p(\hat{n})$ are the surface spherical harmonic functions. A similar Fourier representation exists for the grain boundary character distribution function, with coefficients ${}^{\phi\phi'\mathrm{q}}_{\mathrm{p}} G^{\mu\mu'\nu\nu'}_{ll'rr'}$. Thus, an expression like (13) for $\tilde{M}(\varepsilon^o)$ is

$$\tilde{M}(\varepsilon^o) = \sum_{\substack{all\ \phi,\phi',\mathrm{l},\mathrm{l}',\mathrm{r}, \\ \mathrm{r}',\mu,\mu',\nu,\nu'}} {}^{\phi\phi'\mathrm{q}}_{\mathrm{p}} \tilde{m}^{\mu\mu'\nu\nu'}_{ll'rr'}(\varepsilon^o) \, {}^{\phi\phi'\mathrm{q}}_{\mathrm{p}} G^{\mu\mu'\nu\nu'}_{ll'rr'}, \tag{19}$$

where ${}^{\phi\phi'\mathrm{q}}_{\mathrm{p}} \tilde{m}^{\mu\mu'\nu\nu'}_{ll'rr'} = \beta_{ll'} \, {}^{\phi\phi'\mathrm{q}}_{\mathrm{p}} m^{\mu\mu'\nu\nu'}_{ll'rr'}$.

3.3 Exemplary Microscopic Conditions

Next, consider an example of how certain elements of the microscopic conditions can be implemented. We shall consider only criterion a), minimum net Burger's vector in the grain boundary. Let $\hat{n}$ denote the normal to the grain boundary. The net density of Burger's vector left behind in the grain boundary is just

$$\vec{b}_{GB} = \sum_{S_B'''} \gamma^{(s)} \left(\hat{b}^{(s)} \cdot \hat{n}\right) \hat{b}^{(s)} - \sum_{S_A'''} \gamma^{(s)} \left(\hat{b}^{(s)} \cdot \hat{n}\right) \hat{b}^{(s)} . \tag{20}$$

In accordance with microscopic condition a) we shall select S_A''', S_B''' so that $\left\|\vec{b}_{GB}\right\| = \min$. These will be considered to be the operative sets.

Consider the three independent $\{10\bar{1}0\}\langle 11\bar{2}0\rangle$ slip systems in hexagonal crystals. Restrict consideration to $\langle 0001\rangle$ columnar polycrystals. For this case the orientation distribution function is simply defined over the angular interval $[0, \pi/3)$ of rotations about $\langle 0001\rangle$. Figure 2 shows the Excess TF calculated from the minimum residual Burger's vector criterion, where θ_A, θ_B describe the orientations of grains A, B relative to a common reference frame. For this calculation, $\varepsilon_{11}^{o} = 1$ is the only non-zero component of plastic strain, and lies in the (0001) plane. (The symmetry about $\theta_A = \theta_B$ is a consequence of the homophase nature of the boundary, and setting *a*=*b*. The value of the Excess TF is precisely zero on this line.) Evidently, the Excess TF is a complex function of macroscopic grain boundary parameters.

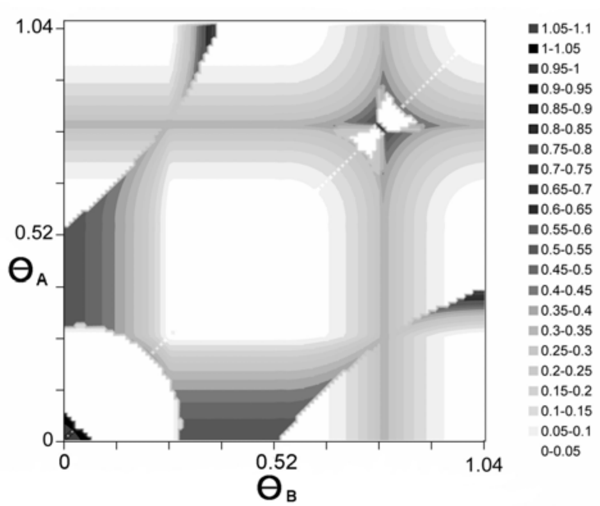

Figure 2. Excess Taylor Factor as a function of orientation parameters θ_A, θ_B (radians).

4. Discussion and Conclusions

We conclude that the incorporation of any of the observed microscopic conditions for slip transfer at grain boundaries, within the classical Taylor theory of plasticity, gives rise to an inverse grain size dependence of the Excess TF. All eight 'macroscopic parameters' of grain boundary character associated with the grain boundary character distribution function are also predicted to affect the Excess TF.

It is evident that the uniform strain criterion of Taylor enforces rather restrictive requirements on plastic deformation, and these will often violate local conditions of stress equilibrium. However, within the Taylor framework it will be important to examine the details of the geometrically-necessary dislocations that are observed to form at the transition region between the boundary layers shown in Figure 1, and the grain interior region. Such considerations may provide sensitive insight into the most appropriate microscopic conditions to apply in conjunction with the Taylor theory.

5. Acknowledgements

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