Supplementary Material for: Grain Size-Inclusion Size Interaction in Metal Matrix Composites Using Mechanism-Based Gradient Crystal Plasticity

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Computational Implementation of MSGCP

For completeness, we give a brief outline of the computational implementation of MSGCP within UMAT.

Plastic slip constitutive law

The kinematics and kinetics of MSGCP approach implemented in this work closely follows the conventional continuum crystal plasticity framework of Asaro and co-workers (Asaro, 1983; Peirce, et al., 1983), except that a length-scale effect is introduced in the slip system hardening. The constitutive law for plastic slip rate $\dot{\gamma}^{\alpha}$ is assumed as

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 . \left|\frac{\tau^{\alpha}}{g_T^{\alpha}}\right|^n . sign(\tau^{\alpha}) \quad \text{(S1)}$$

where $\dot{\gamma}_0$ and τ^{α} are the reference plastic slip rate and resolved shear stress on slip system α and g_T^{α} is the overall hardening of lattice due to both SSD and GND densities. The evolution law for the SSD induced hardening for multiple slip deformation is given by

$$\dot{g}_{SSD}^{\alpha} = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^{\beta} \quad \text{(S2)}$$

where $h_{\alpha\beta}$ is a matrix representing self and latent hardening coefficients given by (Asaro, 1983a,b),

$$h_{\alpha\alpha}(\gamma) = h_0^\alpha sech^2 \left|\frac{h_0\gamma}{\tau_s^\alpha - \tau_0^\alpha}\right| \quad \text{(no sum on } \alpha\text{)} \tag{S3}$$

$$h_{\alpha\beta}(\gamma) = q h_{\alpha\alpha}(\gamma), \quad \alpha \neq \beta \tag{S4}$$

In Eq. (S3), h_0^α is initial hardening modulus, τ_s^α is the saturation value for the resolved shear stress, τ_0^α is the critical resolved shear stress, $\gamma = \sum_\alpha \gamma^\alpha$ is the total cumulative shear strain on all slip systems and q (~ 1-2) is a accounts for the interaction between different slip systems.

In the MSGCP approach, the GND density ρ_g^αon α^{th} slip system is assumed to contribute to its overall hardening via Taylor hardening model. Consequently, g_T^α is given by (Han, et. al. 2005)

$$g_T^\alpha = \tau_0^\alpha \sqrt{\left(\frac{g_{SSD}^\alpha}{\tau_0^\alpha}\right)^2 + l\eta^\alpha} \tag{S5}$$

where the internal material length-scale $l = (a^2 \mu_m^2 b / \tau_0^{\alpha 2})$, with b as the magnitude of Burgers vector, μ_m as the overall shear modulus and a as an empirical material constant ranging between 0.1-0.5. In Eq. (S5), η^α is an effective scalar measure of the GND density tensor on the slip system α

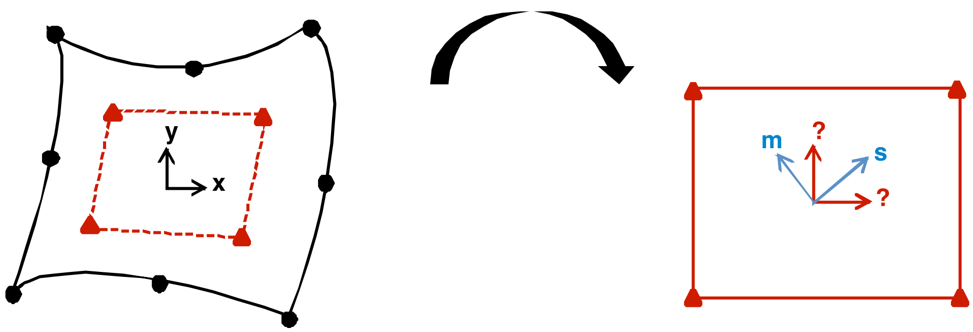
$$\eta^{\alpha} = \left| m^{\alpha} \times \left\{ \sum_{\beta} [s^{\alpha} . s^{\beta}] \nabla \gamma^{\beta} \times m^{\beta} \right\} \right| \tag{S6}$$

where s^{α} and m^{α} are respectively, the slip direction and slip-plane normal for α^{th} slip system. The effective slip gradient is related to the GND density in each slip system via $\rho_g^{\alpha} = \eta^{\alpha}/b$.

Slip gradient calculation

In implementing this length-scale feature within a UMAT, one needs to calculate the slip gradients at each Gauss point (GP). We exploit the concept of shape functions that is at the core of a typical finite element (FE) formulation for evaluating the slip gradients corresponding to each slip systems. For illustration purposes, we present the formulation applicable for an 8-node plane strain finite element, but the approach can be extended to different types of FE's. As is widely known, the number of GP's in a FE determines the order of integration. The 8-node plane strain element that we adopt here (CPE8R) uses a reduced integration procedure in order to minimize the effects due to shear locking. Therefore, for each FE all the state variables (i.e. individual and total slip, slip gradients, etc.) and stresses are calculated at these GP's. To calculate the plastic slip gradients within an FE, we apply the approach similar to the one is used in calculating strains from displacements in a conventional FE formulation (Cook, et al., 2002). Within a FE, we consider a 4-node *pseudo*-element (Fig. S1) constructed by joining the GP's describable by linear shape functions $N_i^{'}$ $(i = 1 - 4)$. The local isoparametric coordinates (ζ and η) of the pseudo-element are related to the global coordinates x and y via the determinant J of the Jacobian matrix (Cook, et al., 2002)

$$\begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{bmatrix} = J^{-1} \begin{bmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \end{bmatrix} \tag{S7}$$



(a) (b)

Figure S1. (a) An Eight-node plane strain FE with four GPs and (b) a linear pseudo-element constructed from the GPs of the actual FE where ξ and η are the local isoparametric coordinates. The slip and normal directions (s and m) of a typical slip system α are also shown (b).

The slip gradient vector $\nabla\gamma^{\alpha}$ in the slip direction s^{α} within each element is obtained using the chain rule of partial differentiation

$$\nabla\gamma^{\alpha} = \frac{\partial\gamma^{\alpha}}{\partial x}\frac{\partial x}{\partial s^{\alpha}} + \frac{\partial\gamma^{\alpha}}{\partial y}\frac{\partial y}{\partial s^{\alpha}} \tag{S8}$$

and the Cartesian slip gradients are related to the pseudo-element shape functions by

$$\frac{\partial \gamma^{\alpha}}{\partial x} = \sum_{i=1}^{4} \frac{\partial N_i{}'}{\partial x} \gamma_i^{\alpha}; \qquad \frac{\partial \gamma^{\alpha}}{\partial y} = \sum_{i=1}^{4} \frac{\partial N_i{}'}{\partial y} \gamma_i^{\alpha} \tag{S9}$$

where γ_i^{α} is the plastic slip at i^{th} pseudo-node (i.e. GP of the actual FE) and on α^{th} slip system[1]. The Cartesian derivatives of N_i' (Eq. S9) are calculated using Eq. (S7).

Time integration scheme

The time integration used in the UMAT is based on the implementation by Huang (1991), but contains augmented information about the GND effects. For completeness, we summarize the method here. The incremental slip on α^{th} slip system is

$$\Delta\gamma^{\alpha} = \Delta t[(1-\theta)\dot{\gamma}^{\alpha}(t) + \theta\dot{\gamma}^{\alpha}(t+\Delta t)] \tag{S10}$$

where the parameter θ is introduces a linear interpolation between value of slip rate $\dot{\gamma}^{\alpha}$ at the beginning and end of the time increment (Peirce et al, 1984). The $\theta = 0$ degenerates to Euler forward time integration scheme, but the recommended value is 0.5. Eq. (S10) can be solved using Newton-Raphson technique

$$\Delta\gamma^{\alpha} - \Delta t(1-\theta)\dot{\gamma}^{\alpha}(t) - \Delta t\theta\dot{\gamma}^{\alpha}(t+\Delta t) = 0 \tag{S11}$$

Then, the plastic slip rate is computed as

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[1] This is similar to the one adopted in ABAQUS to calculate strain from nodal displacements u, e.g., $\varepsilon_{xx} = \frac{\partial u}{\partial x} = \sum_{i=1}^{4} \frac{\partial N_i}{\partial x} u_i$

$$\dot{\gamma}^{\alpha}(t+\Delta t) = \dot{\gamma}_0 . \left|\frac{\tau^{\alpha}+\Delta\tau^{\alpha}}{g^{\alpha}+\Delta g^{\alpha}}\right|^{n} . sign(\tau^{\alpha}+\Delta\tau^{\alpha}) \quad \text{(S12)}$$

Here, the values of stress and solution dependent state variables are evaluated at the end of each time increment and this allows using larger time increment. Further details on the basic implementation of the user subroutine UMAT and incremental formulations can be found in the report by Huang (1991).

Additional References

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