Crystal Plasticity Modeling of Al 7075

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Goal

Predict accurate stress and strain (slip) fields at the grain scale for realistic microstructures subject to cyclic loading.

Key phenomena that should be captured by the model:

- Geometric effects (grain structure)
- Texture effects (orientations)
- Material hardening
- Particle effects
- Damage accumulation (irreversible slip)

Methodology

Methodology focuses on the modeling of grain-scale mechanics and includes development of a constitutive model for crystal plasticity and a finite element formulation for polycrystals. The constitutive model is informed by experimental observations and is based on underlying phenomena.

Constitutive Model

A crystal elasto-viscoplastic model is employed to capture the response of Al 7075-T651.

Decomposition of the deformation gradient into elastic and plastic parts.

$$\mathbf{F} = {}^{e}\mathbf{F}\,{}^{p}\mathbf{F}$$

Velocity gradient given in terms of the slip rate on each slip system.

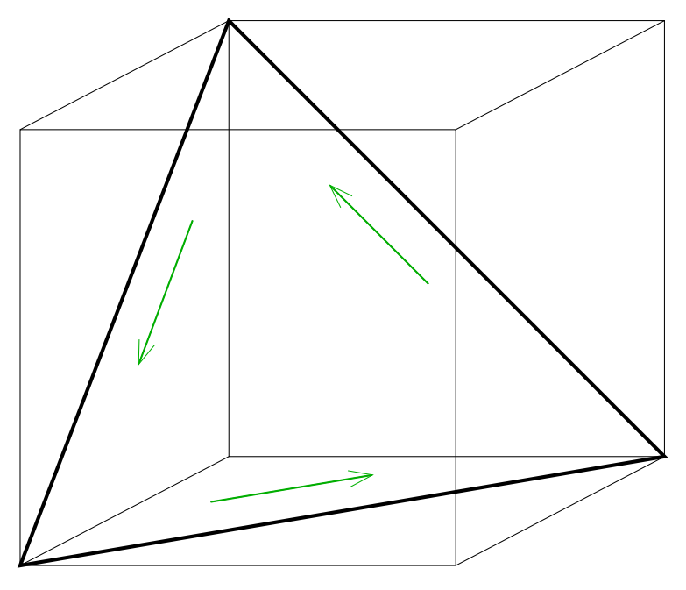
$${}^{p}\hat{\mathbf{L}} = \sum_{\alpha} \dot{\gamma}^{\alpha}\ \mathbf{P}^{\alpha}$$

Plastic Slip Model

The crystal plasticity model captures slip-system activity and the interaction of dislocations with precipitates (Orowan looping).

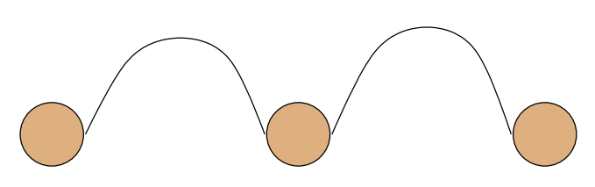
A power law relates rate of shearing on slip systems to resolved shear stress.

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_{o}\frac{\tau^{\alpha}}{g^{\alpha}}\left|\frac{\tau^{\alpha}}{g^{\alpha}}\right|^{\frac{1}{m}-1}$$



Evolution of resistance to plastic slip (hardening) is based on the Orowan looping mechanism.[1–3]

$$\dot{g}^{\alpha} = G_{o}\left(\frac{g_{s}-g^{\alpha}}{g_{s}-g_{o}}\right)\sum_{\beta} 2\left|\mathrm{S}_{ij}^{\alpha}\,\mathrm{S}_{ij}^{\beta}\right|\left|\dot{\gamma}^{\beta}\right|$$



Finite Element Formulation

The finite element implementation allows for the modeling of realistic grain structures. A three-dimensional formulation with additional pressure variable is utilized for stability.

Governing equations:

$$\left(\sigma_{ij}^{\prime} + p\,\delta_{ij}\right)_{,j} = 0 \qquad \frac{1}{3}\sigma_{ii} - p = 0$$

Corresponding weak forms (total Lagrangian) with interpolation functions:

$$\underbrace{\int_{\Omega_o}\left(\sigma_{ij}^{h^{\prime}} + p^{h}\,\delta_{ij}\right)\psi_{\alpha,K}\mathrm{F}_{Kj}^{-1}J d\Omega_o}_{f_{i\alpha}^{\mathrm{int}}(\bar{\mathbf{u}},\bar{\mathbf{p}})} - \underbrace{\int_{\partial\Omega_{2o}}\hat{t}_i\psi_{\alpha}\frac{d\Gamma}{d\Gamma_o}d\Gamma_o}_{f_{i\alpha}^{\mathrm{ext}}} = 0$$

$$\underbrace{\int_{\Omega_o}\frac{1}{\mathrm{K}}\left(\frac{1}{3}\sigma_{ii}^{h} - p^{h}\right)\widetilde{\psi}_{\rho}J d\Omega_o}_{h_{\rho}(\bar{\mathbf{u}},\bar{\mathbf{p}})} = 0$$

Linearized equations:

$$\begin{aligned}\mathrm{K}_{i\alpha j\beta}^{r}\,\Delta\bar{u}_{j\beta} + \mathrm{G}_{i\alpha\varphi}^{r}\,\Delta\bar{p}_{\varphi} &= f_{i\alpha}^{\mathrm{ext}} - f_{i\alpha}^{\mathrm{int}}\left(\bar{\mathbf{u}}^{r},\bar{\mathbf{p}}^{r}\right)\\ \mathrm{H}_{\rho j\beta}^{r}\,\Delta\bar{u}_{j\beta} + \mathrm{M}_{\rho\varphi}^{r}\,\Delta\bar{p}_{\varphi} &= 0 - h_{\rho}\left(\bar{\mathbf{u}}^{r},\bar{\mathbf{p}}^{r}\right)\end{aligned}$$

Discontinuous interpolations for $\bar{p}_{\varphi}$ allow for a $\Delta\bar{\mathbf{p}}$ solution on the element level:

$$\Delta\bar{p}_{\varphi} = -\mathrm{M}_{\varphi\rho}^{r^{-1}}\left(h_{\rho}\left(\bar{\mathbf{u}}^{r},\bar{\mathbf{p}}^{r}\right) + \mathrm{H}_{\rho j\beta}^{r}\,\Delta\bar{u}_{j\beta}\right)$$

Implementation

Constitutive model and finite-element formulation were implemented in C++.

Key features of the formulation:

- Finite strain
- Stable mixed displacement/pressure formulation
- State update routine for elasto-viscoplastic crystal constitutive model
- Consistent tangent formulation for fast convergence

Finite-element driver:

- Utilizes MPICH for parallel processing
- PETSc software package used for solving global system of equations

Calibration Results

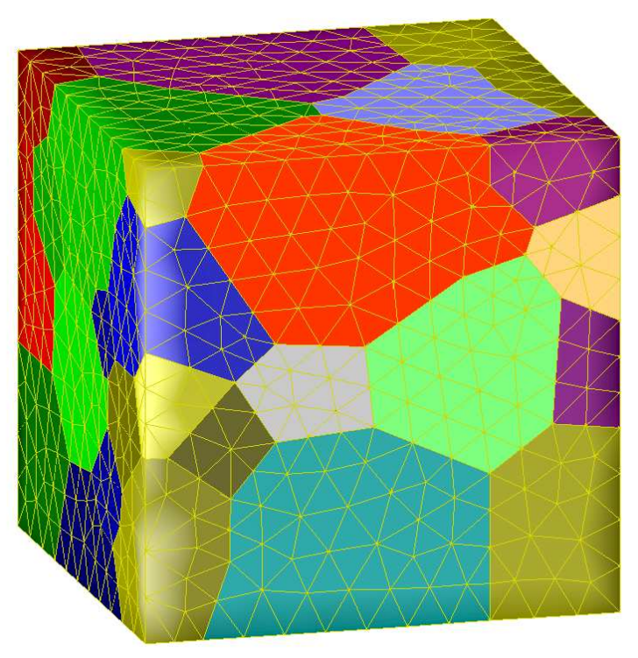
The crystal plasticity model was calibrated against monotonic and cyclic experimental data (Mississippi State, Northrop-Grumman).

MODEL PARAMETERS FOR AL 7075

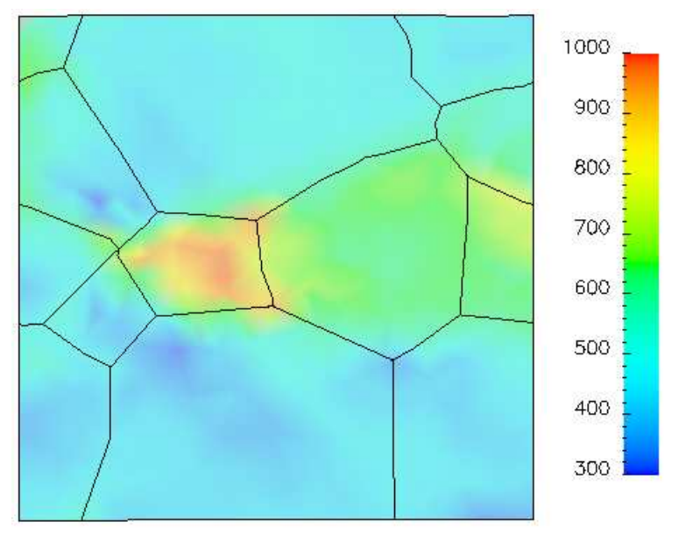
m	0.005	g_s	250 MPa
g_o	220 MPa	μ	28.3 GPa
$\dot{\gamma}_o$	1.0 s^{-1}	λ	60.9 GPa
G_o	120 MPa	η	5.1 GPa

Results

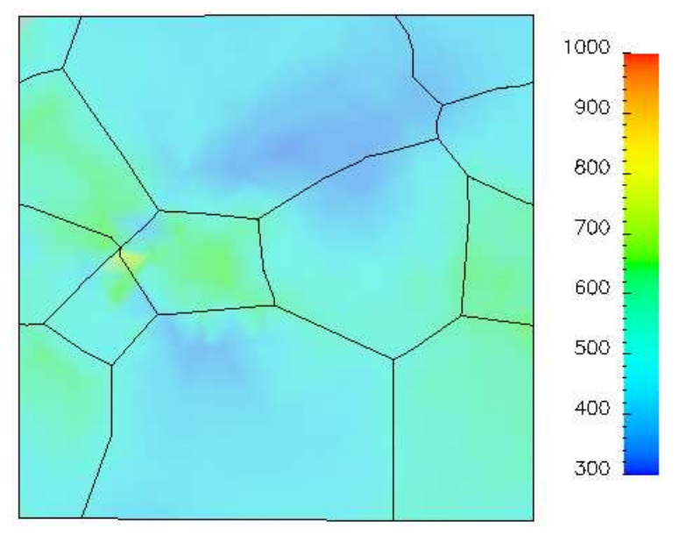
Finite-element analysis of a polycrystal with an embedded particle was carried out using two different sets of grain orientations. The particle was modeled as linear elastic. Results show the influence of grain orientation on material response.



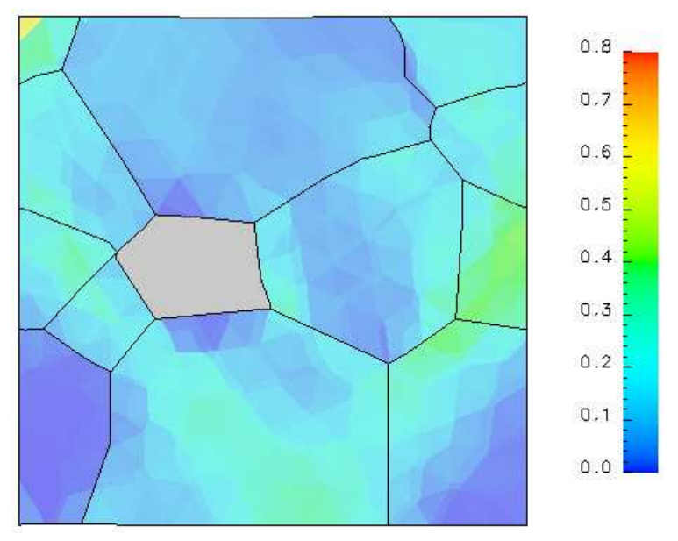
REPRESENTATIONAL VOLUME ELEMENT (PARTICLE SHOWN IN GRAY).



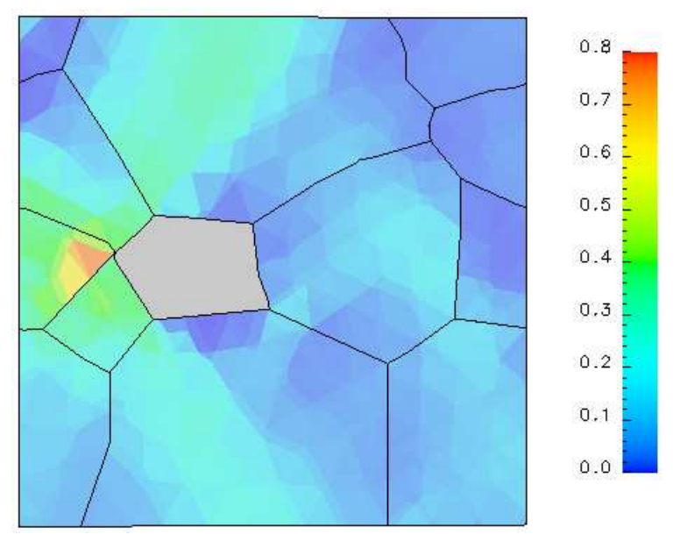
TENSILE STRESS AT 1.5% STRAIN FOR FIRST SET OF ORIENTATIONS.



TENSILE STRESS AT 1.5% STRAIN FOR SECOND SET OF ORIENTATIONS.

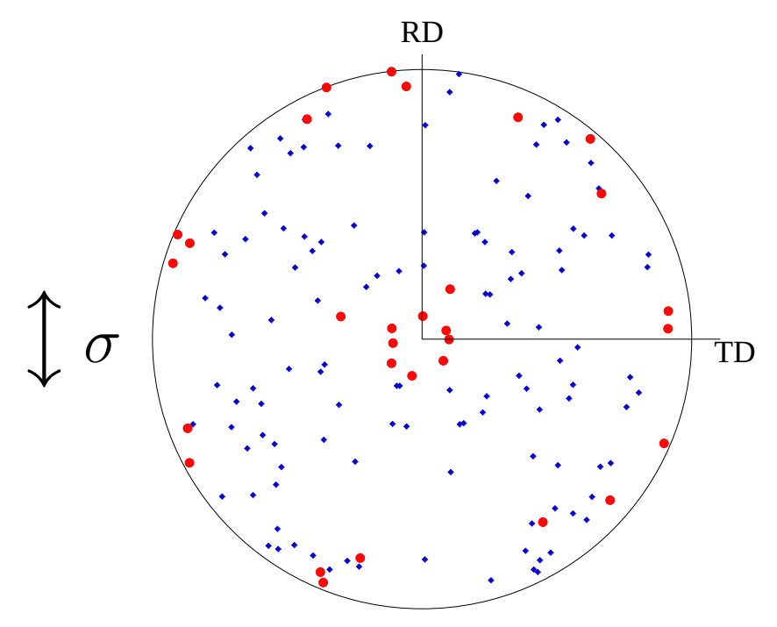


ACCUMULATED PLASTIC SLIP AFTER TWO CYCLES OF 1.5% STRAIN FOR FIRST SET OF ORIENTATIONS.

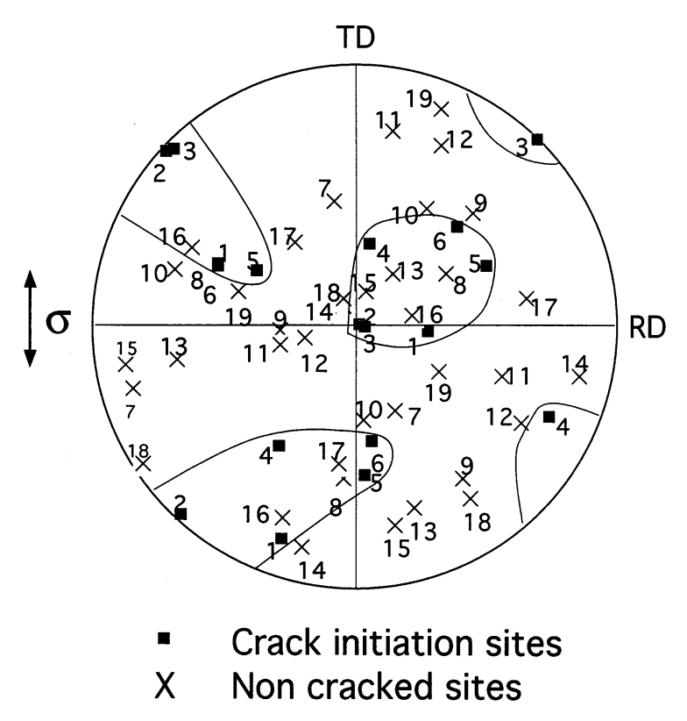


ACCUMULATED PLASTIC SLIP AFTER TWO CYCLES OF 1.5% STRAIN FOR SECOND SET OF ORIENTATIONS.

A series of simulations on a single crystal with an embedded particle show a relationship between grain orientation and plastic slip accumulation.



MODEL RESULTS: (100) POLE FIGURE FOR AL-7075 LOADED IN THE ROLLING DIRECTION (HIGH-SLIP ORIENTATIONS HOWN IN RED).



EXPERIMENTAL RESULTS FROM PATTON *et al.* [4] : (100) POLE FIGURE FOR AL-7010 LOADED IN THE TRANSVERSE DIRECTION.

References

[1] U.F. Kocks. A statistical theory of flow stress and work-hardening. *Philosophical Magazine*, 13(123):541–566, 1966.

[2] E.W. Hart. Theory of dispersion hardening in metals. *Acta Metallurgica*, 20(2):275–289, 1972.

[3] C. Schmitt, P. Lipinski, and M. Berveiller. Micromechanical modelling of the elastoplastic behavior of polycrystals containing precipitates — application to hypo- and hyper-eutectoid steels. *International Journal of Plasticity*, 13(3):183–199, 1997.

[4] G. Patton, C. Rinaldi, Y. Bréchet, G. Lormand, and R. Fougères. Study of fatigue damage in 7010 aluminum alloy. *Materials Science and Engineering A*, A254(1-2):207–218, 1998.

[5] D.J. Littlewood and A.M. Maniatty. Multiscale modeling of crystal plasticity in Al 7075-T651. In *Proceedings of the VIII International Conference on Computational Plasticity Fundamentals and Applications*, pages 618–621, Barcelona, Spain, 2005.