Multiscale Polycrystalline Plasticity Model using the Optimal Transportation Meshfree (OTM) Method

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**Introduction**

We present a method for the simulation of crystalline materials under extreme conditions. The thermo-mechanical behavior of polycrystalline metals at the macroscopic scale is inherently multiscale. Therefore, a predictive material model should consider the underlying micro-mechanical processes for the determination of the macroscopic response.

Hypervelocity impact simulations involve very large strains and high pressures and temperatures. The Optimal Transportation Meshfree (OTM) method provides a robust numerical framework for the simulation of solids of arbitrary geometry under such extreme conditions, while exactly conserving linear and angular momentum.

**The Optimal Transportation Meshfree Method**

- The OTM method for general solid flows
- Simulation of Taylor-Bar Impact Test

**Single Crystal Plasticity Model**

We adopt a finite-deformation continuum-mechanics approach to describe plasticity at the subgrain level. Crystallographic slip in metallic materials is the fundamental mechanism of plastic deformations.

As dislocations move along crystallographic planes, slip is generated. Plastic deformations are the result of slip in multiple crystallographic planes, motivating the crystallographic flow rule

\[ \mathbf{L}^p = \mathbf{F}^{p-1} \mathbf{F}^p = \sum \mathbf{f} \otimes \mathbf{m}^k \]

Dislocation-based forest-hardening model accounts for dislocation evolution and interaction, yielding predictive response.

Crystal Elasticity: Work Hardening: Rate Dependency:

\[ \mathbf{F} = \frac{\partial W}{\partial \mathbf{F}} \quad \mathbf{g}^p = \frac{\partial W}{\partial \mathbf{g}^p} \quad \mathbf{y}^p = \frac{\partial \mathbf{g}^p}{\partial \mathbf{y}^p} \left\{ \begin{array}{ll} \mathbf{g}^p \frac{1}{m} & \text{if } \mathbf{y}^p \geq 0 \\ 0 & \text{otherwise} \end{array} \right. \]

Numerical time integration of elasto-viscoplastic crystal model is done using variational constitutive updates.

**Constitutive Model Validation**

- Universal Tension Test in Cu Single Crystal
- Single crystal uniaxial tension tests and numerical simulations using a dislocation-based hardening model.

**Simulation of Taylor-Bar Impact Test**

Using the proposed model, we have simulated a Taylor-bar impact test for polycrystalline copper.

- Sample dimensions: diameter = 6.4mm, length = 32.4mm
- Impact velocity : 227 m/s
- Untextured polycrystal - crystals are currently assigned random orientation.
- See “Full-Field Experimental Methods for Validation of Multiscale Polycrystalline Plasticity Models” for efforts toward textured polycrystals
- Goal: Simulation up to t=80μs, after which all kinetic energy is transformed into plastic deformation

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