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PII: S0749-6419(15)00125-4
DOI: 10.1016/j.ijplas.2015.07.007
Reference: INTPLA 1946

To appear in: *International Journal of Plasticity*

Received Date: 27 March 2015

Revised Date: 17 July 2015

Please cite this article as: Luscher, D.J., Mayeur, J.R., Mourad, H.M., Hunter, A., Kenamond, M.A., Coupling continuum dislocation transport with crystal plasticity for application to shock loading conditions, *International Journal of Plasticity* (2015), doi: 10.1016/j.ijplas.2015.07.007.

Coupling continuum dislocation transport with crystal plasticity for application to shock loading conditions

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Abstract

We have developed a multi-physics modeling approach that couples continuum dislocation transport, nonlinear thermoelasticity, crystal plasticity, and consistent internal stress and deformation fields to simulate the single-crystal response of materials under extreme dynamic conditions. Dislocation transport is modeled by enforcing dislocation conservation at a slip-system level through the solution of advection-diffusion equations. Nonlinear thermoelasticity provides a thermodynamically consistent equation of state to relate stress (including pressure), temperature, energy densities, and dissipation. Crystal plasticity is coupled to dislocation transport via Orowan's expression where the constitutive description makes use of recent advances in dislocation velocity theories applicable under extreme loading conditions. The configuration of geometrically necessary dislocation density gives rise to an internal stress field that can either inhibit or accentuate the flow of dislocations. An internal strain field associated with the internal stress field contributes to the kinematic decomposition of the overall deformation. The paper describes each theoretical component of the framework, key aspects of the constitutive theory, and some details of a one-dimensional implementation. Results from single-crystal copper plate impact simulations are discussed in order to highlight the role of dislocation transport and pile-up in shock loading regimes. The main conclusions of the paper reinforce the utility of the modeling approach to shock problems.

Keywords: crystal plasticity, shock waves, dislocations, dynamics

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1. Introduction

An improved mechanistic understanding of the mesoscale response of materials under extreme dynamic loading conditions is required to enable predictive physics-based modeling of macroscale response under such conditions. These environmental extremes often include large pressures, deformations, and deformation rates. The response of materials to such environments involves complex physical processes, for example, the nucleation of voids and their subsequent growth and interaction, nucleation of twins, phase changes, and the formation of shear bands. Many of these physical processes occur over length and time scales that are prohibitively small to explicitly resolve within macroscale calculations.

Mesoscale modeling and simulation can provide a physical connection between important microstructural processes (e.g. plasticity, damage nucleation, phase transformation, twinning) occurring under environmental extremes and macroscale models of engineered performance. In the case of polycrystalline materials, this connection can be established via theoretical and numerical mesoscale models of polycrystal response, only if such models include accurate descriptions of the underlying single crystal physics. In addition, mesoscale simulation results can assist in the interpretation of experimental observations in many cases. Together, mesoscale modeling and experiments with high-resolution diagnostics can inform the development of improved macroscale damage and plasticity models.

For example, plate impact experiments have been conducted to gain a better understanding of the conditions leading to nucleation of voids in single and polycrystalline copper (Cao et al., 2010; Perez-Bergquist et al., 2011; Cerreta et al., 2012; Han et al., 2012). These experimental results can be used to formulate