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A dislocation density-based continuum model of the anisotropic shock response of single crystal α-cyclotrimethylene trinitramine

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ABSTRACT

We have developed a model for the finite deformation thermomechanical response of α-cyclotrimethylene trinitramine (RDX). Our model accounts for nonlinear thermoelastic lattice deformation through a free energy-based equation of state developed by Cawkwell et al. (2016) in combination with temperature and pressure dependent elastic constants, as well as dislocation-mediated plastic slip on a set of slip systems motivated by experimental observation. The kinetics of crystal plasticity are modeled using the Orowan equation relating slip rate to dislocation density and the dislocation velocity developed by Austin and McDowell (2011), which naturally accounts for transition from thermally activated to dislocation drag limited regimes. Evolution of dislocation density is specified in terms of local ordinary differential equations reflecting dislocation–dislocation interactions.

This paper presents details of the theory and parameterization of the model, followed by discussion of simulations of flyer plate impact experiments. Impact conditions explored within this combined simulation and experimental effort span shock pressures ranging from 1 to 3 GPa for four crystallographic orientations and multiple specimen thicknesses. Simulation results generated using this model are shown to be in strong agreement with velocimetry measurements from the corresponding plate impact experiments. Finally, simulation results are used to motivate conclusions about the nature of dislocation-mediated plasticity in RDX.
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1. Introduction

Explosives can initiate under impacts whose energy, if distributed homogeneously throughout the material, translates to temperature increases that are insufficient to drive the rapid chemistry observed (Bowden and Yoffe, 1948, 1952). Heterogeneous thermomechanical interactions at the meso-scale (i.e. between single crystal and homogenized macroscale) lead to the formation of localized hot spots within the material. Direct numerical simulations of meso-scale responses can contribute to our understanding of the evolution of hot spots if they include the relevant deformation mechanisms that are essential to the nonlinear thermomechanical response of explosive molecular crystals.

Crystal plasticity modeling is a mature field in the context of applications to quasi-static deformation problems. Early crystal plasticity models employed phenomenological expressions for the plastic slip kinetics and hardening relations and did not include an explicit representation of dislocations (e.g. Asaro, 1983; Mathur and Dawson, 1989; Kalidindi et al., 1992;

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Bronkhorst et al., 1992). More recent contributions have introduced dislocation density as an evolving field variable (e.g. Roters et al., 2000; Prasad et al., 2005; Ma et al., 2006; Lee et al., 2010; Alankar et al., 2011). Most of these works have focused on metallic single crystals typically comprising cubic or hexagonal crystal symmetry.

There are fewer examples of previous work focused on modeling molecular single crystals, where each lattice site contains a molecule rather than an individual atom. Energetic composites typically employ explosive molecular crystals bonded together with a polymeric adhesive. Thus, meso-scale modeling of explosives motivates improved dynamical models for the response of energetic molecular crystals.

Winey and Gupta (2006) developed a thermomechanical framework for simulating the shock response of single crystals that is strongly connected with its incremental update scheme. For example, their nonlinear thermoelasticity is not based on a governing potential, which could be parameterized from measurement or finer scale atomistic simulations, and instead uses an incremental update approach based on a set of co-rotating elastic moduli and constant Grüneisen tensor. Their approach yielded excellent agreement between measured and simulated velocimetry for impact along the [100] crystallographic direction in single crystal LiF over a range of specimen thicknesses. They extended their dislocation-based plasticity model for application to shock response of the energetic molecular crystal PETN by including a crystallographic shear cracking model. They further extended the incremental linear elasticity to account for nonlinearity by using third-order elastic constants and showed that the nonlinear extension is critical for correctly capturing shock wave profiles. Their dislocation theory defines the velocity of dislocations within the drag-limited regime although it does not restrict dislocation velocity to be less than the shear wave speed. As a consequence, the model may not perform as well for situations in which the material is dislocation starved (i.e. high dislocation velocity) nor at lower dislocation velocities when thermally activated motion past dislocation barriers is the dominant mechanism.

Barton et al. (2009) developed a dislocation-based model for the shock response of the energetic molecular single crystal HMX and calibrated it against interface velocimetry results from four impacts spanning two crystal orientations and two specimen thicknesses. Their model accounts for the phenomenology of both thermally activated and drag-limited dislocation motion. Barton et al. (2009) and Austin et al. (2014, 2015) have applied extensions of this model to predicting the evolving temperature field and coupled thermochemical reactions in the vicinity of a collapsing pore in single crystal HMX.

Clayton and Becker (2012) have developed a single crystal model for the quasi-static deformation of α-RDX which they applied to simulating thermomechanical responses during nanoindentation experiments. They included six slip systems identified from previous indentation experiments (Gallagher et al., 1992; Ramos et al., 2009). The crystallographic slip rate used in their model is based on a power law dependence of the resolved shear stress. Simulated results of the indenter force versus applied displacement demonstrate consistent trends with measurements, although they exhibit discrepancies of approximately 50% with the experimental data points in some cases. They further demonstrated that the simulation results are sensitive to elastic moduli and assumed slip system strength parameters over credible ranges in these parameter values.

De and Zamiri (2014) developed a model for the anisotropic single crystal response of RDX to shock loading conditions, which they calibrated and compared to interface velocimetry data from Hooks et al. (2006) and Cawkwell et al. (2010) for shock impacts on the (111) and (210) crystallographic planes. Competing mechanisms of thermally activated dislocation motion and phonon drag at high velocity are used as motivation for a phenomenological viscoplastic flow stress applied at a slip system level in their model; however, they do not explicitly account for the evolving dislocation density field, nor the corresponding velocities of mobile dislocations. Furthermore, the model of De and Zamiri (2014) only includes three distinct slip systems. Thus while they were able to capture aspects of the measured velocimetry data for two impact orientations, that model is unable to reproduce the elastic–plastic two-wave structure observed for impact on (100) orientations as reported in Hooks et al. (2006, 2011). Furthermore, De and Zamiri (2014) compare their simulation results with experimental data reported by Hooks et al. (2006) that was superseded by data published in an erratum by Hooks et al. (2011).

Josyula et al. (2016) applied a variation on the model developed by De and Zamiri (2014) to simulate quasi-static compression. Whereas Josyula et al. (2016) emphasize the importance of representing dislocation behavior, they omit some of the dislocation-inspired phenomenology of De and Zamiri (2014) instead employing a power-law viscoplastic slip rate. While the modified model includes four additional slip systems not included by De and Zamiri (2014), the results exhibit purely elastic response for compression on (100) planes because the considered slip systems have zero Schmid factor for that orientation.

Advances in experimental diagnostics under development within the shock physics community, such as *in situ* X-ray diffraction and imaging, will provide a better understanding of the mechanisms that accommodate deformation imposed through impact loading (Ramos et al., 2014b). In order to simulate, and ultimately predict, the types of data that will be measured by such diagnostics, models must have a consistent physical basis that explicitly accounts for the evolution of crystal defects.

A new model for the anisotropic, dynamic response of α-RDX is developed here. The model adopts a multiplicative decomposition of deformation consistent with classical finite deformation crystal plasticity models. Nonlinear thermoelasticity is handled in a thermodynamically consistent framework. The thermoelastic deformation is decoupled in order to carefully account for contributions to free energy from purely volumetric deformation based on the equations of state developed by Cawkwell et al. (2016) and parts representing the coupling between dilatation and isochoric deformation of the lattice. The evolution of plastic deformation is based on crystallographic slip, in which the slip rates are related to dislocation activity through the Orowan equation. The velocity of mobile dislocations reflects the natural temporal competition between thermally activated motion past obstacles impeding dislocation motion and phonon drag-limited

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