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Simulation of shock wave propagation in single crystal and polycrystalline aluminum

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ABSTRACT

A thermoelastic–viscoplastic constitutive model has been developed to model high strain rate deformation in single crystal metals. The thermoelastic formulation employs a material Eulerian strain measure, which has recently been shown to converge more rapidly than traditional Lagrangian strain measures for material undergoing large compression. The viscoplastic formulation is based on the physics of dislocation glide and generation as well as their interaction. This model has been implemented into a one-dimensional, extended finite-difference formulation for anisotropic materials and is used to model shock wave propagation in aluminum single crystals, polycrystals, and pre-textured polycrystals for peak shock pressures ranging from 2 to 110 GPa. The model was able to reproduce experimentally measured particle velocity profiles from both plate impact and laser shock experiments performed on single crystals and polycrystals. Simulations showed that the orientation distribution in vapor-deposited polycrystalline samples can affect the observed elastic precursor decay by a factor of two, as well as change the observed response in laser shock experiments from a dual to single-wave shock structure. Simulations performed on cold rolled aluminum samples showed that an increase in the cold rolling reduction caused a decrease in the number of active slip systems, as well as a decrease in the heterogeneity of total accumulated slip. Finally, a coarse-grained analytical model was developed from results of plane wave simulations and was shown to effectively reproduce plastic heterogeneity induced by single crystal orientations. Simulations in this work showed that single crystal effects play a key role in dictating the macroscopically observed response, which suggests high strain rate experiments that omit detailed initial microstructural characterization do not provide sufficient information for complete mechanistic understanding or model validation.

1. Introduction

A significant amount of experimental work has been performed to measure microstructure development in high strain rate and shock loading of single crystal and polycrystalline metals, as well as quantifying the influence of prior processing on the subsequent response (Gilman, 1969; Murr, 1981b). In single crystals, dislocation velocities (Johnston and Gilman, 1959) as well as possible dislocation multiplication mechanisms (Johnston and Gilman, 1960) have been identified using

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etch-pitting experiments. Constitutive relations based on these observations have been tested by comparing the elastic precursor decay observed experimentally with theoretical predictions for symmetrically oriented single crystals (Johnson et al., 1970). For inferred dislocation densities based on elastic precursor decay experiments to match realistic densities, it was shown that stress-based nucleation must also be included, even in single crystals (Gupta et al., 1975). Despite these experimental and constitutive model developments, few studies have aimed at modeling individual dislocation processes at the single crystal level for shock loading, with a few notable past (Johnson et al., 1970; Johnson, 1972) and recent investigations (Winey and Gupta, 2006; Barton et al., 2009; Barton et al., 2011; Lusher et al., 2013; Hansen et al., 2013).

From the viewpoint of extending knowledge of high strain rate single-crystal deformation to the evolving spatio-temporal deviatoric response of polycrystalline metals, experimental characterization has outpaced constitutive modeling efforts. The experimentally observed dependence of macroscopic flow strength on strain, strain rate, and temperature history (Dorn et al., 1948; Lindholm and Yeakley, 1968; Klepaczko, 1975) can be captured using a phenomenological description of the material's evolving structure (Hoge and Mukherjee, 1977; Estrin and Mecking, 1984; Follansbee and Kocks, 1988; Klepaczko and Chiem, 1986). However, to model effects due to material purity (Rohatgi et al., 2001; Murr and Esquivel, 2004) and prior processing or deformation (Murr, 1981a; Kazmi and Murr, 1981; Follansbee and Gray, 1991), which have experimentally been shown to affect the high strain rate and shock response by altering the substructure and instantaneous loading response, a physically-based model that appeals to the actual deformation mechanisms must be employed. The material's initial state has also been shown to influence the spall response. Experiments on pure metals have shown that single crystals possess a significantly higher spall strength than polycrystals (Kanel, 2010). Grain size (Escobedo et al., 2011) and orientation (Vignjevic et al., 2002; Garkushin et al., 2008) have also been shown to influence the void nucleation, growth, and coalescence process, which in turn affects spall strength. Experiments have also shown that prior processing can govern the dominant spall mechanism, where annealed material exhibited ductile fracture mechanisms whereas rolled material exhibited brittle fracture mechanisms (Williams et al., 2013). However, due to the lack of understanding of the substructure development that occurs during the shock loading process, it is difficult to make conclusive arguments concerning the influence of substructure developed during shock loading on the spall response.

Although limited in number, there have been some computational efforts to quantify the high rate continuum response of annealed and pre-textured polycrystals using crystal plasticity simulations. Schoenfeld (1998), Schoenfeld and Kad (2002) and Kad et al. (2002) developed crystal plasticity models for Ta and Ti–6Al–4V based on existing high rate strength models (Johnson and Cook, 1983; Follansbee and Kocks, 1988) and explored the effect of pre-texturing on experiments such as Taylor impact cylinders, penetration of rolled plates, and explosive deep drawing. Although these models were able to quantify the influence of the initial orientation distribution due cold rolling on ballistic performance, these models were unable to include realistic dislocation densities due to cold rolling or interpret the influence of cold rolling on particular deformation mechanisms. A similar phenomenological crystal plasticity model was combined with a high pressure volumetric thermoelastic relation by Becker (2004) to study the influence of peak shock pressure and loading rate on polycrystalline Ta. It was shown that the ratio of shock width to grain size governs residual plastic deformation heterogeneity; however, the physical plastic deformation mechanisms responsible for the change in heterogeneity or the influence of pre-processing cannot be distinguished using this hardening model.

A constitutive model recently developed by Austin and McDowell (2011) has been used to model the high strain rate response of copper, aluminum (Al), and nickel from strain rates ranging from 10^4–10^{10} s^{-1} (Austin and McDowell, 2012). This model distinguishes the mobile and immobile dislocation densities as well as the mechanisms that govern their evolution, including nucleation, multiplication, annihilation, and trapping of dislocations. It has also recently been extended to include single-crystal dislocation evolution laws as well as finite-deformation single-crystal thermoelasticity; however, so far it has only been used in a steady plane wave numerical method to quantify the orientation-dependence of high strain rate single crystal deformation and compare simulation results with existing experiments (Lloyd et al., 2014). In this work the recently-developed single crystal viscoplastic constitutive model will be implemented into a one-dimensional, extended finite-difference method for anisotropic materials to model the spatio-temporal evolution of single crystals subjected to longitudinal shock loading. This finite-difference method allows all three velocity components to vary with respect to the wave propagation direction, which is necessary to model the quasi-longitudinal and quasi-transverse waves that can form in shock wave experiments performed on anisotropic materials. Shock deformation of annealed, preferentially oriented, and cold rolled polycrystals will be examined and compared with existing experimental results. In all three of these cases, experimental microstructures are modeled by employing realistic dislocation densities, orientation distributions, and grain sizes. For cold rolled simulations, results from quasistatic crystal plasticity simulations are used to generate dislocation densities on individual slip systems. Finite-difference simulations of discrete polycrystals are then compared with a coarse-grained model that can be solved analytically for shock wave propagation given an input shock strength, which is based parameterizing results of plane wave propagation simulations.

2. Constitutive model and numerical method

2.1. Thermoelastic–viscoplastic formulation

The volumetric compression achieved in plate impact and laser-shock experiments can comprise a significant portion of the total deformation. In metals and in many other materials, material stiffness has been shown to increase with increasing