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Analysis of shock compression of strong single crystals with logarithmic thermoelastic-plastic theory

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ABSTRACT

A finite strain theory is developed for anisotropic single crystals undergoing shock loading. Inelastic deformation may arise from dislocation slip, twinning, or fracture and crack sliding. Internal energy can generally depend on a logarithmic measure of finite elastic strain, entropy, and an internal variable associated with defect accumulation. A closed form analytical solution is derived for the planar shock response in the thermoelastic regime, at axial stresses up to the Hugoniot elastic limit. In the plastic regime, for highly symmetric orientations and rate independent shear strength, the Rankine–Hugoniot conditions and constitutive relations can be reduced to a set of algebraic equations that can be solved for the material response. The theory is applied towards planar shock loading of single crystals of sapphire, diamond, and quartz. Logarithmic elasticity is demonstrated to be more accurate (i.e., require fewer higher-order elastic constants) than Lagrangian or Eulerian theories for sapphire, diamond, and Z-cut quartz. Results provide new insight into criteria for initiation of twinning, slip, and/or fracture in these materials as well as their strength degradation when shocked at increasingly higher pressures above the Hugoniot elastic limit.

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1. Introduction

The response of solids to shock compression under planar impact has been a subject of intensive study over the past half-century (McQueen, Marsh, Taylor, Fritz, & Carter, 1970), including numerous advances in experiments, theoretical/analytical methods, and numerical techniques. Regarding modeling of related phenomena, much effort has centered on development of the pressure–volume equation-of-state (EOS) applicable for loading regimes or materials (e.g., very high pressures, or isotropic fluids and ductile solids) wherein shear strength and anisotropy are of little or no concern. However, for strong solids–ceramics, minerals, and some metals and alloys, for example – significant shear strength is retained under impact loading at moderate to high pressures. This strength can affect the global response of the material in loading conditions pertinent to ballistic penetration, geologic events, explosions, high-speed vehicular collisions, etc. Microstructure, including grain or constituent orientation and presence of multiple phases, can also significantly affect the shock response (Grady, 1984). In shocked single crystals of high purity which are the focus of the present work, crystal lattice orientation is the primary descriptor of initial microstructure, and it affects anisotropic themoelasticity and orientation-dependent inelasticity (e.g., slip, twinning, and cleavage fracture).

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In Section 2 of this paper, a new finite deformation, anisotropic thermoelastic theory is developed for single crystals, and is applied to study the shock response of oriented crystals of sapphire (α-Al_2O_3), diamond (C), and quartz (α-SiO_2). These materials are considered because (i) they exhibit a high Hugoniot Elastic Limit (HEL), enabling assessment of finite strain effects in their elastic shock response and (ii) ample data on higher-order elastic constants (Graham, 1972; Hankey & Schuele, 1970; Nielsen, 1986; Thurston, McSkimin, & Andreatch, 1966) and planar shock compression experiments (Graham & Brooks, 1971; Fowles, 1967; Lang & Gupta, 2010) exist, enabling model development and validation.

In recent prior work (Clayton, 2013), a finite strain theory based on strain measure $\boldsymbol{D} = \frac{1}{2}(\boldsymbol{1} - \boldsymbol{F}^{-1}\boldsymbol{F}^{-\mathrm{T}})$ was developed and compared to usual nonlinear crystal thermoelasticity (Clayton, 2011a; Thurston, 1974; Wallace, 1972) based on the Green strain $\boldsymbol{E} = \frac{1}{2}(\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F} - \boldsymbol{1})$, where $\boldsymbol{F}$ is the deformation gradient. These are respectively referred to as "Eulerian" and "Lagrangian" theories (Nielsen, 1986; Thomsen, 1972), though both strain measures are referred to material coordinates and are thus admissible in thermodynamic potentials for anisotropic solids [in contrast to the Almansi strain $\boldsymbol{A} = \frac{1}{2}(\boldsymbol{1} - \boldsymbol{F}^{-\mathrm{T}}\boldsymbol{F}^{-1})$, for example, used in isotropic nonlinear elasticity]. Eulerian theory demonstrated advantages with regards to describing the compression and shear reponses of ideal cubic crystals with Cauchy symmetry, and demonstrated greater intrinsic stability (Clayton & Bliss, 2014) than Lagrangian theory for these conditions. Analytical solutions to the planar shock problem were also derived using both models, with predictions compared for sapphire, diamond, and quartz (Clayton, 2013). Neither model was definitively superior for describing the shock response of these real anisotropic single crystals, with elastic constants of up to order three or four necessary in either case. Anisotropic Lagrangian-type nonlinear elastic models of crystals have been used by other authors in numerical simulations of wave propagation (Winey & Gupta, 2004) and spall (Foulk & Vogler, 2010). Recently, the aforementioned Eulerian theory has been applied towards new nonlinear elastic solutions of boundary value problems involving discrete lattice defects (Clayton, in press).

In the novel thermoelastic theory developed in the current work, internal energy is a function of entropy and material logarithmic strain $\boldsymbol{e} = \ln \boldsymbol{U}$, where $\boldsymbol{U}$ is the right stretch in the polar decomposition $\boldsymbol{F} = \boldsymbol{RU} = \boldsymbol{VR}$, with $\boldsymbol{R}$ the rotation. Elastic theory based on Hencky's strain measure $\ln \boldsymbol{V}$ has been used to accurately model isotropic solids at moderate-to-large strains (Anand, 1979), but this Eulerian theory does not apply for anisotropic solids. Regarding the latter, hyperelastic theory based on $\boldsymbol{e}$ has been considered with regards to derivation of higher-order elastic constants in cubic crystals (Dlużewski, 2000), but such theory has remained, until now, untested for stress states involving both pressure and shear such as uniaxial strain shock compression. Success of the logarithmic pressure–volume EOS, to which $\boldsymbol{e}$-based theory degenerates under hydrostatic loading, has been demonstrated (Poirier & Tarantola, 1998). In Section 2.1, a complete thermodynamically consistent nonlinear thermoelasticity theory incorporating $\boldsymbol{e}$ is derived and presented for the first time. A new analytical solution to the planar shock problem for solids obeying this constitutive theory is derived in Section 2.2. Application of the solution to sapphire, diamond, and quartz follows in Section 2.3, wherein advantages of the proposed logarithmic formulation over existing Lagrangian and Eulerian thermoelasticity models become clear.

Recently (Srinivasa, 2012), a promising structure for anisotropic hyperelasticity has been developed that involves decomposition of $\boldsymbol{F}$ into the product of an orthogonal matrix and an upper triangular matrix, with strain energy depending on the latter. This approach, though not explored in the current paper, demonstrates certain advantages regarding computational efficiency and physical interpretation relative to models that use a polar decomposition (e.g., logarithmic theory).

In Section 3, the logarithmic theory is extended to address inelastic deformation, wherein the deformation gradient is split into thermoelastic ($\boldsymbol{F}^{\mathrm{E}}$) and inelastic ($\boldsymbol{F}^{\mathrm{P}}$) parts: $\boldsymbol{F} = \boldsymbol{F}^{\mathrm{E}}\boldsymbol{F}^{\mathrm{P}}$ (Clayton, 2011a; Teodosiu & Sidoroff, 1976), implying existence of a stress free intermediate or natural configuration (Rajagopal & Srinivasa, 1998) from which the material exhibits an instantaneous thermoelastic response. Typical crystal plasticity models of high rate behavior have used the elastic Green strain measure $\boldsymbol{E} = \frac{1}{2}(\boldsymbol{F}^{\mathrm{ET}}\boldsymbol{F}^{\mathrm{E}} - \boldsymbol{1})$ in their nonlinear elastic stress–strain relations (Clayton, 2005a, 2005b; Luscher, Bronkhorst, Alleman, & Addessio, 2013; Vogler & Clayton, 2008; Winey & Gupta, 2006). In Section 3.1 of the current work, logarithmic thermoelastic strain $\boldsymbol{e} = \ln \boldsymbol{U}^{\mathrm{E}}$ is used as a state variable in the internal energy, where $\boldsymbol{F}^{\mathrm{E}} = \boldsymbol{R}^{\mathrm{E}}\boldsymbol{U}^{\mathrm{E}} = \boldsymbol{V}^{\mathrm{E}}\boldsymbol{R}^{\mathrm{E}}$. Inelastic deformation $\boldsymbol{F}^{\mathrm{P}}$ may result from a host of physical mechanisms in single crystals, including dislocation slip (Clayton, McDowell, & Bammann, 2004; Teodosiu & Sidoroff, 1976), deformation twinning (Clayton, 2009), pore collapse (Barton, Winter, & Reaugh, 2009; Clayton, 2008), and/or cleavage fracture on preferred planes (Aslan, Cordero, Gaubert, & Forest, 2011; Clayton, 2006). Thermodynamically consistent elastic–plastic models incorporating logarithmic strain measures have been developed elsewhere for isotropic solids (Xiao, Bruhns, & Meyers, 2007); several known previous logarithmic models for anisotropic elastic–plastic crystals (Barton et al., 2009; Clayton & Becker, 2012) have posited constitutive equations for deviatoric stress and pressure directly (the latter with an EOS), in a way not necessarily consistent with existence of a hyperelastic total energy potential.

Solution of the planar elastic–plastic shock problem is derived in Section 3.2, wherein a rate independent, but history dependent, deformation system-level shear strength model is applied in the context of the logarithmic theory. The Rankine–Hugoniot conditions (Germain & Lee, 1973) and constitutive relations yield a set of coupled nonlinear algebraic equations that can be solved iteratively for the themomechanical state downstream from a plastic shock, with the upstream state corresponding to the elastic precursor. The analysis extends a prior treatment of isotropic solids (Perrin & Delannoy-Coutris, 1983). Previous analytical solutions for elastic–plastic wave propagation in crystals have been restricted to small strain theory (linear elasticity) and isentropic conditions (Johnson, 1972, 1974; Johnson, Jones, & Michaels, 1970); the present work, in contrast, incorporates large deformation, nonlinear themoelasticity, and entropy production. In Section 3.3, model predictions are compared with experimental data on sapphire, diamond, and quartz shocked in pure mode directions above the