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Crystal thermoelasticity at extreme loading rates and pressures: Analysis of higher-order energy potentials

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ABSTRACT

Several finite elastic strain measures are evaluated for use in constitutive models of crystalline elasticity and elasto-plasticity. These include the Green material strain tensor, the Eulerian material strain tensor, and the logarithmic material strain tensor, all of which are referred to locally relaxed coordinates invariant under spatial rotations. New applications of logarithmic strain-based theory towards shock compression of aluminum, copper, and magnesium single crystals and polycrystals are presented. Solutions to the planar shock problem from previous work are summarized and compared with the present results. Consideration of these new results in conjunction with previous analysis for a number of different metals, ceramics, and minerals suggests that Eulerian strain-based theory is most accurate for modeling the dynamic high-pressure response of ductile metallic crystals wherein ratios of elastic shear to bulk moduli tend to be relatively small, while logarithmic strain-based theory is recommended for modeling shocks in ceramics and minerals with larger ratios of effective elastic shear to bulk modulus.

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1. Introduction

The shock response of solids is important in applications related to structural crashworthiness, defense (e.g., projectile–target interactions), and geophysics (e.g., explosive mining operations and hypervelocity collisions of planetary rock masses) [1]. Accurate, efficient, stable, and thermodynamically consistent models for nonlinear anisotropic elasticity are required for proper mesoscale modeling of crystalline solids subjected to impact or ballistic loading. Nonlinear hyperelasticity addresses the thermodynamically reversible response component of solids subjected to large deformation; classes of crystalline materials of interest include metals [2], ceramics and minerals [3], energetic materials [4], and electronic materials [5].

This Letter considers three particular nonlinear thermoelasticity models–each based on a different finite strain tensor referred to locally unstressed material coordinates–and their performance regarding depiction of shock compression of crystalline solids. The three strain measures are the elastic Green–Lagrange strain $\boldsymbol{E}$ (often simply referred to here as Green strain), Eulerian material strain $\boldsymbol{D}$, and logarithmic material strain $\boldsymbol{e}$, all defined mathematically later in the text.

Conventional Lagrangian formulations of nonlinear elasticity for crystals [6,7] incorporate the elastic Green strain tensor. However, benefits of Eulerian strain tensors for isotropic materials were predicted [8] and demonstrated for cubic crystals under hydrostatic stress [9]. Thermal effects were considered in [10] for cubic crystals, and a theory for non-cubic crystals was initiated in [11]. A complete $\boldsymbol{D}$-based continuum thermoelastic theory for large deformation of crystals of arbitrary symmetry was developed in [12]. Analytical solutions for homogeneous deformations of ideal cubic crystals were studied over a prescribed range of elastic coefficients; stress states and

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intrinsic stability measures were compared. For realistic coefficients, Eulerian theory predicted more physically realistic and stable behavior than Lagrangian theory under large compression and shear. Analytical solutions for shock compression of anisotropic single crystals were derived for internal energy functions quartic in Lagrangian or Eulerian strain and linear in entropy; results were analyzed for nonmetals quartz, sapphire, and diamond in [12] and metals aluminum, copper, and magnesium in [13]. Eulerian theory was recently used to numerically model the viscoplastic response of aluminum single crystals and textured polycrystals in wave propagation simulated using the finite difference method [14], wherein Lagrangian theory was found insufficient for modeling strong/overdriven elastic–plastic shocks.

A complete $\boldsymbol{e}$-based continuum thermoelastic theory was analogously developed in [15] and applied to study the shock response of the same three nonmetals. The theory was extended to describe elastic–plastic response using a multiplicative decomposition of the deformation gradient (formally given later in Eq. (2)), and solutions for plastic shocks (involving slip, twinning, and/or shear fractures) following an elastic precursor in rate independent solids were derived [15]. Logarithmic theory delivered superior accuracy to Lagrangian and Eulerian theories for modeling shocks in single crystals of sapphire (X- and Z-cut), quartz (Z-cut), and diamond (X-cut) [15]. Logarithmic theory incorporating third-order elastic constants was also applied to analytically model the elastic–inelastic response of isotropic polycrystalline titanium diboride ceramic [16], including double yield and effects of static lateral pre-stress.

The remainder of this Letter is organized as follows. Kinematics and strain tensors are formally defined in Section 2, along with three-dimensional forms of internal energy functions. Specialization of the general theory to shock loading and large volumetric deformation is reviewed in Section 3. Analytical solutions corresponding to energy potentials associated with different strain tensors are compared with each other, experimental data, and atomic simulation data in Section 4, leading to suggested/preferred potentials for use in various situations. Conclusions follow in Section 5. Notation of continuum mechanics is used: vectors and tensors in bold font, scalars in italics, and summation over repeated indices (subscripts) referred to Cartesian coordinates. As befitting the brief style of a Letter, derivations that can be found in the cited references are usually omitted.

2. General constitutive theory

At a material element with reference coordinates $\boldsymbol{X}$ and spatial coordinates $\boldsymbol{x}$, the deformation gradient $\boldsymbol{F}$ and volume ratio J are

$$\begin{aligned} &\boldsymbol{F}(\boldsymbol{X}) = \partial \boldsymbol{x}/\partial \boldsymbol{X}, \\ &F_{ij}(X_K) = \partial x_i/\partial X_J = \delta_{ij} + \partial u_i/\partial X_J; \\ &J(\boldsymbol{X}) = V/V_0 = \det \boldsymbol{F}; \end{aligned} \tag{1}$$

where $\boldsymbol{u}$ is the particle displacement. For an elastic–plastic material, where "plastic" refers here to any thermodynamically irreversible mechanism such as dislocation glide, deformation twinning, fracture, void growth, or pore collapse, the total deformation gradient is typically split into a product of a thermoelastic term (superscript E) and a plastic term (superscript P, and which can be further decomposed into a product of deformation mappings associated with different physical mechanisms) [2–4,6,17]:

$$\begin{aligned} &\boldsymbol{F} = \boldsymbol{F}^E\boldsymbol{F}^P, \qquad F_{ij} = F^E_{iK}F^P_{Kj}; \\ &J = J^EJ^P = \det \boldsymbol{F}^E \det \boldsymbol{F}^P. \end{aligned} \tag{2}$$

The elastic Green material strain tensor (i.e., Green–Lagrange strain) is defined as [6,7]

$$\boldsymbol{E} = \frac{1}{2}(\boldsymbol{F}^{ET}\boldsymbol{F}^E - \boldsymbol{1}), \qquad E_{IJ} = \frac{1}{2}(F^E_{kI}F^E_{kJ} - \delta_{IJ}). \tag{3}$$

Also considered here are theories incorporating the elastic Eulerian material strain tensor [12–14]

$$\boldsymbol{D} = \frac{1}{2}(\boldsymbol{1} - \boldsymbol{F}^{E-1}\boldsymbol{F}^{E-T}), \qquad D_{ij} = \frac{1}{2}(\delta_{ij} - F^{E-1}_{Ik}F^{E-1}_{Jk}) \tag{4}$$

and the elastic material logarithmic strain tensor [15,16]

$$\begin{aligned} &\boldsymbol{e} = \ln \boldsymbol{U}^E = \frac{1}{2}\ln(\boldsymbol{F}^{ET}\boldsymbol{F}^E) = \frac{1}{2}\ln \boldsymbol{C}^E, \\ &e_{IJ} = \frac{1}{2}\ln(\boldsymbol{F}^{ET}\boldsymbol{F}^E)_{IJ}. \end{aligned} \tag{5}$$

Complete presentations of thermodynamic theories can be found in [12–16] and are too lengthy to reproduce in entirety in this Letter. Several important relations are listed next for reference. Local balance laws are, in the absence of discontinuities, body forces, and heat conduction,

$$\rho_0 = \rho J, \qquad \nabla \cdot \boldsymbol{\sigma} = \rho \ddot{\boldsymbol{x}}, \qquad \dot{U} = J\boldsymbol{\sigma} : (\dot{\boldsymbol{F}}\boldsymbol{F}^{-1}), \tag{6}$$

with ρ_0 and ρ reference and spatial mass densities, $\boldsymbol{\sigma}$ symmetric Cauchy stress, and U internal energy per reference volume. Letting ξ denote an internal state variable linked to evolution of microstructure (e.g., defects) and η the entropy density, forms of internal energy functions are

$$\begin{aligned} &U = \bar{U}(\boldsymbol{E}, \eta, \xi), \qquad U = \hat{U}(\boldsymbol{D}, \eta, \xi), \\ &U = \breve{U}(\boldsymbol{e}, \eta, \xi). \end{aligned} \tag{7}$$

Corresponding thermoelastic relationships for stress $\boldsymbol{\sigma}$ and temperature θ follow as [12,15]

$$\begin{aligned} &\boldsymbol{\sigma} = J^{E-1}\boldsymbol{F}^E(\partial \bar{U}/\partial \boldsymbol{E})\boldsymbol{F}^{ET}, \\ &\boldsymbol{\sigma} = J^{E-1}\boldsymbol{F}^{E-T}(\partial \hat{U}/\partial \boldsymbol{D})\boldsymbol{F}^{E-1}, \\ &\boldsymbol{\sigma} = J^{E-1}\boldsymbol{F}^E[(\partial \breve{U}/\partial \boldsymbol{e}) : (\partial \ln \boldsymbol{C}^E/\partial \boldsymbol{C}^E)]\boldsymbol{F}^{ET}; \end{aligned} \tag{8}$$

$$\theta = \partial \bar{U}/\partial \eta, \qquad \theta = \partial \hat{U}/\partial \eta, \qquad \theta = \partial \breve{U}/\partial \eta. \tag{9}$$

At fixed entropy and internal state variables, assuming a stress-free reference configuration, and written explicitly with elastic constants up to fourth order, internal energy