

Nonlinear Eulerian Thermoelasticity for Anisotropic Crystals

by John D. Clayton

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Nonlinear Eulerian thermoelasticity for anisotropic crystals

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A complete continuum thermoelastic theory for large deformation of crystals of arbitrary symmetry is developed. The theory incorporates as a fundamental state variable in the thermodynamic potentials what is termed an Eulerian strain tensor (in material coordinates) constructed from the inverse of the deformation gradient. Thermodynamic identities and relationships among Eulerian and the usual Lagrangian material coefficients are derived, significantly extending previous literature that focused on materials with cubic or hexagonal symmetry and hydrostatic loading conditions. Analytical solutions for homogeneous deformations of ideal cubic crystals are studied over a prescribed range of elastic coefficients; stress states and intrinsic stability measures are compared. For realistic coefficients, Eulerian theory is shown to predict more physically realistic behavior than Lagrangian theory under large compression and shear. Analytical solutions for shock compression of anisotropic single crystals are derived for internal energy functions quartic in Lagrangian or Eulerian strain and linear in entropy; results are analyzed for quartz, sapphire, and diamond. When elastic constants of up to order four are included, both Lagrangian and Eulerian theories are capable of matching Hugoniot data. When only the second-order elastic constant is known, an alternative theory incorporating a mixed Eulerian–Lagrangian strain tensor provides a reasonable approximation of experimental data.

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1. Introduction

Nonlinear continuum thermoelasticity provides a physical description of behavior of crystalline solids in the study of acoustic and shock waves, ballistic impact, and high-pressure geophysics problems. For extremely high pressure events, much work has focused on development of scalar equations of state, e.g., scalar relations among pressure, volume, entropy, and temperature and associated thermodynamic (energy) potentials. For ductile substances (e.g., many metals) and those that fracture easily, such a description is sufficient in many cases wherein the deviatoric stress (i.e., shear components) are restricted in magnitude due to plastic slip, twinning, or fracture that limit shear strength to a small fraction of the applied pressure. However, some crystalline materials such as ceramics and hard minerals may retain significant shear strength at finite strain under high pressure loading, e.g., as observed in plate impact or explosive loading (Wackerle, 1962; Fowles, 1967; Graham and Brooks, 1971; Kondo and Ahrens, 1983; Lang and Gupta, 2010). In these cases, a three-dimensional tensor theory of nonlinear thermoelasticity is required. Furthermore, apart from exceptional cases such as hydrostatic loading of cubic crystals, material anisotropy must be addressed in descriptions of single crystal behavior.

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The present work distinguishes among theories based on what are labeled Lagrangian and Eulerian finite strain measures. Let $\mathbf{x}$ denote the time-dependent spatial position of a material element located at point $\mathbf{X}$ in the undeformed body. The deformation gradient is $\mathbf{F} = \nabla_0 \mathbf{x}$, where ∇_0 is the material gradient operator and $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$. The inverse deformation gradient is $\mathbf{F}^{-1} = \nabla \mathbf{X}$, with ∇ the spatial gradient and the inverse motion $\mathbf{X} = \mathbf{X}(\mathbf{x}, t)$. The ratio of current to initial volume of the element is $J = V/V_0 = \det \mathbf{F}$; inverting this gives $J^{-1} = V_0/V = \det \mathbf{F}^{-1}$. A theory whose independent state variable entering the thermodynamic potentials is constructed from stretch raised to some positive power/exponent is labeled here as “Lagrangian”; a theory utilizing stretch raised to some negative power/exponent is labeled here as “Eulerian”. This terminology will be explained in more detail later by example.

Let a superscript T denote transposition. Conventional nonlinear elasticity for crystalline solids (Wallace, 1972; Thurston, 1974; Clayton, 2011a) incorporates the Lagrangian strain measure $\mathbf{E}(\mathbf{X}, t) = \frac{1}{2}(\mathbf{F}^T \mathbf{F} - \mathbf{1})$, often called the Green–St. Venant tensor or simply the Green strain, in the thermodynamic potentials. This approach, when elastic constants of up to third order are included, has been successful for modeling many crystalline solids under compression $V/V_0 \gtrsim 0.95$, including ceramics and pure minerals (Winey and Gupta, 2004; Clayton, 2009, 2011b; Foulk and Vogler, 2010; Clayton et al., 2012), metals (Clayton, 2005a,b, 2006; Vogler and Clayton, 2008), and locally heterogeneous geologic materials (Clayton, 2008, 2010a), but its accuracy degrades at larger compressions (smaller volume ratios) possible in shock loading or ballistic events. In such cases, elastic constants of order four and higher, difficult to measure and unknown for most anisotropic crystals, may be needed (Thurston, 1974).

For hydrostatic compression of cubic crystals or isotropic polycrystalline solids, it has been shown (Birch, 1978; Jeanloz, 1989) that pressure–volume equations of state incorporating Eulerian volumetric strain measures, i.e., a series of term(s) consisting of V_0/V raised to some positive exponent, are almost always more accurate than those incorporating Lagrangian measures [i.e., dominant term(s) consisting of V/V_0 raised to some positive exponent] when each representation contains the same number of bulk elastic constants. A canonical example of an Eulerian description is the Birch–Murnaghan EOS (Birch, 1947, 1978; Murnaghan, 1951) which often demonstrates high accuracy even when truncated at second order and at third order is often almost indistinguishable from the linear shock velocity–particle velocity relation that applies exceptionally well for many shock-compressed solids (Jeanloz, 1989).

The Birch–Murnaghan EOS is by definition restricted to pressure–volume space. A complete description for all stress states requires a tensor formulation. For single crystals, as well as textured polycrystals and composites, this formulation must account for anisotropy. A mathematically and thermodynamically consistent way to construct such a description is to assign scalar thermodynamic potentials (e.g., free energy or internal energy) that are irreducible functions of requisite invariants of an objective finite strain tensor for the given material's symmetry. By conjecture, extending arguments for Eulerian equations of state to arbitrary stress states and anisotropic solids, it is proposed that thermodynamic potentials incorporating an Eulerian strain measure, as defined above, will provide analogous advantages in six-dimensional stress–strain space as Eulerian equations of state provide in pressure–volume space.¹ For example, if the analogy holds as anticipated, Eulerian theory with elastic constants of up to order two might provide comparable accuracy as Lagrangian theory with constants of up to order three. Higher-order elastic constants are difficult to measure—standard tests include wave speed measurements in stressed crystals (Thurston, 1974; Thurston et al., 1966; Hankey and Schuele, 1970) or costly shock compression experiments in multiple directions (Graham and Brooks, 1971; Graham, 1972a, 1972b)—and have been reported for few low-symmetry materials. Third-order constants can also be predicted via first principles calculations (Zhao et al., 2007). Therefore, any theory that alleviates the need for measurements or atomic calculations of elastic constants above a certain order would be valuable.

The present paper develops a theory that incorporates Eulerian finite strain tensor $\mathbf{D}(\mathbf{x}, t) = \frac{1}{2}(\mathbf{1} - \mathbf{F}^{-1} \mathbf{F}^{-T})$, suggested (but not implemented) for describing elasticity of anisotropic solids by Murnaghan² and perhaps first implemented in calculations (of stressed cubic crystals) by Thomsen (1972). Because $\mathbf{D}$ has components referred to the reference coordinate system, it is invariant under spatial rotations (Davies, 1973), and can be used in elastic potentials for anisotropic bodies. Because $\mathbf{D}$ is symmetric and referred to material coordinates, functional forms of thermoelastic potentials for anisotropic materials expressed in terms of $\mathbf{D}$ will be the same as those in terms of $\mathbf{E}$ (Thomsen, 1972; Weaver, 1976). For example, elastic constant tensors of all orders will have the same symmetries, though magnitudes of higher-order constants will differ between the two theories. Transformation formulae can be derived relating material constants of the two theories (Weaver, 1976; Perrin and Delannoy, 1978), obviating the need for additional experiments or quantum calculations if Lagrangian constants have already been obtained.

Further clarification of terms “Lagrangian” and “Eulerian” is in order. In this paper, a “Lagrangian” strain refers to a tensor depending on principal stretch ratios raised to some positive exponent, while an “Eulerian” strain refers to a tensor depending on principal stretch ratios raised to some negative exponent. This is consistent with terminology adopted in the physics and chemistry literature (Thomsen, 1972; Weaver, 1976; Perrin and Delannoy, 1978; Davies, 1974; Nielsen, 1986). According to this scheme $\mathbf{D}$ is labeled “Eulerian” in the sense that it is constructed from the inverse deformation gradient $\mathbf{F}^{-1}(\mathbf{x}, t)$ (precisely, right stretch $\mathbf{U}$ raised to the -2 power) and its field is implicitly a function of spatial coordinates $\mathbf{x}$,

¹ This conjecture is later shown to be true for ideal cubic solids with an ambient pressure derivative of bulk modulus $B'_0 \approx 4$, but not necessarily true for shock compression of highly anisotropic single crystals.

² Murnaghan (1937, p. 257) proposed a strain energy depending on deformation measure $j = 1 - 2\mathbf{D}$.

even though indices of $\mathbf{D}$ are referred to a material coordinate system (associated with $\mathbf{X}$). In contrast, according to conventions often used in continuum mechanics literature, a tensor is said to be “Lagrangian” if it is referred to material/initial coordinates and “Eulerian” if referred to spatial/current coordinates. According to this scheme $\mathbf{D}$ would be Lagrangian, while $\mathbf{E}$ would be Lagrangian in either scheme (right stretch $\mathbf{U}$ raised to the +2 power, and expressed in material coordinates). Almansi strain $\mathbf{e}(\mathbf{x}, t) = \frac{1}{2}(\mathbf{1} - \mathbf{F}^{-T}\mathbf{F}^{-1})$ entering Murnaghan's (1937) theory for isotropic solids would be Eulerian according to either scheme. The negative of tensor $\mathbf{D}$ has been referred to elsewhere as Piola strain (Haupt, 2000).

Recent work (Clayton and Bliss, submitted for publication) has demonstrated that under finite shear, isotropic $\mathbf{E}$ -based Lagrangian theory is prone to intrinsic instability in terms of attainment of null eigenvalue(s) of an incremental stiffness matrix (Wang et al., 1993; Morris and Krenn, 2000) with increasing magnitude of third-order elastic constants, regardless of their sign. This is often referred to as a “Born instability” (Thomsen, 1972; Born, 1940), though different elastic stiffness tensors for perfect crystals have been suggested as most appropriate depending on boundary conditions (Hill, 1975; Hill and Milstein, 1977). While certain crystals such as quartz (Gregoryanz et al., 2000) and boron carbide (Clayton, 2012, 2013) can demonstrate true physical instabilities, in a model such instabilities should result from material physics rather than pathologies associated with extrapolation of a strain-based theory to large deformations outside the domain for which elastic properties have been measured.

Benefits of using Eulerian strain measures for nonlinear elasticity of isotropic materials were extolled by Murnaghan (1937) in the 1930s and were demonstrated for cubic crystals under hydrostatic stress by Birch (1947). Thermal effects were considered later in a $\mathbf{D}$ -based Eulerian formulation (Davies, 1974), and a mechanical theory for several non-cubic crystals incorporating $\mathbf{D}$ was initiated and exercised in the late 1970s (Weaver, 1976; Perrin and Delannoy, 1978). With the exception of the early works of Murnaghan and Birch, these Eulerian treatments remain obscure, and theoretical developments and comparisons with experiment are limited to hydrostatic pressure loading. Nonetheless, the Eulerian framework has demonstrated superior accuracy over Lagrangian theory for predicting the hydrostatic isothermal response of a few anisotropic crystals (Weaver, 1976; Perrin and Delannoy, 1978). Despite such promise, Eulerian $\mathbf{D}$ -based thermoelasticity theory has not been completely developed for crystals of arbitrary anisotropy, and until now has been untested for general non-hydrostatic stress states. In the present work, the theory is fully developed and is applied to several loading protocols, including adiabatic uniaxial strain conditions (involving simultaneous shear and compression) characteristic of shock-wave problems (Thurston, 1974; Perrin and Delannoy-Coutis, 1983).

The remainder of this paper is structured as follows. Derivations are presented in parallel for Eulerian and Lagrangian theories in Section 2, including governing equations, thermodynamic identities, intrinsic stability criteria, and material coefficients. Analytical solutions for homogeneous deformations of a cubic crystal are examined in Section 3. These solutions, which apparently have not been given elsewhere, apply for cubic crystals with fully anisotropic second-order elasticity but symmetrized anharmonicity characterized by a single third-order constant. A new solution is derived in Section 4 for shock compression of a single crystal of arbitrary symmetry described by fourth-order Eulerian theory. Predictions of this solution are compared with those of the Lagrangian solution for three materials which remain elastic under large uniaxial compression: quartz, sapphire, and diamond. Conclusions are given in Section 5. Appendices contain supporting material on kinematics and thermomechanics. Standard notation of continuum field theory is used: vectors and tensors are generally written in bold italic; when indicial notation is used, components of vectors and tensors are referred to a Cartesian frame of reference and are written in plain italic, with summation over repeated indices.

2. Theory

2.1. Nonlinear continuum mechanics of hyperelastic solids

Spatial coordinates are related to reference coordinates by the motion $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$. The deformation gradient $\mathbf{F}$ and its determinant are³

$$\mathbf{F} = \nabla_0 \mathbf{x} \quad (F_{ij} = \partial_j x_i), \quad J = \det \mathbf{F} > 0. \quad (2.1)$$

Let $\mathbf{P}(\mathbf{X}, t)$ and $\boldsymbol{\sigma}(\mathbf{x}, t)$ denote, respectively, first Piola–Kirchhoff and Cauchy stress:

$$\mathbf{P} = J \boldsymbol{\sigma} \mathbf{F}^{-T}; \quad P_{ij} = J \sigma_{ik} F_{jk}^{-1} = \frac{\rho_0}{\rho} \sigma_{ik} \partial_k x_j. \quad (2.2)$$

Let $(\dot{\cdot}) = \partial(\cdot)/\partial t|_{\mathbf{x}}$ denote the material time derivative and $\mathbf{v}$ particle velocity. Balance of linear momentum in the absence of body force and balance of angular momentum are

$$\nabla_0 \cdot \mathbf{P} = \rho_0 \dot{\mathbf{v}}; \quad \partial_j P_{ij} = \rho_0 \ddot{x}_i; \quad (2.3)$$

$$\mathbf{P} \mathbf{F}^T = \mathbf{F} \mathbf{P}^T; \quad P_{ij} F_{kl} = P_{kl} F_{ij}. \quad (2.4)$$

³ See Appendix A for a thorough discussion of kinematics.

Let Ψ denote Helmholtz free energy per unit initial volume, and let θ and η denote absolute temperature and entropy per initial volume. Internal energy density U obeys

$$U = \Psi + \theta\eta. \quad (2.5)$$

The following usual functional forms are assumed for homogeneous solids:

$$\Psi = \Psi(\mathbf{F}, \theta), \quad U = U(\mathbf{F}, \eta). \quad (2.6)$$

Dependence on $\mathbf{F}$ will be replaced later by dependence on symmetric strain measures that respect rotational invariance of the thermodynamic potentials.

The local balance of energy, in the absence of scalar heat sources, is

$$\dot{U} = \mathbf{P} : \dot{\mathbf{F}} - \nabla_0 \cdot \mathbf{Q}; \quad \dot{U} = P_{ij} \partial_j \dot{x}_i - \partial_j Q_j; \quad (2.7)$$

with $\mathbf{Q}$ the referential heat flux vector. The local entropy production inequality is

$$\dot{\eta} + \nabla_0 \cdot (\theta^{-1} \mathbf{Q}) \geq 0; \quad \theta \dot{\eta} + \partial_j Q_j - \theta^{-1} Q_j \partial_j \theta \geq 0. \quad (2.8)$$

Using (2.5) and (2.7) in (2.8),

$$\mathbf{P} : \dot{\mathbf{F}} - \eta \dot{\theta} - \dot{\Psi} - \theta^{-1} \mathbf{Q} \cdot \nabla_0 \theta \geq 0. \quad (2.9)$$

Substituting from the first of (2.6),

$$(\mathbf{P} - \partial \Psi / \partial \mathbf{F}) : \dot{\mathbf{F}} - (\eta + \partial \Psi / \partial \theta) \dot{\theta} - \mathbf{Q} \cdot \nabla_0 \theta \geq 0, \quad (2.10)$$

from which the usual constitutive equations of hyperelasticity can be deduced:

$$\mathbf{P} = \partial \Psi / \partial \mathbf{F}, \quad \eta = -\partial \Psi / \partial \theta. \quad (2.11)$$

From (2.5), (2.6) and letting $\theta = \theta(\mathbf{F}, \eta)$,

$$\frac{\partial U}{\partial \mathbf{F}} = \frac{\partial \Psi}{\partial \mathbf{F}} + \frac{\partial \Psi}{\partial \theta} \frac{\partial \theta}{\partial \mathbf{F}} + \eta \frac{\partial \theta}{\partial \mathbf{F}}, \quad \frac{\partial U}{\partial \eta} = \frac{\partial \Psi}{\partial \theta} \frac{\partial \theta}{\partial \eta} + \eta \frac{\partial \theta}{\partial \eta} + \theta. \quad (2.12)$$

Then, from the second of (2.11), it follows that

$$\mathbf{P} = \partial U / \partial \mathbf{F}, \quad \theta = \partial U / \partial \eta. \quad (2.13)$$

2.2. Lagrangian and Eulerian variables

Lagrangian Green strain $\mathbf{E}(\mathbf{X}, t)$ is defined as

$$\mathbf{E} = \frac{1}{2} (\mathbf{F}^T \mathbf{F} - \mathbf{1}); \quad E_{IJ} = \frac{1}{2} (\partial_I x_k \partial_J x_k - \delta_{IJ}). \quad (2.14)$$

Eulerian strain $\mathbf{D}(\mathbf{x}, t)$ is defined as

$$\mathbf{D} = \frac{1}{2} (\mathbf{1} - \mathbf{F}^{-1} \mathbf{F}^{-T}); \quad D_{IJ} = \frac{1}{2} (\delta_{IJ} - \partial_k X_I \partial_k X_J). \quad (2.15)$$

Considered in parallel are two thermoelastic formulations more specific than (2.6), one based on $\mathbf{E}$ and termed “Lagrangian”, the other based on $\mathbf{D}$ and termed “Eulerian”:

$$\Psi = \bar{\Psi}[\mathbf{E}(\mathbf{F}), \theta], \quad U = \bar{U}[\mathbf{E}(\mathbf{F}), \eta]; \quad (2.16)$$

$$\Psi = \hat{\Psi}[\mathbf{D}(\mathbf{F}), \theta], \quad U = \hat{U}[\mathbf{D}(\mathbf{F}), \eta]. \quad (2.17)$$

These thermodynamic potentials are all invariant under spatial rotations since both $\mathbf{E}$ and $\mathbf{D}$ are referred to the material coordinate system. First Piola–Kirchhoff stress in the Lagrangian description is, from (2.11), (2.13), and (A.8),

$$P_{kL} = \frac{\partial \bar{\Psi}}{\partial E_{IJ}} \frac{\partial E_{IJ}}{\partial F_{kL}} = F_{kJ} \frac{\partial \bar{\Psi}}{\partial E_{JL}} = F_{kJ} \frac{\partial \bar{U}}{\partial E_{JL}} = F_{kJ} \bar{S}_{JL}. \quad (2.18)$$

Second Piola–Kirchhoff stress is

$$\bar{S}_{JL} = \partial \bar{\Psi} / \partial E_{JL} = \partial \bar{U} / \partial E_{JL} = F_{Jk}^{-1} P_{kL} = J F_{Jk}^{-1} F_{Li}^{-1} \sigma_{ki}. \quad (2.19)$$

First Piola–Kirchhoff stress in the Eulerian description is, from (2.11), (2.13), and (A.13),

$$P_{kL} = \frac{\partial \hat{\Psi}}{\partial D_{IJ}} \frac{\partial D_{IJ}}{\partial F_{kL}} = F_{Ik}^{-1} (\delta_{JL} - 2D_{JL}) \frac{\partial \hat{\Psi}}{\partial D_{JL}} = F_{Ik}^{-1} (\delta_{JL} - 2D_{JL}) \frac{\partial \hat{U}}{\partial D_{JL}} = F_{Ik}^{-1} F_{Lm}^{-1} F_{Jm}^{-1} \hat{S}_{IJ}. \quad (2.20)$$

The Eulerian analog of second Piola–Kirchhoff stress is

$$\hat{S}_{JL} = \partial \hat{\Psi} / \partial D_{JL} = \partial \hat{U} / \partial D_{JL} = F_{kJ} F_{iL} F_{iM} P_{kM} = F_{kJ} F_{kN} F_{iL} F_{iM} \bar{S}_{NM} = J F_{ij} F_{kl} \sigma_{ik}. \quad (2.21)$$

Cauchy stress becomes, from (2.2),

$$\sigma_{ij} = J^{-1} F_{iK} F_{jL} \frac{\partial \bar{\Psi}}{\partial E_{KL}} = J^{-1} F_{Ki}^{-1} F_{Lj}^{-1} \frac{\partial \hat{\Psi}}{\partial D_{KL}}. \quad (2.22)$$

Let $c(\mathbf{F}, \theta) = \bar{c}(\mathbf{E}, \theta) = \hat{c}(\mathbf{D}, \theta)$ denote specific heat per unit reference volume at constant deformation, where from (2.11):

$$c = \partial U / \partial \theta = \theta (\partial \eta / \partial \theta) = -\theta (\partial^2 \Psi / \partial \theta^2). \quad (2.23)$$

The rate of internal energy can be expanded as

$$\dot{U} = (\partial U / \partial \mathbf{F}) : \dot{\mathbf{F}} + (\partial U / \partial \eta) \dot{\eta} = \mathbf{P} : \dot{\mathbf{F}} + \theta [(\partial \eta / \partial \mathbf{F}) : \dot{\mathbf{F}} + (\partial \eta / \partial \theta) \dot{\theta}]. \quad (2.24)$$

Substituting (2.24) and (2.23) into (2.7) leads to

$$c \dot{\theta} = \theta (\partial^2 \Psi / \partial \mathbf{F} \partial \theta) : \dot{\mathbf{F}} - \nabla_0 \cdot \mathbf{Q}. \quad (2.25)$$

Defining thermal stress coefficients $\bar{\beta}(\mathbf{E}, \theta)$ and $\hat{\beta}(\mathbf{D}, \theta)$ as

$$\bar{\beta} = \partial \eta / \partial \mathbf{E} = -\partial^2 \bar{\Psi} / \partial \mathbf{E} \partial \theta, \quad \hat{\beta} = \partial \eta / \partial \mathbf{D} = -\partial^2 \hat{\Psi} / \partial \mathbf{D} \partial \theta; \quad (2.26)$$

$$\partial^2 \Psi / \partial \theta \partial F_{ij} = -\beta_{ij} = -\bar{\beta}_{jL} F_{iL} = -\hat{\beta}_{KL} F_{Ki}^{-1} F_{Lm}^{-1} F_{jm}^{-1}; \quad (2.27)$$

and using (A.20), (2.25) can be written as

$$\bar{c} \dot{\theta} = -\theta \bar{\beta} : \dot{\mathbf{E}} - \nabla_0 \cdot \mathbf{Q}, \quad \hat{c} \dot{\theta} = -\theta \hat{\beta} : \dot{\mathbf{D}} - \nabla_0 \cdot \mathbf{Q}. \quad (2.28)$$

Second-order tensor Grüneisen parameters are defined as

$$\bar{\Gamma} = \bar{\beta} / \bar{c}, \quad \hat{\Gamma} = \hat{\beta} / \hat{c}. \quad (2.29)$$

The following Maxwell-type equalities can be derived using procedures in Thurston (1974) and Clayton (2011a):

$$\theta \bar{\Gamma} = (\theta / \bar{c}) (\partial \eta / \partial \mathbf{E}) = -\partial \bar{\mathbf{S}} / \partial \eta = -\partial \theta / \partial \mathbf{E}, \quad (2.30)$$

$$\theta \hat{\Gamma} = (\theta / \hat{c}) (\partial \eta / \partial \mathbf{D}) = -\partial \hat{\mathbf{S}} / \partial \eta = -\partial \theta / \partial \mathbf{D}; \quad (2.31)$$

$$(\theta / \bar{c}^S) \bar{\alpha} = (\theta / \bar{c}^S) (\partial \mathbf{E} / \partial \theta) = \partial \mathbf{E} / \partial \eta = -\partial \theta / \partial \bar{\mathbf{S}}, \quad (2.32)$$

$$(\theta / \hat{c}^S) \hat{\alpha} = (\theta / \hat{c}^S) (\partial \mathbf{D} / \partial \theta) = \partial \mathbf{D} / \partial \eta = -\partial \theta / \partial \hat{\mathbf{S}}; \quad (2.33)$$

$$\bar{\alpha} = \partial \mathbf{E} / \partial \theta = \partial \eta / \partial \bar{\mathbf{S}}, \quad \hat{\alpha} = \partial \mathbf{D} / \partial \theta = \partial \eta / \partial \hat{\mathbf{S}}. \quad (2.34)$$

Analogously to (2.26) and (2.27),

$$\theta \bar{\Gamma} = -\partial^2 \bar{U} / \partial \mathbf{E} \partial \eta, \quad \theta \hat{\Gamma} = -\partial^2 \hat{U} / \partial \mathbf{D} \partial \eta; \quad (2.35)$$

$$\partial^2 U / \partial \eta \partial F_{ij} = -\theta \Gamma_{ij} = -\theta \bar{\Gamma}_{jL} F_{iL} = -\theta \hat{\Gamma}_{KL} F_{Ki}^{-1} F_{Lm}^{-1} F_{jm}^{-1}. \quad (2.36)$$

Defining $\alpha_{KL} = \partial F_{KL} / \partial \theta$ at constant $\mathbf{P}$, thermal expansion coefficients are related implicitly by

$$2\bar{\alpha}_{IJ} = \alpha_{KL} (\delta_{IL} F_{KJ} + \delta_{JL} F_{KI}), \quad 2\hat{\alpha}_{IJ} = \alpha_{KL} F_{Lm}^{-1} (F_{IK}^{-1} F_{Jm}^{-1} + F_{JK}^{-1} F_{Im}^{-1}). \quad (2.37)$$

Specific heats per unit volume at constant deformation ($c = \bar{c} = \hat{c}$) and constant stress ($c^S = \bar{c}^S = \hat{c}^S$) obey (Thurston, 1974; Clayton, 2011a)

$$c = \theta (\partial \eta / \partial \theta)_{\mathbf{E}, \mathbf{D}} = -\theta (\partial^2 \Psi / \partial \theta^2) = \partial U / \partial \theta, \quad c^S = \theta (\partial \eta / \partial \theta)_{\bar{\mathbf{S}}, \hat{\mathbf{S}}}. \quad (2.38)$$

Isothermal second-order thermodynamic elastic coefficients are

$$\bar{C}_{IJKL}^\theta = \left. \frac{\partial \bar{\mathbf{S}}_{KL}}{\partial E_{IJ}} \right|_\theta = \frac{\partial^2 \bar{\Psi}}{\partial E_{IJ} \partial E_{KL}}, \quad \hat{C}_{IJKL}^\theta = \left. \frac{\partial \hat{\mathbf{S}}_{KL}}{\partial D_{IJ}} \right|_\theta = \frac{\partial^2 \hat{\Psi}}{\partial D_{IJ} \partial D_{KL}}. \quad (2.39)$$

Isentropic second-order thermodynamic elastic coefficients are

$$\bar{C}_{IJKL}^\eta = \left. \frac{\partial \bar{\mathbf{S}}_{KL}}{\partial E_{IJ}} \right|_\eta = \frac{\partial^2 \bar{U}}{\partial E_{IJ} \partial E_{KL}}, \quad \hat{C}_{IJKL}^\eta = \left. \frac{\partial \hat{\mathbf{S}}_{KL}}{\partial D_{IJ}} \right|_\eta = \frac{\partial^2 \hat{U}}{\partial D_{IJ} \partial D_{KL}}. \quad (2.40)$$

Thermal expansion and thermal stress coefficients are related by

$$\bar{\beta} = (\partial \eta / \partial \mathbf{E})|_\theta = (\partial \eta / \partial \bar{\mathbf{S}})|_\theta : (\partial \bar{\mathbf{S}} / \partial \mathbf{E})|_\theta = \bar{\alpha} : \bar{\mathbf{C}}^\theta, \quad \bar{\beta}_{IJ} = \bar{\alpha}_{KL} \bar{C}_{KLIJ}^\theta. \quad (2.41)$$

$$\hat{\beta} = (\partial \eta / \partial \mathbf{D})|_\theta = (\partial \eta / \partial \hat{\mathbf{S}})|_\theta : (\partial \hat{\mathbf{S}} / \partial \mathbf{D})|_\theta = \hat{\alpha} : \hat{\mathbf{C}}^\theta, \quad \hat{\beta}_{IJ} = \hat{\alpha}_{KL} \hat{C}_{KLIJ}^\theta. \quad (2.42)$$

Specific heats per unit reference volume are related, using the procedure in [Thurston \(1974\)](#), as

$$\mathcal{C}^S - \mathcal{C} = \theta \bar{\alpha} : \bar{\beta} = \theta \hat{\alpha} : \hat{\beta}. \quad (2.43)$$

Isentropic and isothermal coefficients are related, using Maxwell relations, by

$$\bar{\mathcal{C}}^\eta = (\partial \bar{\mathcal{S}} / \partial \mathbf{E})|_\eta = (\partial \bar{\mathcal{S}} / \partial \mathbf{E})|_\theta + (\partial \bar{\mathcal{S}} / \partial \theta|_{\mathbf{E}}) \otimes (\partial \theta / \partial \mathbf{E})|_\theta = \bar{\mathcal{C}}^\theta + (\theta / \bar{\mathcal{C}}) \bar{\beta} \otimes \bar{\beta}, \quad (2.44)$$

$$\hat{\mathcal{C}}^\eta = (\partial \hat{\mathcal{S}} / \partial \mathbf{D})|_\eta = (\partial \hat{\mathcal{S}} / \partial \mathbf{D})|_\theta + (\partial \hat{\mathcal{S}} / \partial \theta|_{\mathbf{D}}) \otimes (\partial \theta / \partial \mathbf{D})|_\theta = \hat{\mathcal{C}}^\theta + (\theta / \hat{\mathcal{C}}) \hat{\beta} \otimes \hat{\beta}, \quad (2.45)$$

or in indicial notation,

$$\bar{\mathcal{C}}_{ijkl}^\eta = \bar{\mathcal{C}}_{ijkl}^\theta + (\theta / \bar{\mathcal{C}}) \bar{\beta}_{ij} \bar{\beta}_{kl}, \quad \hat{\mathcal{C}}_{ijkl}^\eta = \hat{\mathcal{C}}_{ijkl}^\theta + (\theta / \hat{\mathcal{C}}) \hat{\beta}_{ij} \hat{\beta}_{kl}. \quad (2.46)$$

Strain energy density, per unit reference volume, is defined as follows for a homogeneous solid:

$$W(\mathbf{F}) = \bar{W}[\mathbf{E}(\mathbf{F})] = \hat{W}[\mathbf{D}(\mathbf{F})] = \Psi(\mathbf{F}, \theta_0). \quad (2.47)$$

where θ_0 is a fixed reference temperature. When temperature/entropy effects are omitted, second-order elastic coefficients reduce to

$$\bar{\mathcal{C}} = \partial^2 \bar{W} / \partial \mathbf{E} \partial \mathbf{E}, \quad \hat{\mathcal{C}} = \partial^2 \hat{W} / \partial \mathbf{D} \partial \mathbf{D}. \quad (2.48)$$

Tangent modulus $\mathbf{A}(\mathbf{F})$ is defined as

$$\mathbf{A} = \partial \mathbf{P} / \partial \mathbf{F} = \partial^2 W / \partial \mathbf{F} \partial \mathbf{F}, \quad A_{ijkl} = \partial P_{kl} / \partial F_{ij} = \partial^2 W / \partial F_{ij} \partial F_{kl}. \quad (2.49)$$

Coefficients $\mathbf{A}$ and $\bar{\mathcal{C}}$ are related by

$$A_{ijkl} = \partial (F_{km} \bar{\mathcal{S}}_{ML}) / \partial F_{ij} = F_{in} F_{km} \bar{\mathcal{C}}_{NJML} + \delta_{ik} \bar{\mathcal{S}}_{JL} = F_{in} F_{km} \bar{\mathcal{C}}_{NJML} + \delta_{ik} F_{jn}^{-1} P_{nL}. \quad (2.50)$$

Similarly, coefficients $\mathbf{A}$ and $\hat{\mathcal{C}}$ are related by

$$A_{ijkl} = \partial (F_{lk}^{-1} F_{lm}^{-1} F_{pm}^{-1} \hat{\mathcal{S}}_{lp}) / \partial F_{ij} = F_{Qi}^{-1} F_{lk}^{-1} F_{jm}^{-1} F_{rm}^{-1} F_{ln}^{-1} F_{pn}^{-1} \hat{\mathcal{C}}_{QRlp} - F_{jk}^{-1} P_{iL} - F_{Li}^{-1} P_{kj} - F_{jm}^{-1} F_{lm}^{-1} F_{kn}^{-1} P_{iN}. \quad (2.51)$$

Equating (2.50) and (2.51),

$$\bar{\mathcal{C}}_{ijkl} = F_{li}^{-1} F_{mi}^{-1} F_{jj}^{-1} F_{nj}^{-1} F_{kk}^{-1} F_{ok}^{-1} F_{ll}^{-1} F_{pl}^{-1} \hat{\mathcal{C}}_{MNOP} - F_{lk}^{-1} F_{jk}^{-1} F_{jn}^{-1} P_{nL} - F_{li}^{-1} F_{km}^{-1} F_{jm}^{-1} P_{iL} - F_{li}^{-1} F_{km}^{-1} F_{mj}^{-1} F_{jn}^{-1} F_{lm}^{-1} P_{ik}. \quad (2.52)$$

Relations analogous to (2.52) hold when either isothermal or isentropic coefficients are used. The local linear momentum balance for a homogeneous elastic solid in the absence of body force becomes, with $\mathbf{A}^\theta = \partial^2 \Psi(\mathbf{F}, \theta) / \partial \mathbf{F} \partial \mathbf{F}$,

$$\rho_0 \ddot{\mathbf{x}}_i = A_{ijkl}^\theta \partial_j \partial_l x_k - \beta_{ij} \partial_j \theta. \quad (2.53)$$

Stress power per unit reference volume is, from (A.20),

$$\dot{W} = (\partial W / \partial \mathbf{F}) : \dot{\mathbf{F}} = \mathbf{P} : \dot{\mathbf{F}} = \bar{\mathbf{S}} : \dot{\mathbf{E}} = \hat{\mathbf{S}} : \dot{\mathbf{D}} = \mathbf{J} \boldsymbol{\sigma} : \mathbf{d}. \quad (2.54)$$

Let δW be a first-order increment in strain energy associated with deformation gradient variation $\delta \mathbf{F}$. Then analogously to (2.54),

$$\delta W = (\partial W / \partial \mathbf{F}) : \delta \mathbf{F} = \mathbf{P} : \delta \mathbf{F} = \bar{\mathbf{S}} : \delta \mathbf{E} = \hat{\mathbf{S}} : \delta \mathbf{D} = \mathbf{J} \boldsymbol{\sigma} : \delta \boldsymbol{\epsilon}, \quad (2.55)$$

where

$$\delta \boldsymbol{\epsilon} = \mathbf{F}^{-T} \delta \mathbf{E} \mathbf{F}^{-1} = \mathbf{F} \delta \mathbf{D} \mathbf{F}^T; \quad \delta \epsilon_{ij} = F_{Ki}^{-1} \delta E_{KL} F_{Lk}^{-1} = F_{iK} \delta D_{KL} F_{jL}; \quad (2.56)$$

$$\delta \mathbf{E} = \frac{1}{2} [\mathbf{F}^T \delta \mathbf{F} + (\delta \mathbf{F})^T \mathbf{F}], \quad \delta \boldsymbol{\epsilon} = \frac{1}{2} [(\delta \mathbf{F}) \mathbf{F}^{-1} + \mathbf{F}^{-1} (\delta \mathbf{F})^T]. \quad (2.57)$$

The first equality in each of (2.56), or the second equality of (2.57), can be used as a definition for spatial increment $\delta \boldsymbol{\epsilon}$; the second equality in each of (2.56) is consistent with transformation formulae between $\delta \mathbf{D}$ and $\delta \mathbf{E}$ analogous to (A.20). This definition for $\delta \boldsymbol{\epsilon}$ is unique when incremental deformation gradient $\delta \mathbf{F}$ is prescribed, and is identical to that used widely elsewhere in the analysis of internal elastic stability (e.g., [Morris and Krenn, 2000](#), their Eq. (9)). Making the connection $\delta W \leftrightarrow \dot{W} dt$, it follows that $\delta \boldsymbol{\epsilon} \leftrightarrow \mathbf{d} dt$. Integrated quantity $\int \delta \boldsymbol{\epsilon} \leftrightarrow \int \mathbf{d} dt$ is path dependent (in contrast to $\mathbf{E}$ or $\mathbf{D}$ that depend only on current values of $\mathbf{F}$ or $\mathbf{F}^{-1}$), and is not used in analysis in this paper or others ([Wang et al., 1993](#); [Morris and Krenn, 2000](#); [Hill, 1975](#)) dealing with intrinsic stability.

Spatial modulus $\bar{\mathcal{C}}$ is defined as

$$\bar{\mathcal{C}}_{ijkl} = J^{-1} F_{il} F_{jj} F_{kk} F_{ll} \bar{\mathcal{C}}_{JJKL} = J^{-1} F_{li}^{-1} F_{jj}^{-1} F_{kk}^{-1} F_{ll}^{-1} \hat{\mathcal{C}}_{JJKL} - \sigma_{il} \delta_{jk} - \sigma_{jl} \delta_{ik} - \sigma_{ik} \delta_{jl} - \sigma_{jk} \delta_{il}. \quad (2.58)$$

The fully symmetric form of incremental tangent modulus $\mathbf{B}$ is ([Wang et al., 1993](#); [Morris and Krenn, 2000](#); [Clayton, 2012](#))

$$B_{ijkl} = \bar{\mathcal{C}}_{ijkl} + \frac{1}{2} (\sigma_{ik} \delta_{jl} + \sigma_{il} \delta_{jk} + \sigma_{jl} \delta_{ik} + \sigma_{jk} \delta_{il} - \sigma_{ij} \delta_{kl} - \sigma_{kl} \delta_{ij}) \\ = J^{-1} F_{li}^{-1} F_{jj}^{-1} F_{kk}^{-1} F_{ll}^{-1} \hat{\mathcal{C}}_{JJKL} - \frac{1}{2} (\sigma_{ik} \delta_{jl} + \sigma_{il} \delta_{jk} + \sigma_{jl} \delta_{ik} + \sigma_{jk} \delta_{il} + \sigma_{ij} \delta_{kl} + \sigma_{kl} \delta_{ij}). \quad (2.59)$$

Consider an elastic solid undergoing homogeneous deformation, omitting thermal effects. Intrinsic mechanical stability can be defined as local convexity of strain energy with respect to a given strain or deformation measure (Hill, 1975; Parry, 1978; Clayton, 2013) and therefore depends on the choice of conjugate stress–strain variables. For intrinsic stability consistent with classical stability under all-around dead loading (Hill, 1975),

$$\delta \mathbf{P} : \delta \mathbf{F} = \delta \mathbf{F} : (\partial^2 W / \partial \mathbf{F} \partial \mathbf{F}) : \delta \mathbf{F} = \delta \mathbf{F} : \mathbf{A} : \delta \mathbf{F} > 0 \Leftrightarrow \det[\mathbf{A}] > 0. \quad (2.60)$$

For intrinsic stability consistent with classical stability under controlled Cauchy stress (Wang et al., 1993; Morris and Krenn, 2000),

$$\delta \boldsymbol{\sigma} : \delta \boldsymbol{\epsilon} = [(\partial \boldsymbol{\sigma} / \partial \mathbf{E}) : \delta \mathbf{E}] : \delta \boldsymbol{\epsilon} = \delta \boldsymbol{\epsilon} : \mathbf{B} : \delta \boldsymbol{\epsilon} > 0 \Leftrightarrow \det[\mathbf{B}] > 0. \quad (2.61)$$

The first two equalities in (2.61) strictly apply only when $\mathbf{F}$ is symmetric, but the inequalities apply regardless since since 6×6 matrix $[\mathbf{B}]$ is rotationally invariant. Symmetric coefficients B_{ijkl} (e.g., evaluated from isentropic thermodynamic moduli) enter the linear momentum equation for propagation of small amplitude elastic waves from a hydrostatically stressed initial configuration (Thomsen, 1972); when the initial configuration is stressed anisotropically, different tangent moduli may enter the wave equation (Thurston, 1965).

2.3. Thermoelastic potentials and material constants

An unstrained reference state is defined by $(\mathbf{E}, \theta) = (\mathbf{0}, \theta_0)$, $(\mathbf{D}, \theta) = (\mathbf{0}, \theta_0)$, and temperature change from this reference state is $\Delta\theta = \theta - \theta_0$. In what follows, Greek subscripts denote Voigt notation for symmetric indices, e.g., $(\cdot)_{IJ} = (\cdot)_{JI} \leftrightarrow (\cdot)_{\alpha}$:

$$11 \leftrightarrow 1, \quad 22 \leftrightarrow 2, \quad 33 \leftrightarrow 3, \quad 23 = 32 \leftrightarrow 4, \quad 13 = 31 \leftrightarrow 5, \quad 12 = 21 \leftrightarrow 6. \quad (2.62)$$

Following the standard convention (Brugger, 1964; Thurston, 1974; Clayton, 2011a), shear strain components contain a factor of two, but stresses and stiffness coefficients do not. For example, $E_6 = 2E_{12}$, $D_6 = 2D_{12}$, $\bar{S}_6 = \bar{S}_{12}$, $\bar{C}_{45} = \bar{C}_{2313}$. First consider free energy per unit reference volume, which can be expressed as in either of the following series expansions about energy Ψ_0 from the reference state:

$$\bar{\Psi}(\mathbf{E}, \theta) = \Psi_0 + \bar{C}_{0\alpha}^\theta E_\alpha + \frac{1}{2!} \bar{C}_{0\alpha\beta}^\theta E_\alpha E_\beta + \frac{1}{3!} \bar{C}_{0\alpha\beta\gamma}^\theta E_\alpha E_\beta E_\gamma + \cdots - \bar{\beta}_{0\alpha} E_\alpha \Delta\theta - \frac{1}{2!} \bar{\beta}_{0\alpha\beta} E_\alpha E_\beta \Delta\theta - \frac{1}{2!} \bar{\beta}'_{0\alpha} E_\alpha (\Delta\theta)^2 - \cdots + g(\theta), \quad (2.63)$$

$$\hat{\Psi}(\mathbf{D}, \theta) = \Psi_0 + \hat{C}_{0\alpha}^\theta D_\alpha + \frac{1}{2!} \hat{C}_{0\alpha\beta}^\theta D_\alpha D_\beta + \frac{1}{3!} \hat{C}_{0\alpha\beta\gamma}^\theta D_\alpha D_\beta D_\gamma + \cdots - \hat{\beta}_{0\alpha} D_\alpha \Delta\theta - \frac{1}{2!} \hat{\beta}_{0\alpha\beta} D_\alpha D_\beta \Delta\theta - \frac{1}{2!} \hat{\beta}'_{0\alpha} D_\alpha (\Delta\theta)^2 - \cdots + g(\theta). \quad (2.64)$$

Letting $(\cdot)|_0 = (\cdot)|_{\mathbf{E}=\mathbf{D}=\mathbf{0}, \theta=\theta_0}$, material coefficients with zero subscripts are constants evaluated at the reference state, which is assumed stress free:

$$\Psi_0 = \bar{\Psi}(\mathbf{0}, \theta_0), \quad \bar{C}_{0\alpha}^\theta = (\partial \bar{\Psi} / \partial E_\alpha)|_0 = 0; \quad (2.65)$$

$$\bar{C}_{0\alpha\beta}^\theta = \left(\frac{\partial^2 \bar{\Psi}}{\partial E_\alpha \partial E_\beta} \right)_0, \quad \bar{C}_{0\alpha\beta\gamma}^\theta = \left(\frac{\partial^3 \bar{\Psi}}{\partial E_\alpha \partial E_\beta \partial E_\gamma} \right)_0; \quad (2.66)$$

$$\bar{\beta}_{0\alpha} = - \left(\frac{\partial^2 \bar{\Psi}}{\partial \theta \partial E_\alpha} \right)_0, \quad \bar{\beta}_{0\alpha\beta} = - \left(\frac{\partial^3 \bar{\Psi}}{\partial \theta \partial E_\alpha \partial E_\beta} \right)_0, \quad \bar{\beta}'_{0\alpha} = - \left(\frac{\partial^3 \bar{\Psi}}{\partial \theta^2 \partial E_\alpha} \right)_0; \quad (2.67)$$

and

$$\Psi_0 = \hat{\Psi}(\mathbf{0}, \theta_0), \quad \hat{C}_{0\alpha}^\theta = (\partial \hat{\Psi} / \partial D_\alpha)|_0 = 0; \quad (2.68)$$

$$\hat{C}_{0\alpha\beta}^\theta = \left(\frac{\partial^2 \hat{\Psi}}{\partial D_\alpha \partial D_\beta} \right)_0, \quad \hat{C}_{0\alpha\beta\gamma}^\theta = \left(\frac{\partial^3 \hat{\Psi}}{\partial D_\alpha \partial D_\beta \partial D_\gamma} \right)_0; \quad (2.69)$$

$$\hat{\beta}_{0\alpha} = - \left(\frac{\partial^2 \hat{\Psi}}{\partial \theta \partial D_\alpha} \right)_0, \quad \hat{\beta}_{0\alpha\beta} = - \left(\frac{\partial^3 \hat{\Psi}}{\partial \theta \partial D_\alpha \partial D_\beta} \right)_0, \quad \hat{\beta}'_{0\alpha} = - \left(\frac{\partial^3 \hat{\Psi}}{\partial \theta^2 \partial D_\alpha} \right)_0. \quad (2.70)$$

Letting c_0 denote a constant specific heat for the unstrained material, thermal free energy is prescribed as

$$g = -c_0 \theta \ln(\theta/\theta_0) \Rightarrow c_0 = -\theta_0 (\partial^2 g / \partial \theta^2)|_0. \quad (2.71)$$

Internal energy can be treated in a similar way, letting U_0 denote internal energy in the reference state defined by $(\mathbf{E}, \eta) = (\mathbf{0}, \eta_0)$, $(\mathbf{D}, \eta) = (\mathbf{0}, \eta_0)$, and entropy change from this reference state is $\Delta\eta = \eta - \eta_0$:

$$\bar{U}(\mathbf{E}, \eta) = U_0 + \bar{C}_{0\alpha}^\eta E_\alpha + \frac{1}{2!} \bar{C}_{0\alpha\beta}^\eta E_\alpha E_\beta + \frac{1}{3!} \bar{C}_{0\alpha\beta\gamma}^\eta E_\alpha E_\beta E_\gamma + \cdots - \theta_0 \left[\bar{F}_{0\alpha} E_\alpha \Delta\eta + \frac{1}{2!} \bar{F}_{0\alpha\beta} E_\alpha E_\beta \Delta\eta + \frac{1}{2!} \bar{F}'_{0\alpha} E_\alpha (\Delta\eta)^2 + \cdots - h(\eta) \right], \quad (2.72)$$

$$\hat{U}(\mathbf{D}, \eta) = U_0 + \hat{C}_{0\alpha}^\eta D_\alpha + \frac{1}{2!} \hat{C}_{0\alpha\beta}^\eta D_\alpha D_\beta + \frac{1}{3!} \hat{C}_{0\alpha\beta\gamma}^\eta D_\alpha D_\beta D_\gamma + \dots - \theta_0 \left[\hat{F}_{0\alpha} D_\alpha \Delta\eta + \frac{1}{2!} \hat{F}_{0\alpha\beta} D_\alpha D_\beta \Delta\eta + \frac{1}{2!} \hat{F}'_{0\alpha} D_\alpha (\Delta\eta)^2 + \dots - h(\eta) \right]. \quad (2.73)$$

Material coefficients evaluated at the unstressed reference state are

$$U_0 = \bar{U}(\mathbf{0}, \eta_0), \quad \bar{C}_{0\alpha}^\eta = (\partial \bar{U} / \partial E_\alpha)|_0 = 0; \quad (2.74)$$

$$\bar{C}_{0\alpha\beta}^\eta = \left(\frac{\partial^2 \bar{U}}{\partial E_\alpha \partial E_\beta} \right)_0, \quad \bar{C}_{0\alpha\beta\gamma}^\eta = \left(\frac{\partial^3 \bar{U}}{\partial E_\alpha \partial E_\beta \partial E_\gamma} \right)_0; \quad (2.75)$$

$$\begin{aligned} \theta_0 \bar{F}_{0\alpha} &= \left(\frac{\theta}{\bar{c}} \frac{\partial \eta}{\partial E_\alpha} \right)_0 = - \left(\frac{\partial \theta}{\partial E_\alpha} \right)_0 = - \left(\frac{\partial^2 \bar{U}}{\partial \eta \partial E_\alpha} \right)_0, \\ \theta_0 \bar{F}_{0\alpha\beta} &= - \left(\frac{\partial^3 \bar{U}}{\partial \eta \partial E_\alpha \partial E_\beta} \right)_0, \quad \theta_0 \bar{F}'_{0\alpha} = - \left(\frac{\partial^3 \bar{U}}{\partial \eta^2 \partial E_\alpha} \right)_0; \end{aligned} \quad (2.76)$$

and

$$U_0 = \hat{U}(\mathbf{0}, \eta_0), \quad \hat{C}_{0\alpha}^\eta = (\partial \hat{U} / \partial D_\alpha)|_0 = 0; \quad (2.77)$$

$$\hat{C}_{0\alpha\beta}^\eta = \left(\frac{\partial^2 \hat{U}}{\partial D_\alpha \partial D_\beta} \right)_0, \quad \hat{C}_{0\alpha\beta\gamma}^\eta = \left(\frac{\partial^3 \hat{U}}{\partial D_\alpha \partial D_\beta \partial D_\gamma} \right)_0; \quad (2.78)$$

$$\begin{aligned} \theta_0 \hat{F}_{0\alpha} &= \left(\frac{\theta}{\hat{c}} \frac{\partial \eta}{\partial D_\alpha} \right)_0 = - \left(\frac{\partial \theta}{\partial D_\alpha} \right)_0 = - \left(\frac{\partial^2 \hat{U}}{\partial \eta \partial D_\alpha} \right)_0, \\ \theta_0 \hat{F}_{0\alpha\beta} &= - \left(\frac{\partial^3 \hat{U}}{\partial \eta \partial D_\alpha \partial D_\beta} \right)_0, \quad \theta_0 \hat{F}'_{0\alpha} = - \left(\frac{\partial^3 \hat{U}}{\partial \eta^2 \partial D_\alpha} \right)_0. \end{aligned} \quad (2.79)$$

Letting c_0 denote a constant specific heat for the unstrained material, and noting when the material is unstrained that $\partial h / \partial \eta = \theta / \theta_0$,

$$\theta_0 h = c_0 \theta_0 (e^{\Delta\eta/c_0} - 1) = c_0 (\partial h / \partial \theta - \theta_0) \Rightarrow c_0 = \theta_0 [\partial h / (\partial \eta)]|_0. \quad (2.80)$$

Expanding the exponential as a Taylor series gives the isolated entropic contribution

$$h = \Delta\eta + \frac{1}{2!} (\Delta\eta)^2 / c_0 + \frac{1}{3!} (\Delta\eta)^3 / c_0^2 + \dots \quad (2.81)$$

Material coefficients defined as derivatives of either free or internal energy with respect to $\mathbf{E}$ are related to those defined as derivatives of either free or internal energy with respect to $\mathbf{D}$ in [Appendix B](#).

3. Analytical solutions: homogeneous isothermal deformation of a cubic crystal

3.1. Cubic crystals

Analytical predictions of constitutive theories based on strain measures $\mathbf{E}$ and $\mathbf{D}$ are compared in what follows. In [Section 3](#), attention is restricted to homogeneous, isothermal deformation of solids whose strain energy functions are truncated at third order in strain, i.e., [\(2.63\)](#) and [\(2.64\)](#) degenerate to

$$\bar{\Psi}(\mathbf{E}, \theta_0) = \frac{1}{2} \bar{C}_{0\alpha\beta}^\theta E_\alpha E_\beta + \frac{1}{6} \bar{C}_{0\alpha\beta\gamma}^\theta E_\alpha E_\beta E_\gamma = \frac{1}{2} C_{\alpha\beta} E_\alpha E_\beta + \frac{1}{6} \bar{C}_{\alpha\beta\gamma} E_\alpha E_\beta E_\gamma, \quad (3.1)$$

$$\hat{\Psi}(\mathbf{D}, \theta_0) = \frac{1}{2} \hat{C}_{0\alpha\beta}^\theta D_\alpha D_\beta + \frac{1}{6} \hat{C}_{0\alpha\beta\gamma}^\theta D_\alpha D_\beta D_\gamma = \frac{1}{2} C_{\alpha\beta} D_\alpha D_\beta + \frac{1}{6} \hat{C}_{\alpha\beta\gamma} D_\alpha D_\beta D_\gamma, \quad (3.2)$$

where, without further consequence, datum energy $\Psi_0 = 0$ has been assigned. When homogeneous deformation $\mathbf{F}$ is imposed, differences in predictions of the two theories arise due to differences in strain measures $\mathbf{E}(\mathbf{F})$ and $\mathbf{D}(\mathbf{F})$, which from [\(A.14\)](#) or [\(A.15\)](#) are second order in strain, as well as differences in third-order elastic constants indicated in [\(B.9\)](#). Second-order elastic constants are equal, as shown in [\(B.3\)](#). Following the second equalities in each of [\(3.1\)](#) and [\(3.2\)](#), θ superscripts and 0 subscripts are dropped from the elastic constants, and $C_{\alpha\beta} = \bar{C}_{0\alpha\beta} = \hat{C}_{0\alpha\beta}$.

Cubic crystals have at most three independent second-order elastic constants and can belong to point groups falling into one of the two Laue groups; those belonging to the Laue group with higher symmetry have six independent third-order constants ([Thurston, 1974](#); [Clayton, 2011a](#)):

$$C_{11}, C_{12}, C_{44}; \quad C_{111}, C_{112}, C_{123}, C_{144}, C_{155}, C_{456}. \quad (3.3)$$

The same components of $\bar{C}_{\alpha\beta\gamma}$ and $\hat{C}_{\alpha\beta\gamma}$ corresponding to $C_{\alpha\beta\gamma}$ in (3.3) are functionally independent, but numerical values of the same components of $\bar{C}_{\alpha\beta\gamma}$ and $\hat{C}_{\alpha\beta\gamma}$ can differ. The latter two are related by (B.9) or (B.10), yielding

$$\begin{aligned}\hat{C}_{111} &= \bar{C}_{111} + 12C_{11}, & \hat{C}_{112} &= \bar{C}_{112} + 4C_{12}, & \hat{C}_{123} &= \bar{C}_{123}, \\ \hat{C}_{144} &= \bar{C}_{144} + 2C_{12}, & \hat{C}_{155} &= \bar{C}_{155} + C_{11} + C_{12} + 4C_{44}, & \hat{C}_{456} &= \bar{C}_{456} + 3C_{44}.\end{aligned}\quad (3.4)$$

In the reference state, bulk modulus B_0 , shear modulus G_0 , and Poisson ratio ν are defined as

$$\begin{aligned}B_0 &= \frac{1}{3}(C_{11} + 2C_{12}), & G_0 &= \frac{1}{2}(C_{11} - C_{12}), \\ \nu &= (3B_0 - 2G_0)/(6B_0 + 2G_0) = \frac{1}{3}C_{12}/(C_{11} + C_{12}).\end{aligned}\quad (3.5)$$

Anisotropy ratio A is

$$A = 1 - G_0/C_{44} = 1 - \frac{1}{2}(C_{11} - C_{12})/C_{44}; \quad A = 0 \Leftrightarrow \text{isotropic}.\quad (3.6)$$

Notice that of the constants (B_0, G_0, ν, A), only A depends on C_{44} . Second-order elastic constants can be expressed in terms of (B_0, ν, A) as follows:

$$\frac{C_{11}}{B_0} = 3 \frac{1-\nu}{1+\nu}, \quad \frac{C_{12}}{B_0} = \frac{3\nu}{1+\nu}, \quad \frac{C_{44}}{B_0} = \frac{3}{2(1-A)} \frac{1-2\nu}{1+\nu}.\quad (3.7)$$

Requiring the quadratic (in strain) contribution to energy to be positive for all nonzero strains leads to the restrictions

$$B_0 > 0, \quad -1 < \nu < \frac{1}{2}, \quad A < 1.\quad (3.8)$$

Combinations of second- and third-order constants are related to pressure derivatives of tangent bulk and shear moduli at the reference state (Thurston, 1965; Guinan and Steinberg, 1974):

$$B'_0 = \left. \frac{dB}{dp} \right|_0 = \left. \frac{d[\frac{1}{3}(B_{11} + 2B_{12})]}{dp} \right|_0 = -\frac{1}{3B_0} \left(\frac{1}{3}\bar{C}_{111} + 2\bar{C}_{112} + \frac{2}{3}\bar{C}_{123} \right),\quad (3.9)$$

$$G'_0 = \left. \frac{dG}{dp} \right|_0 = \left. \frac{d[\frac{1}{2}(B_{11} - B_{12})]}{dp} \right|_0 = -\frac{1}{6B_0} (\bar{C}_{111} - \bar{C}_{123} + 2G_0) - 1.\quad (3.10)$$

Here $B_{\alpha\beta}$ are components of incremental stiffness (2.59) in Voigt notation, when stress is hydrostatic ($\sigma_{ij} = -p\delta_{ij}$). These can be converted to expressions in terms of $\hat{C}_{\alpha\beta\gamma}$ using (3.4):

$$B'_0 = -\frac{1}{3B_0} \left(\frac{1}{3}\hat{C}_{111} + 2\hat{C}_{112} + \frac{2}{3}\hat{C}_{123} \right) + 4,\quad (3.11)$$

$$G'_0 = -\frac{1}{6B_0} (\hat{C}_{111} - \hat{C}_{123} - 11C_{11} - C_{12}) - 1.\quad (3.12)$$

In some problems analyzed subsequently, certain assumptions are used to further reduce the number of independent elastic constants. For a cubic crystal of the higher symmetry Laue group also obeying Cauchy's relations (Clayton, 2011a)–which in Lagrangian theory correspond to pairwise central force interactions among atoms and may omit thermal-kinetic and zero-point vibrational contributions to stiffness–two independent second-order constants and three independent third-order constants remain:

$$C_{44} = C_{12}; \quad C_{155} = C_{112}, \quad C_{456} = C_{144} = C_{123}.\quad (3.13)$$

From (3.7), the first of (3.13) is equivalent to $A = 1 - (1 - 2\nu)/(2\nu)$. Although (3.13) is incompatible with correspondences (3.4), (3.9) and (3.11) can still be applied independently. For an isotropic solid not necessarily obeying Cauchy's relations, two independent second-order constants and three third-order constants also remain:

$$\begin{aligned}C_{44} &= \frac{1}{2}(C_{11} - C_{12}); & C_{144} &= \frac{1}{2}(C_{112} - C_{123}), \\ C_{155} &= \frac{1}{4}(C_{111} - C_{112}), & C_{456} &= \frac{1}{8}(C_{111} - 3C_{112} + 2C_{123}).\end{aligned}\quad (3.14)$$

For a third-order elastic material simultaneously obeying Cauchy and isotropic symmetry restrictions, (3.13) and (3.14) applied together, the response is parameterized by a single second-order constant (e.g., C_{11} or B_0):

$$C_{12} = \frac{1}{3}C_{11} \Leftrightarrow G_0/B_0 = \frac{3}{5} \Leftrightarrow \nu = \frac{1}{4} \Leftrightarrow C_{11} = \frac{9}{5}B_0;\quad (3.15)$$

and a single third-order constant (e.g., C_{111} or B'_0/B_0):

$$\begin{aligned}C_{112} &= 3C_{123} = \frac{1}{5}C_{111} \Rightarrow \\ B'_0 &= -\frac{7}{27}\bar{C}_{111}/B_0, & G'_0 &= -\frac{7}{45}\bar{C}_{111}/B_0 - \frac{6}{5}; \quad (\text{Lagrangian}) \\ B'_0 &= -\frac{7}{27}\hat{C}_{111}/B_0 + 4, & G'_0 &= -\frac{7}{45}\hat{C}_{111}/B_0 + \frac{3}{5}; \quad (\text{Eulerian})\end{aligned}\quad (3.16)$$

Note that one of the three third-order relations in (3.14) becomes redundant when Cauchy conditions (3.13) are applied. Here and in what follows⁴ in Section 3, (3.9), (3.11), and (3.16) all apply, but (3.4) no longer necessarily holds since all relations in the latter are not generally compatible with (3.16). Behavior analyzed in what follows in Section 3 can be described by the following energy functions, normalized by bulk modulus B_0 :

$$\begin{aligned} \frac{\bar{\Psi}}{3B_0} = & \frac{1-\nu}{2(1+\nu)}(E_{11}^2 + E_{22}^2 + E_{33}^2) + \frac{\nu}{1+\nu}(E_{11}E_{22} + E_{22}E_{33} + E_{33}E_{11}) + \frac{1}{1-A} \frac{1-2\nu}{1+\nu}(E_{12}^2 + E_{23}^2 + E_{13}^2) - \frac{1}{70} B_0' E_{IJ} E_{KL} E_{MN} \\ & \times [\delta_{IJ} \delta_{KL} \delta_{MN} + \delta_{IJ}(\delta_{KM} \delta_{LN} + \delta_{KN} \delta_{LM}) + \delta_{KL}(\delta_{IM} \delta_{JN} + \delta_{IN} \delta_{JM}) + \delta_{MN}(\delta_{IK} \delta_{JL} + \delta_{IL} \delta_{JK}) + \delta_{IK}(\delta_{JM} \delta_{LN} + \delta_{JN} \delta_{LM}) \\ & + \delta_{JL}(\delta_{IM} \delta_{KN} + \delta_{IN} \delta_{KM}) + \delta_{IL}(\delta_{JM} \delta_{KN} + \delta_{JN} \delta_{KM}) + \delta_{JK}(\delta_{IM} \delta_{LN} + \delta_{IN} \delta_{LM})], \end{aligned} \quad (3.17)$$

$$\begin{aligned} \frac{\hat{\Psi}}{3B_0} = & \frac{1-\nu}{2(1+\nu)}(D_{11}^2 + D_{22}^2 + D_{33}^2) + \frac{\nu}{1+\nu}(D_{11}D_{22} + D_{22}D_{33} + D_{33}D_{11}) + \frac{1}{1-A} \frac{1-2\nu}{1+\nu}(D_{12}^2 + D_{23}^2 + D_{13}^2) \\ & - \frac{1}{70} (B_0' - 4) D_{IJ} D_{KL} D_{MN} \times [\delta_{IJ} \delta_{KL} \delta_{MN} + \delta_{IJ}(\delta_{KM} \delta_{LN} + \delta_{KN} \delta_{LM}) + \delta_{KL}(\delta_{IM} \delta_{JN} + \delta_{IN} \delta_{JM}) + \delta_{MN}(\delta_{IK} \delta_{JL} + \delta_{IL} \delta_{JK}) \\ & + \delta_{IK}(\delta_{JM} \delta_{LN} + \delta_{JN} \delta_{LM}) + \delta_{JL}(\delta_{IM} \delta_{KN} + \delta_{IN} \delta_{KM}) + \delta_{IL}(\delta_{JM} \delta_{KN} + \delta_{JN} \delta_{KM}) + \delta_{JK}(\delta_{IM} \delta_{LN} + \delta_{IN} \delta_{LM})]. \end{aligned} \quad (3.18)$$

In these expressions, normalized quadratic contributions to energy, $(1/2B_0)C_{\alpha\beta}E_{\alpha}E_{\beta}$ and $(1/2B_0)C_{\alpha\beta}D_{\alpha}D_{\beta}$, retain full cubic anisotropy and depend on two dimensionless parameters ν and A , while normalized cubic contributions to energy, $(1/6B_0)\bar{C}_{\alpha\beta\gamma}E_{\alpha}E_{\beta}E_{\gamma}$ and $(1/6B_0)\hat{C}_{\alpha\beta\gamma}D_{\alpha}D_{\beta}D_{\gamma}$, assume isotropic and Cauchy symmetries and depend only on dimensionless parameter B_0' in (3.17) and (3.18).

Values considered subsequently span a realistic range for crystalline solids: $0 \leq B_0' \leq 8$, $\frac{1}{10} \leq \nu \leq \frac{2}{5}$, and $-1 \leq A \leq \frac{1}{2}$. When $\nu = \frac{1}{4}$, the value $B_0' = 4$ corresponds to $G_0' = \frac{6}{5}$, both of which are characteristic of pure polycrystalline substances (Guinan and Steinberg, 1974; Steinberg, 1982). Third-order contributions drop out of Lagrangian and Eulerian energies when $B_0' = 0$ and $B_0' = 4$, respectively. The Cauchy relations for third-order constants are reasonable for some real materials such as noble metals (copper, silver, gold) wherein closed-shell repulsive interactions dominate anharmonic properties (Hiki and Granato, 1966). Therefore, the present model with property set $(\nu, A, B_0') = (\frac{1}{4}, 0, 4)$ would be a realistic representation of an untextured polycrystalline noble metal. Different, stronger Cauchy-type relations have been proposed elsewhere (Hiki and Granato, 1966) for cubic solids wherein the nonlinearity is again characterized by a single third-order constant, but these other relations are incompatible with isotropy unless all third-order constants vanish, so they could not be applied to describe an untextured polycrystal and are not investigated further here.

3.2. Hydrostatic loading

For uniform spherical deformation from initial volume V_0 to final volume $V = JV_0$,

$$x_i = J^{1/3} \delta_{ij} X_j, \quad \partial_K J = (\partial J / \partial F_{ij}) \partial_K F_{ij} = J F_{ji}^{-1} \partial_K F_{ij} = 0; \quad (3.19)$$

$$\mathbf{F} = J^{1/3} \mathbf{1} = \left(\frac{V}{V_0} \right)^{1/3} \mathbf{1}, \quad \mathbf{E} = \frac{1}{2} (J^{2/3} - 1) \mathbf{1}, \quad \mathbf{D} = \frac{1}{2} (1 - J^{-2/3}) \mathbf{1}. \quad (3.20)$$

Axial components of strain tensors $\mathbf{E}$ and $\mathbf{D}$ for spherical deformation (3.20) and uniaxial strain (to be discussed in this section) are shown in Fig. 1 from 20% expansion to 40% compression. Strain component D_{11} tends to become more strongly negative relative to E_{11} as J decreases.

In homogeneous cubic crystals or isotropic bodies, the stress state resulting from such deformation is hydrostatic:

$$\sigma_{ij} = -p \delta_{ij}, \quad P_{iK} = -p J^{2/3} \delta_{iK}, \quad \bar{S}_{JK} = -p J^{1/3} \delta_{JK}, \quad \hat{S}_{JK} = -p J^{5/3} \delta_{JK}. \quad (3.21)$$

Therefore, Cauchy pressure is, using (A.8) and (A.13),

$$p = -\frac{1}{3} J^{-1/3} \bar{S}_{KK} = -\frac{1}{3} J^{-1/3} \left(\frac{\partial \bar{\Psi}}{\partial J} \frac{\partial J}{\partial E_{KK}} \right) \Big|_{\mathbf{F} = J^{1/3} \mathbf{1}} = -\frac{\partial \bar{\Psi}}{\partial J} = -\frac{1}{3} J^{-5/3} \hat{S}_{KK} = -\frac{1}{3} J^{-5/3} \left(\frac{\partial \hat{\Psi}}{\partial J} \frac{\partial J}{\partial D_{KK}} \right) \Big|_{\mathbf{F}^{-1} = J^{-1/3} \mathbf{1}} = -\frac{\partial \hat{\Psi}}{\partial J}. \quad (3.22)$$

Energy densities per unit reference volume in (3.17) and (3.18) reduce to

$$\bar{\Psi}/B_0 = \frac{9}{8} (J^{2/3} - 1)^2 [1 - \frac{1}{2} B_0' (J^{2/3} - 1)], \quad (3.23)$$

$$\hat{\Psi}/B_0 = \frac{9}{8} (1 - J^{-2/3})^2 [1 - \frac{1}{2} (B_0' - 4) (1 - J^{-2/3})]. \quad (3.24)$$

These expressions are independent of anisotropy factor A and Poisson ratio ν ; they also hold for any cubic crystal, regardless of any possible isotropic or Cauchy symmetries. From (3.22), Cauchy pressures resulting from third-order Lagrangian and

⁴ A perhaps more physically plausible, yet more mathematically cumbersome, approach would impose (3.13) only on Lagrangian constants and then use (3.4) to obtain an alternative set of Eulerian constants.

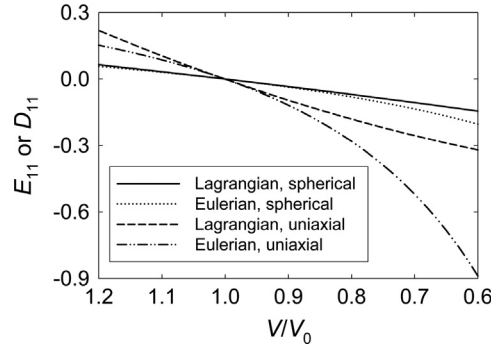


Fig. 1. Lagrangian (E_{11}) and Eulerian (D_{11}) strain components under spherical and uniaxial deformation.

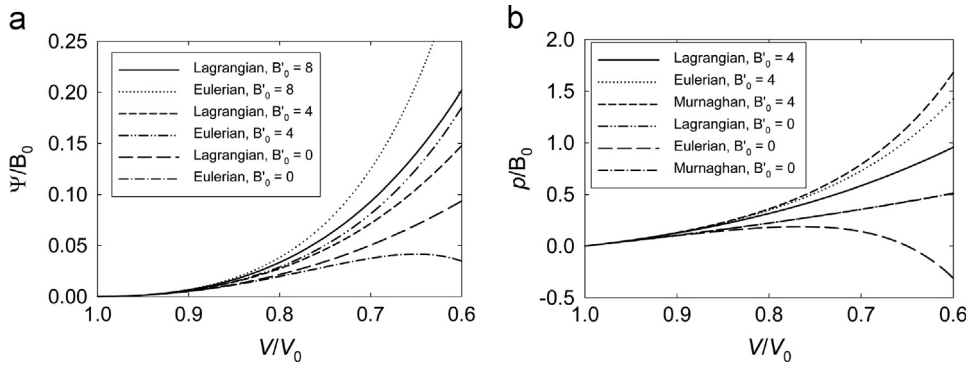


Fig. 2. Normalized (a) energy density and (b) hydrostatic pressure for spherical deformation.

Eulerian models are, respectively,

$$p/B_0 = \frac{3}{2}(J^{-1/3} - J^{1/3})[1 - \frac{3}{4}B'_0(J^{2/3} - 1)], \quad (\text{Lagrangian}) \quad (3.25)$$

$$p/B_0 = \frac{3}{2}(J^{-7/3} - J^{-5/3})[1 + \frac{3}{4}(B'_0 - 4)(J^{-2/3} - 1)]. \quad (\text{Eulerian}) \quad (3.26)$$

These can be compared with the well known respective Birch–Murnaghan and Murnaghan equations of state (Birch, 1947; Murnaghan, 1951, 1937; Thomsen, 1970):

$$p/B_0 = \frac{3}{2}(J^{-7/3} - J^{-5/3})[1 + \frac{3}{4}(B'_0 - 4)(J^{-2/3} - 1)], \quad (\text{Birch–Murnaghan}) \quad (3.27)$$

$$p/B_0 = (J^{-B'_0} - 1)/B'_0, \quad \lim_{B'_0 \rightarrow 0} p/B_0 = -\ln J. \quad (\text{Murnaghan}) \quad (3.28)$$

Since pressures in (3.26) and (3.27) coincide, the Birch–Murnaghan EOS is obtained directly from the present third-order Eulerian elastic theory based on strain measure $\mathbf{D}$ when applied to a cubic crystal subjected to spherical deformation. Values of normalized energy density $\bar{\psi}/B_0$ and $\dot{\psi}/B_0$ are shown in Fig. 2(a) for several values of B'_0 over compression range $0.6 \leq J \leq 1$. Normalized pressures from (3.25) to (3.28) are shown in Fig. 2(b). As B'_0 increases, energy and pressure increase more rapidly with decreasing volume for Eulerian theory compared to Lagrangian theory. For physically characteristic value $B'_0 = 4$, Eulerian theory provides much closer agreement with the Murnaghan EOS, giving a strongly increasing pressure at large compression representative of real materials; for physically low value $B'_0 = 0$, Lagrangian theory nearly coincides with the Murnaghan EOS.

Now consider incremental modulus $\mathbf{B}$ of (2.59), which for cubic crystals under spherical deformation reduces to

$$B_{ijkl} = J^{1/3} \bar{\mathbf{C}}_{ijkl} \delta_{ij} \delta_{kl} + p(\delta_{ij} \delta_{kl} - \delta_{ik} \delta_{jl} - \delta_{il} \delta_{jk}) = J^{-7/3} \hat{\mathbf{C}}_{ijkl} \delta_{ij} \delta_{kl} + p(\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}). \quad (3.29)$$

This tensor has the same symmetries as second-order elastic moduli $\bar{\mathbf{C}}$ and $\hat{\mathbf{C}}$, and thus three independent components. For Lagrangian theory with energy function (3.17), these are

$$B_{111}/B_0 = 3J^{1/3} \left\{ \frac{1-\nu}{1+\nu} - \frac{9}{10} B'_0 (J^{2/3} - 1) - \frac{1}{2} (J^{-2/3} - 1) \left[1 - \frac{3}{4} B'_0 (J^{2/3} - 1) \right] \right\}, \quad (3.30)$$

$$B_{12}/B_0 = 3J^{1/3} \left\{ \frac{\nu}{1+\nu} - \frac{3}{10} B'_0 (J^{2/3} - 1) + \frac{1}{2} (J^{-2/3} - 1) \left[1 - \frac{3}{4} B'_0 (J^{2/3} - 1) \right] \right\}, \quad (3.31)$$

$$B_{44}/B_0 = 3J^{1/3} \left\{ \frac{1-2\nu}{2(1-A)(1+\nu)} - \frac{3}{10} B'_0 (J^{2/3} - 1) - \frac{1}{2} (J^{-2/3} - 1) \left[1 - \frac{3}{4} B'_0 (J^{2/3} - 1) \right] \right\}. \quad (3.32)$$

For Eulerian theory with energy function (3.18), these are

$$B_{11}/B_0 = 3J^{-7/3} \left\{ \frac{1-\nu}{1+\nu} - \frac{9}{10} (B'_0 - 4)(1-J^{-2/3}) + \frac{3}{2} (1-J^{2/3}) \left[1 + \frac{3}{4} (B'_0 - 4)(J^{-2/3} - 1) \right] \right\}, \quad (3.33)$$

$$B_{12}/B_0 = 3J^{-7/3} \left\{ \frac{\nu}{1+\nu} - \frac{3}{10} (B'_0 - 4)(1-J^{-2/3}) + \frac{1}{2} (1-J^{2/3}) \left[1 + \frac{3}{4} (B'_0 - 4)(J^{-2/3} - 1) \right] \right\}, \quad (3.34)$$

$$B_{44}/B_0 = 3J^{-7/3} \left\{ \frac{1-2\nu}{2(1-A)(1+\nu)} - \frac{3}{10} (B'_0 - 4)(1-J^{-2/3}) + \frac{1}{2} (1-J^{2/3}) \left[1 + \frac{3}{4} (B'_0 - 4)(J^{-2/3} - 1) \right] \right\}. \quad (3.35)$$

For homogeneous hydrostatic loading in which pressure is applied incrementally, (2.61) is an exact criterion for elastic stability (Milstein and Hill, 1979), and there is no practical need to consider other criteria such as (2.60). Intrinsic stability criterion (2.61) can here be reduced to the following three normalized conditions:

$$\Lambda_B = \frac{B}{B_0} = \frac{B_{11} + 2B_{12}}{3B_0} > 0, \quad \Lambda_G = \frac{G}{G_0} = \frac{B_{11} - B_{12}}{2G_0} > 0, \quad \Lambda_\mu = \frac{\mu}{C_{44}} = \frac{B_{44}}{C_{44}} > 0. \quad (3.36)$$

For Lagrangian theory, left sides of these equalities become, explicitly,

$$\Lambda_B = \left\{ 1 - \frac{3}{2} B'_0 (J^{2/3} - 1) + \frac{1}{2} (J^{-2/3} - 1) \left[1 - \frac{3}{4} B'_0 (J^{2/3} - 1) \right] \right\} J^{1/3}, \quad (3.37)$$

$$\Lambda_G = \left\{ 1 - \frac{3(1+\nu)}{5(1-2\nu)} B'_0 (J^{2/3} - 1) - \frac{1+\nu}{1-2\nu} (J^{-2/3} - 1) \left[1 - \frac{3}{4} B'_0 (J^{2/3} - 1) \right] \right\} J^{1/3}, \quad (3.38)$$

$$\Lambda_\mu = \left\{ 1 - \frac{3(1-A)(1+\nu)}{5(1-2\nu)} B'_0 (J^{2/3} - 1) - \frac{(1-A)(1+\nu)}{(1-2\nu)} (J^{-2/3} - 1) \left[1 - \frac{3}{4} B'_0 (J^{2/3} - 1) \right] \right\} J^{1/3}. \quad (3.39)$$

Notice Λ_B depends only on (J, B'_0) , whereas Λ_G depends on (J, ν, B'_0) and Λ_μ depends on (J, A, ν, B'_0) . Also, $\Lambda_\mu \rightarrow \Lambda_G$ as $A \rightarrow 0$. Analogously, for Eulerian theory,

$$\Lambda_B = \left\{ 1 - \frac{3}{2} (B'_0 - 4)(1-J^{-2/3}) + \frac{5}{2} (1-J^{2/3}) \left[1 + \frac{3}{4} (B'_0 - 4)(J^{-2/3} - 1) \right] \right\} J^{-7/3}, \quad (3.40)$$

$$\Lambda_G = \left\{ 1 - \frac{3(1+\nu)}{5(1-2\nu)} (B'_0 - 4)(1-J^{-2/3}) + \frac{1+\nu}{1-2\nu} (1-J^{2/3}) \left[1 - \frac{3}{4} (B'_0 - 4)(1-J^{-2/3}) \right] \right\} J^{-7/3}, \quad (3.41)$$

$$\Lambda_\mu = \left\{ 1 - \frac{3(1-A)(1+\nu)}{5(1-2\nu)} (B'_0 - 4)(1-J^{-2/3}) + \frac{(1-A)(1+\nu)}{(1-2\nu)} (1-J^{2/3}) \left[1 - \frac{3}{4} (B'_0 - 4)(1-J^{-2/3}) \right] \right\} J^{-7/3}. \quad (3.42)$$

Table 1 shows stable domains for spherical/hydrostatic strain, defined as J for which (3.37)–(3.47) are positive. For the range of properties analyzed, stability predictions of either theory are similar, with Lagrangian theory stable to slightly larger compression (at $B'_0 = 0$) and Eulerian to slightly larger tension (at $B'_0 = 8$).

3.3. Uniaxial strain

For uniform uniaxial strain in the X_1 direction,

$$x_1 = JX_1, \quad x_2 = X_2, \quad x_3 = X_3; \quad \partial_K J = 0; \quad (3.43)$$

Table 1

Stable domains for spherical deformation over property ranges $0 \leq B'_0 \leq 8$, $\frac{1}{10} \leq \nu \leq \frac{2}{5}$, and $-1 \leq A \leq \frac{1}{2}$.

Theory	$\Lambda_B > 0$	$\Lambda_G > 0$	$\Lambda_\mu > 0$
Lagrangian	$0.00 < J < 1.13$ $\infty > p/B_0 > -0.12$	$0.81 < J < 1.06$ $0.21 > p/B_0 > -0.06$	$0.90 < J < 1.03$ $0.11 > p/B_0 > -0.03$
Eulerian	$0.76 < J < 1.23$ $0.19 > p/B_0 > -0.08$	$0.88 < J < 1.07$ $0.12 > p/B_0 > -0.07$	$0.93 < J < 1.04$ $0.07 > p/B_0 > -0.04$

$$\mathbf{F} = [F_{ij}] = [\partial x_i / \partial X_j] = \begin{bmatrix} J & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{F}^{-1} = [F_{ij}^{-1}] = [\partial X_i / \partial x_j] = \begin{bmatrix} J^{-1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}; \quad (3.44)$$

$$\mathbf{E} = [E_{ij}] = \begin{bmatrix} \frac{1}{2}(J^2 - 1) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{D} = [D_{ij}] = \begin{bmatrix} \frac{1}{2}(1 - J^{-2}) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (3.45)$$

Specifically considered here is deformation along a $\langle 100 \rangle$ direction, wherein both referential and spatial Cartesian coordinate axes are aligned parallel to cubic axes of the undeformed crystal lattice. Energies per unit volume in (3.17) and (3.18) reduce to

$$\bar{\Psi}/B_0 = \frac{C_{11}}{8B_0}(J^2 - 1)^2 + \frac{\bar{C}_{111}}{48B_0}(J^2 - 1)^3 = \frac{3}{8}(J^2 - 1)^2 \left[\frac{1 - \nu}{1 + \nu} - \frac{3}{14}B'_0(J^2 - 1) \right], \quad (3.46)$$

$$\hat{\Psi}/B_0 = \frac{C_{11}}{8B_0}(1 - J^{-2})^2 + \frac{\hat{C}_{111}}{48B_0}(1 - J^{-2})^3 = \frac{3}{8}(1 - J^{-2})^2 \left[\frac{1 - \nu}{1 + \nu} - \frac{3}{14}(B'_0 - 4)(1 - J^{-2}) \right]. \quad (3.47)$$

Notice that energy, and hence stresses and pressure, depend on material constants B_0 , B'_0 , and ν , but not anisotropy factor A for uniaxial strain along $\langle 100 \rangle$. Normalized energy densities $\bar{\Psi}/B_0$ and $\hat{\Psi}/B_0$ are shown in Fig. 3(a) for several values of ν (with fixed $B'_0 = 4$) over the compression range $0.6 \leq J \leq 1$, and similarly in Fig. 3(b) for several values of B'_0 with fixed $\nu = \frac{1}{4}$. As ν decreases, shear modulus G_0 increases, and energy increases when J and B'_0 are held fixed. As B'_0 increases, energy increases more rapidly with decreasing volume for Eulerian compared to Lagrangian theory as expected considering the rapid increase in $|D_{11}|$ with decreasing volume in Fig. 1. When $B'_0 = 0$, Eulerian theory predicts unrealistic negative energy for $J < 0.77$.

First consider Lagrangian theory based on strain measure $\mathbf{E}$. In Voigt notation, nonzero second Piola–Kirchhoff stress components $\bar{S}_\alpha = \partial \bar{\Psi} / \partial E_\alpha$ are

$$\bar{S}_1 = \frac{1}{2}(J^2 - 1) \left[C_{11} + \frac{1}{4}\bar{C}_{111}(J^2 - 1) \right] = \frac{3}{2}B_0(J^2 - 1) \left[\frac{1 - \nu}{1 + \nu} - \frac{9}{28}B'_0(J^2 - 1) \right], \quad (3.48)$$

$$\bar{S}_2 = \bar{S}_3 = \frac{1}{2}(J^2 - 1) \left[C_{12} + \frac{1}{4}\bar{C}_{112}(J^2 - 1) \right] = \frac{3}{2}B_0(J^2 - 1) \left[\frac{\nu}{1 + \nu} - \frac{9}{140}B'_0(J^2 - 1) \right]. \quad (3.49)$$

Cauchy stresses $\sigma_{ij} = J^{-1}F_{jM}P_{iM} = J^{-1}F_{iL}F_{jM}\bar{S}_{LM}$ and pressure $p = -\frac{1}{3}\sigma_{kk}$ are, in Voigt notation,

$$\sigma_1 = J\bar{S}_1 = \frac{3}{2}B_0(J^3 - J) \left[\frac{1 - \nu}{1 + \nu} - \frac{9}{28}B'_0(J^2 - 1) \right], \quad (3.50)$$

$$\sigma_2 = \sigma_3 = J^{-1}\bar{S}_2 = J^{-1}\bar{S}_3 = \frac{3}{2}B_0(J - J^{-1}) \left[\frac{\nu}{1 + \nu} - \frac{9}{140}B'_0(J^2 - 1) \right], \quad (3.51)$$

$$p = -\frac{1}{2}B_0(J^2 - 1) \left\{ J \left[\frac{1 - \nu}{1 + \nu} - \frac{9}{28}B'_0(J^2 - 1) \right] + 2J^{-1} \left[\frac{\nu}{1 + \nu} - \frac{9}{140}B'_0(J^2 - 1) \right] \right\}. \quad (3.52)$$

The ratio R of pressure under uniaxial strain to that under spherical deformation at the same volume ratio J is found by dividing (3.52) by (3.25):

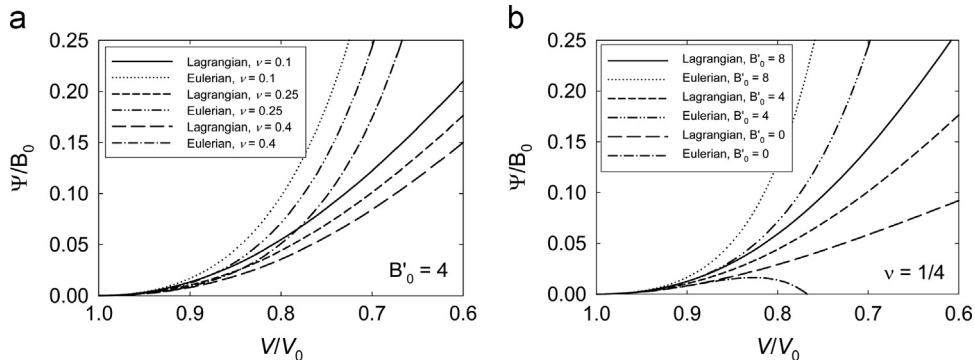


Fig. 3. Normalized energy density under uniaxial compression for (a) variable ν and (b) variable B'_0 .

$$R = \frac{(1-J^2) \left\{ J \left[\frac{1-\nu}{1+\nu} - \frac{9}{28} B'_0 (J^2-1) \right] + 2J^{-1} \left[\frac{\nu}{1+\nu} - \frac{9}{140} B'_0 (J^2-1) \right] \right\}}{3(J^{-1/3} - J^{1/3}) \left[1 - \frac{3}{4} B'_0 (J^{2/3} - 1) \right]}. \quad (3.53)$$

Now consider Eulerian theory based on strain measure $\mathbf{D}$. In Voigt notation, nonzero stress components $\hat{S}_\alpha = \partial \hat{\Psi} / \partial D_\alpha$ are

$$\hat{S}_1 = \frac{1}{2}(1-J^{-2}) \left[C_{11} + \frac{1}{4} \hat{C}_{111}(1-J^{-2}) \right] = \frac{3}{2} B_0(1-J^{-2}) \left[\frac{1-\nu}{1+\nu} - \frac{9}{28} (B'_0-4)(1-J^{-2}) \right], \quad (3.54)$$

$$\hat{S}_2 = \hat{S}_3 = \frac{1}{2}(1-J^{-2}) \left[C_{12} + \frac{1}{4} \hat{C}_{112}(1-J^{-2}) \right] = \frac{3}{2} B_0(1-J^{-2}) \left[\frac{\nu}{1+\nu} - \frac{9}{140} B'_0(1-J^{-2}) \right]. \quad (3.55)$$

Cauchy stresses $\sigma_{ij} = J^{-1} F_{Li}^{-1} F_{Mj}^{-1} \hat{S}_{LM}$ and pressure $p = -\frac{1}{3} \sigma_{kk}$ are, in Voigt notation,

$$\sigma_1 = J^{-3} \hat{S}_1 = \frac{3}{2} B_0(J^{-3} - J^{-5}) \left[\frac{1-\nu}{1+\nu} - \frac{9}{28} (B'_0-4)(1-J^{-2}) \right], \quad (3.56)$$

$$\sigma_2 = \sigma_3 = J^{-1} \hat{S}_2 = J^{-1} \hat{S}_3 = \frac{3}{2} B_0(J^{-1} - J^{-3}) \left[\frac{\nu}{1+\nu} - \frac{9}{140} B'_0(1-J^{-2}) \right], \quad (3.57)$$

$$p = -\frac{1}{2} B_0(J^{-3} - J^{-5}) \left\{ \frac{1-\nu}{1+\nu} - \frac{9}{28} (B'_0-4)(1-J^{-2}) + 2J^2 \left[\frac{\nu}{1+\nu} - \frac{9}{140} (B'_0-4)(1-J^{-2}) \right] \right\}. \quad (3.58)$$

The ratio R of pressure under uniaxial strain to that under spherical deformation at the same volume ratio J is found by dividing (3.58) by (3.26):

$$R = \frac{(J^{-5} - J^{-3}) \left\{ \frac{1-\nu}{1+\nu} - \frac{9}{28} (B'_0-4)(1-J^{-2}) + 2J^2 \left[\frac{\nu}{1+\nu} - \frac{9}{140} (B'_0-4)(1-J^{-2}) \right] \right\}}{3(J^{-7/3} - J^{-5/3}) \left[1 + \frac{3}{4} (B'_0-4)(J^{2/3} - 1) \right]}. \quad (3.59)$$

Normalized axial components of true (equivalently, Cauchy or first Piola–Kirchhoff) stress $P = -P_{11} = -\sigma_{11}$, positive in compression, are compared in Fig. 4(a) for several values of ν at fixed $B'_0 = 4$ over $0.6 \leq J \leq 1$, and similarly in Fig. 4(b) for variable B'_0 with $\nu = \frac{1}{4}$. As ν decreases, shear modulus G_0 increases, and compressive stress increases when J and B'_0 are held fixed. As B'_0 increases, P increases more rapidly with decreasing volume for Eulerian compared to Lagrangian theory, providing a more physically realistic representation of real solid behavior for $V/V_0 \leq 0.9$ (Jeanloz, 1989). Pressure ratios of (3.53) and (3.59) are compared for the same volume ranges and property sets in Fig. 5(a) and (b). For the most physically representative case $B'_0 = 4$, Lagrangian theory predicts $R < 1$ for $J \leq 0.9$, and Eulerian predicts $R > 1$ for $J < 1$. In analysis of shock physics data, material shear strength is often estimated as the difference between P in a uniaxial compression test and p in hydrostatic compression (Graham and Brooks, 1971; Kondo and Ahrens, 1983). The present analysis shows that such a procedure would underestimate strength for Lagrangian theory (for $R < 1$) and overestimate strength for Eulerian theory ($R > 1$).

Under uniaxial strain deformation, stiffness coefficients $\mathbf{A}$ and $\mathbf{B}$ become too lengthy to write down individually in closed form, but can easily be calculated using (2.50), (2.51) and (2.59). Intrinsic stability criteria (2.60) and (2.61) can be tested by considering the following inequalities (Clayton, 2012) that are necessary conditions for stability under homogeneous strain:

$$\det[\mathbf{A}] > 0 \Leftrightarrow \Lambda_A = \lambda_{\min}([A_{\alpha\beta}]) / \lambda_0 > 0; \quad \det[\mathbf{B}] > 0 \Leftrightarrow \Lambda_B = \lambda_{\min}([B_{\alpha\beta}]) / \lambda_0 > 0. \quad (3.60)$$

Here, $\lambda_{\min}([\cdot])$ refers to the minimum eigenvalue of 6×6 matrix $[\cdot]$, and $\lambda_0 = \lambda_{\min}([C_{\alpha\beta}])$ is the minimum eigenvalue of the second-order elastic stiffness matrix in the undeformed material. When $\mathbf{F} = \mathbf{1}$, $\Lambda_A = \Lambda_B = 1$. Incremental stiffness $\mathbf{B}$ in (2.59)

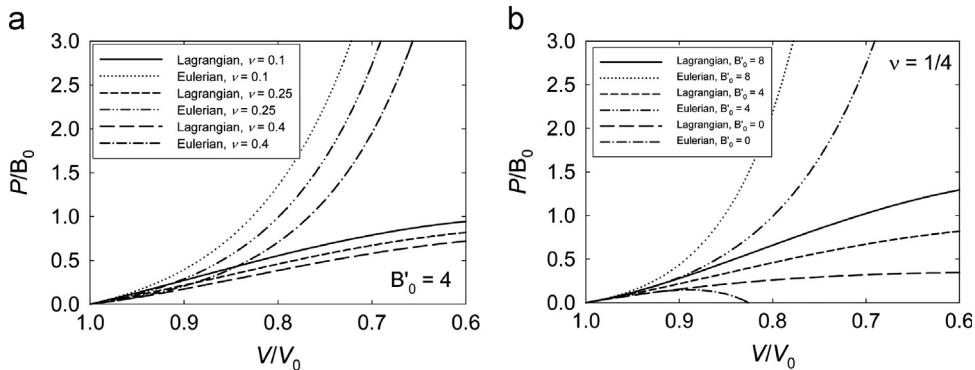


Fig. 4. Normalized axial true stress under uniaxial compression for (a) variable ν and (b) variable B'_0 .

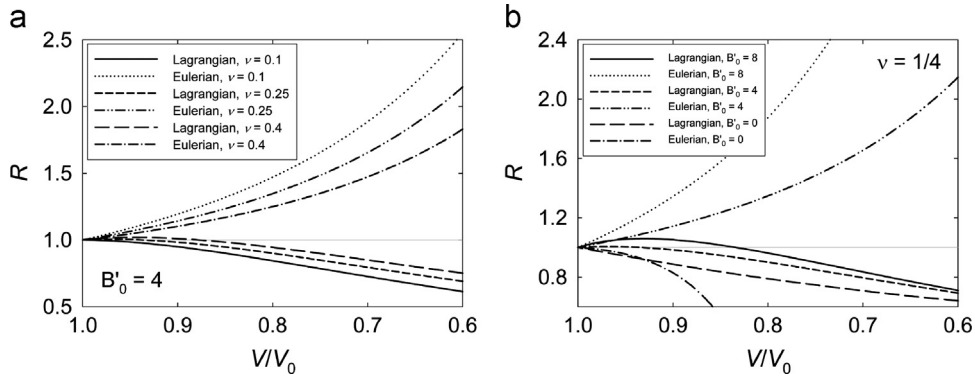


Fig. 5. Ratio R of Cauchy pressure under uniaxial compression to Cauchy pressure under spherical compression for (a) variable ν and (b) variable B'_0 .

Table 2

Stable domains for uniaxial strain over property ranges $0 \leq B'_0 \leq 8$, $\frac{1}{10} \leq \nu \leq \frac{2}{5}$, and $-1 \leq A \leq \frac{1}{2}$.

Theory	$\det[\mathbf{A}] > 0$	$\det[\mathbf{B}] > 0$
Lagrangian	$0.81 < J < 1.02$ $0.18 > P/B_0 > -0.02$	$0.90 < J < 1.02$ $0.10 > P/B_0 > -0.02$
Eulerian	$0.94 < J < 1.03$ $0.06 > P/B_0 > -0.03$	$0.95 < J < 1.03$ $0.05 > P/B_0 > -0.03$

already has full Voigt symmetry and can be written immediately as a 6×6 matrix; the symmetrized form of $\mathbf{A}$ entering (3.60) is formed from converting the following fourth-order tensor to Voigt notation (Clayton, 2012):

$$A_{ijkl} = \frac{1}{4}(A_{ijkl}\delta_{ii}\delta_{kk} + A_{jikl}\delta_{ij}\delta_{kk} + A_{ijlk}\delta_{ii}\delta_{ll} + A_{jilk}\delta_{ij}\delta_{ll}). \quad (3.61)$$

Table 2 shows stable domains for uniaxial strain, defined as J for which either of (3.60) applies. For the range of properties analyzed, stability predictions of either theory are similar, with Lagrangian theory stable to slightly larger compression and Eulerian to slightly larger tension. First instability occurs for $\nu = \frac{2}{5}$ and $A = -1$, properties corresponding to lowest shear modulus C_{44} . In compression, instability occurs for largest J at the minimum considered value of $B_0 = 0$; in tension, instability occurs for smallest J at the maximum considered value of $B_0 = 8$.

3.4. Simple shear

For uniform simple shear of magnitude γ in the X_1 – X_2 plane, let

$$x_1 = X_1 + \gamma X_2, \quad x_2 = X_2, \quad x_3 = X_3; \quad \partial_K \gamma = 0; \quad (3.62)$$

$$\mathbf{F} = [F_{ij}] = \begin{bmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{F}^{-1} = [F_{ij}^{-1}] = \begin{bmatrix} 1 & -\gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}; \quad (3.63)$$

$$\mathbf{E} = [E_{ij}] = \frac{1}{2} \begin{bmatrix} 0 & \gamma & 0 \\ \gamma & \gamma^2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{D} = [D_{ij}] = \frac{1}{2} \begin{bmatrix} -\gamma^2 & \gamma & 0 \\ \gamma & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (3.64)$$

In this case, $J = \det \mathbf{F} = 1 \Leftrightarrow V = V_0$, and nonzero strain components are $E_2 = \frac{1}{2}\gamma^2$ and $E_6 = 2E_{12} = \gamma$ or $D_1 = -\frac{1}{2}\gamma^2$ and $D_6 = 2D_{12} = \gamma$. Specifically considered here is shearing along a $\langle 100 \rangle$ direction on a $\{010\}$ plane, wherein both referential and spatial Cartesian coordinate axes are aligned parallel to cubic axes of the undeformed crystal lattice. Energy densities per unit volume in (3.17) and (3.18) reduce to

$$\bar{\Psi}/B_0 = \frac{1}{2B_0}\gamma^2 \left[C_{44} + \left(\frac{1}{4}C_{11} + \frac{1}{2}\bar{C}_{144} \right) \gamma^2 + \frac{1}{24}\bar{C}_{111}\gamma^4 \right] = \frac{3}{2}\gamma^2 \left\{ \frac{1-2\nu}{2(1-A)(1+\nu)} + \left[\frac{1-\nu}{4(1+\nu)} - \frac{9}{70}B_0 \right] \gamma^2 - \frac{3}{56}B_0\gamma^4 \right\}, \quad (3.65)$$

$$\dot{\Psi}/B_0 = \frac{1}{2B_0}\gamma^2 \left[C_{44} + \left(\frac{1}{4}C_{11} - \frac{1}{2}\hat{C}_{155} \right) \gamma^2 - \frac{1}{24}\hat{C}_{111}\gamma^4 \right] = \frac{3}{2}\gamma^2 \left\{ \frac{1-2\nu}{2(1-A)(1+\nu)} + \left[\frac{1-\nu}{4(1+\nu)} + \frac{9}{70}(B_0-4) \right] \gamma^2 + \frac{3}{56}(B_0-4)\gamma^4 \right\}. \quad (3.66)$$

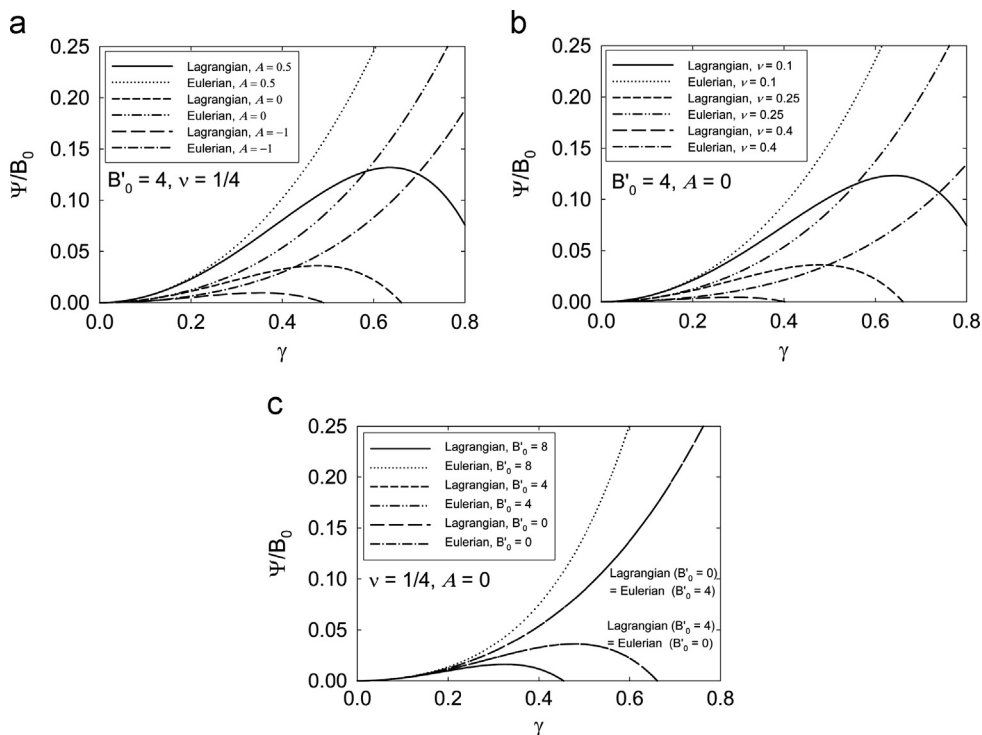


Fig. 6. Normalized energy density under simple shear for (a) variable A , (b) variable ν and (c) variable B'_0 .

Normalized energy densities $\bar{\Psi}/B_0$ and $\hat{\Psi}/B_0$ are shown in Fig. 6(a) for several values of A (with fixed $B'_0 = 4$ and $\nu = \frac{1}{4}$), in Fig. 6(b) for several values of ν (with fixed $B'_0 = 4$ and $A = 0$), and in Fig. 6(c) for several values of B'_0 (with fixed $\nu = \frac{1}{4}$ and $A = 0$), over the shear strain range $0 \leq \gamma \leq 0.8$. As shown in Fig. 6(a) and (b), when $B'_0 = 4$, as γ becomes large, energy may decrease and even become unrealistically negative for Lagrangian theory. As shown in Fig. 6(c), under simple shear, $\bar{\Psi}$ with $B'_0 = 0$ is equal to $\hat{\Psi}$ with $B'_0 = 4$, and $\bar{\Psi}$ with $B'_0 = 4$ is equal to $\hat{\Psi}$ with $B'_0 = 0$, as can be verified by inspection of (3.65) and (3.66). For $\gamma \geq 0.45$, Ψ can become unrealistically negative (indicating unstable behavior) in Lagrangian theory for $B'_0 \geq 4$ and in Eulerian theory for $B'_0 = 0$.

First consider Lagrangian theory based on strain measure $\mathbf{E}$. In Voigt notation, nonzero second Piola–Kirchhoff stress components $\bar{S}_\alpha = \partial \bar{\Psi} / \partial E_\alpha$ are

$$\bar{S}_1 = \frac{1}{2}(C_{12} + \bar{C}_{155})\gamma^2 + \frac{1}{8}\bar{C}_{112}\gamma^4 = \frac{3}{2}B_0\gamma^2\left(\frac{\nu}{1+\nu} - \frac{9}{35}B'_0 - \frac{9}{140}B'_0\gamma^2\right), \quad (3.67)$$

$$\bar{S}_2 = \frac{1}{2}(C_{11} + \bar{C}_{155})\gamma^2 + \frac{1}{8}\bar{C}_{111}\gamma^4 = \frac{3}{2}B_0\gamma^2\left(\frac{1-\nu}{1+\nu} - \frac{9}{35}B'_0 - \frac{9}{28}B'_0\gamma^2\right), \quad (3.68)$$

$$\bar{S}_3 = \frac{1}{2}(C_{12} + \bar{C}_{144})\gamma^2 + \frac{1}{8}\bar{C}_{112}\gamma^4 = \frac{3}{2}B_0\gamma^2\left(\frac{\nu}{1+\nu} - \frac{3}{35}B'_0 - \frac{9}{140}B'_0\gamma^2\right), \quad (3.69)$$

$$\bar{S}_6 = \left(C_{44} + \frac{1}{2}\bar{C}_{155}\gamma^2\right)\gamma = \frac{3}{2}B_0\gamma\left[\frac{1-2\nu}{(1-A)(1+\nu)} - \frac{9}{35}B'_0\gamma^2\right]. \quad (3.70)$$

Cauchy stresses, including shear stress τ and pressure p , are

$$\sigma_1 = \bar{S}_1 + \gamma^2\bar{S}_2 + 2\gamma\bar{S}_6 = \frac{3}{2}B_0\gamma^2\left[\frac{2(1-2\nu) + (1-A)\nu}{(1-A)(1+\nu)} - \frac{9}{35}B'_0 + \gamma^2\left(\frac{1-\nu}{1+\nu} - \frac{117}{140}B'_0 - \frac{9}{28}B'_0\gamma^2\right)\right], \quad (3.71)$$

$$\sigma_2 = \bar{S}_2 = \frac{3}{2}B_0\gamma^2\left(\frac{1-\nu}{1+\nu} - \frac{9}{35}B'_0 - \frac{9}{28}B'_0\gamma^2\right), \quad (3.72)$$

$$\sigma_3 = \bar{S}_3 = \frac{3}{2}B_0\gamma^2\left(\frac{\nu}{1+\nu} - \frac{3}{35}B'_0 - \frac{9}{140}B'_0\gamma^2\right), \quad (3.73)$$

$$\tau = \sigma_6 = \bar{S}_6 + \gamma\bar{S}_2 = \frac{3}{2}B_0\gamma\left[\frac{1-2\nu}{(1-A)(1+\nu)} + \gamma^2\left(\frac{1-\nu}{1+\nu} - \frac{18}{35}B'_0 - \frac{9}{28}B'_0\gamma^2\right)\right], \quad (3.74)$$

$$p = -\frac{1}{2}B_0\gamma^2 \left[\frac{2(1-2\nu) + (1-A)(1+\nu)}{(1-A)(1+\nu)} - \frac{21}{35}B'_0 + \gamma^2 \left(\frac{1-\nu}{1+\nu} - \frac{171}{140}B'_0 - \frac{9}{28}B'_0\gamma^2 \right) \right]. \quad (3.75)$$

When $A=0$, a universal relation (Eringen, 1962) for isotropic hyperelasticity can be verified:

$$\sigma_1 - \sigma_2 = \frac{3}{2}B_0\gamma^2 \left[\frac{1-2\nu}{1+\nu} + \gamma^2 \left(\frac{1-\nu}{1+\nu} - \frac{18}{35}B'_0 - \frac{9}{28}B'_0\gamma^2 \right) \right] = \tau\gamma. \quad (3.76)$$

Now consider Eulerian theory based on strain measure $\mathbf{D}$. In Voigt notation, nonzero stress components $\hat{S}_\alpha = \partial\hat{\Psi}/\partial D_\alpha$ are

$$\hat{S}_1 = \frac{1}{2}(-C_{11} + \hat{C}_{155})\gamma^2 + \frac{1}{8}\hat{C}_{111}\gamma^4 = -\frac{3}{2}B_0\gamma^2 \left[\frac{1-\nu}{1+\nu} + \frac{9}{35}(B'_0-4) + \frac{9}{28}(B'_0-4)\gamma^2 \right], \quad (3.77)$$

$$\hat{S}_2 = \frac{1}{2}(-C_{12} + \hat{C}_{155})\gamma^2 + \frac{1}{8}\hat{C}_{112}\gamma^4 = -\frac{3}{2}B_0\gamma^2 \left[\frac{\nu}{1+\nu} + \frac{9}{35}(B'_0-4) + \frac{9}{140}(B'_0-4)\gamma^2 \right], \quad (3.78)$$

$$\hat{S}_3 = \frac{1}{2}(-C_{12} + \hat{C}_{144})\gamma^2 + \frac{1}{8}\hat{C}_{112}\gamma^4 = -\frac{3}{2}B_0\gamma^2 \left[\frac{\nu}{1+\nu} + \frac{3}{35}(B'_0-4) + \frac{9}{140}(B'_0-4)\gamma^2 \right], \quad (3.79)$$

$$\hat{S}_6 = \left(C_{44} - \frac{1}{2}\hat{C}_{155}\gamma^2 \right)\gamma = \frac{3}{2}B_0\gamma \left[\frac{1-2\nu}{(1-A)(1+\nu)} + \frac{9}{35}(B'_0-4)\gamma^2 \right]. \quad (3.80)$$

Cauchy stresses, including shear stress and pressure, are Cauchy stresses, including shear stress τ and pressure p , are

$$\sigma_1 = \hat{S}_1 = -\frac{3}{2}B_0\gamma^2 \left[\frac{1-\nu}{1+\nu} + \frac{9}{35}(B'_0-4) + \frac{9}{28}(B'_0-4)\gamma^2 \right], \quad (3.81)$$

$$\sigma_2 = \hat{S}_2 + \gamma^2\hat{S}_1 - 2\gamma\hat{S}_6 = -\frac{3}{2}B_0\gamma^2 \left[\frac{2(1-2\nu) + (1-A)\nu}{(1-A)(1+\nu)} + \frac{9}{35}(B'_0-4) + \frac{1-\nu}{1+\nu}\gamma^2 + \gamma^2(B'_0-4) \left(\frac{117}{140} + \frac{9}{28}\gamma^2 \right) \right], \quad (3.82)$$

$$\sigma_3 = \hat{S}_3 = -\frac{3}{2}B_0\gamma^2 \left[\frac{\nu}{1+\nu} + \frac{3}{35}(B'_0-4) + \frac{9}{140}(B'_0-4)\gamma^2 \right], \quad (3.83)$$

$$\tau = \sigma_6 = \hat{S}_6 - \gamma\hat{S}_1 = \frac{3}{2}B_0\gamma \left[\frac{1-2\nu}{(1-A)(1+\nu)} + \frac{1-\nu}{1+\nu}\gamma^2 + \frac{18}{35}(B'_0-4)\gamma^2 + \frac{9}{28}(B'_0-4)\gamma^4 \right], \quad (3.84)$$

$$p = \frac{1}{2}B_0\gamma^2 \left[\frac{2(1-2\nu) + (1-A)(1+\nu)}{(1-A)(1+\nu)} + \frac{21}{35}(B'_0-4) + \gamma^2 \left(\frac{1-\nu}{1+\nu} + \frac{171}{140}(B'_0-4) + \frac{9}{28}(B'_0-4)\gamma^2 \right) \right]. \quad (3.85)$$

When $A=0$, a universal relation (Eringen, 1962) for isotropic hyperelasticity can be verified:

$$\sigma_1 - \sigma_2 = \frac{3}{2}B_0\gamma^2 \left[\frac{1-2\nu}{1+\nu} + \frac{1-\nu}{1+\nu}\gamma^2 + \frac{18}{35}(B'_0-4)\gamma^2 + \frac{9}{28}(B'_0-4)\gamma^4 \right] = \tau\gamma. \quad (3.86)$$

For both Lagrangian and Eulerian theories, τ is $O(\gamma)$ and normal stresses are $O(\gamma^2)$.

Normalized shear stress τ/B_0 for Lagrangian and Eulerian theories [(3.74) and (3.84)] are shown in Fig. 7(a) for several values of A (with fixed $B'_0 = 4$ and $\nu = \frac{1}{4}$), in Fig. 7(b) for several values of ν (with fixed $B'_0 = 4$ and $A=0$), and in Fig. 7(c) for several values of B'_0 (with fixed $\nu = \frac{1}{4}$ and $A=0$), over the shear strain range $0 \leq \gamma \leq 0.8$. As shown in Fig. 7(a) and (b), when $B'_0 = 4$, as γ becomes large, shear stress may decrease and even become unrealistically negative for Lagrangian theory. As shown in Fig. 6(c), under simple shear, τ of Lagrangian theory with $B'_0 = 0$ is equal to τ of Eulerian theory with $B'_0 = 4$, and τ of Lagrangian theory with $B'_0 = 4$ is equal to τ of Eulerian theory with $B'_0 = 0$.

Under shear deformation, stiffness coefficients $\mathbf{A}$ and $\mathbf{B}$ can be calculated using (2.50), (2.51), and (2.59). Intrinsic stability criteria (2.60) and (2.61) can then be tested by considering the necessary conditions

$$\det[\mathbf{A}] > 0 \Leftrightarrow \Lambda_A = \lambda_{\min}([\mathbf{A}_{\alpha\beta}])/\lambda_0 > 0; \quad \det[\mathbf{B}] > 0 \Leftrightarrow \Lambda_B = \lambda_{\min}([\mathbf{B}_{\alpha\beta}])/\lambda_0 > 0; \quad (3.87)$$

where $\lambda_{\min}([\cdot])$ is the minimum eigenvalue of 6×6 matrix $[\cdot]$, and $\lambda_0 = \lambda_{\min}([\mathbf{C}_{\alpha\beta}])$. The symmetric form of $\mathbf{A}$ in (3.87) is computed with (3.61). Because (2.60) and (2.61), when used with fully symmetric 6×6 matrices $[\mathbf{A}_{\alpha\beta}]$ and $[\mathbf{B}_{\alpha\beta}]$, do not strictly apply when the deformation gradient involves rotation (i.e., when $\mathbf{F} \neq \mathbf{F}^T$), in applying (3.87) the substitution $\mathbf{F} \rightarrow \mathbf{U}$ is applied, where $\mathbf{U}$ is the right stretch tensor from the polar decomposition of the simple shear deformation in (3.63) (Clayton and Bliss, submitted for publication):

$$\begin{bmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = [\mathbf{R}_{ik}][\mathbf{U}_{KJ}] = \begin{bmatrix} \frac{2}{(4+\gamma^2)^{1/2}} & \frac{\gamma}{(4+\gamma^2)^{1/2}} & 0 \\ \frac{-\gamma}{(4+\gamma^2)^{1/2}} & \frac{2}{(4+\gamma^2)^{1/2}} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{2}{(4+\gamma^2)^{1/2}} & \frac{\gamma}{(4+\gamma^2)^{1/2}} & 0 \\ \frac{\gamma}{(4+\gamma^2)^{1/2}} & \frac{2+\gamma^2}{(4+\gamma^2)^{1/2}} & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (3.88)$$

With this substitution, strain energies and stresses referred to referential coordinates are unchanged, but Cauchy stress components may differ from those presented analytically above in the absence of rotation. Table 3 shows stable domains for shear strain, defined as γ for which either of (3.87) applies. First instability occurs for $\nu = \frac{2}{5}$ and $A = -1$, properties

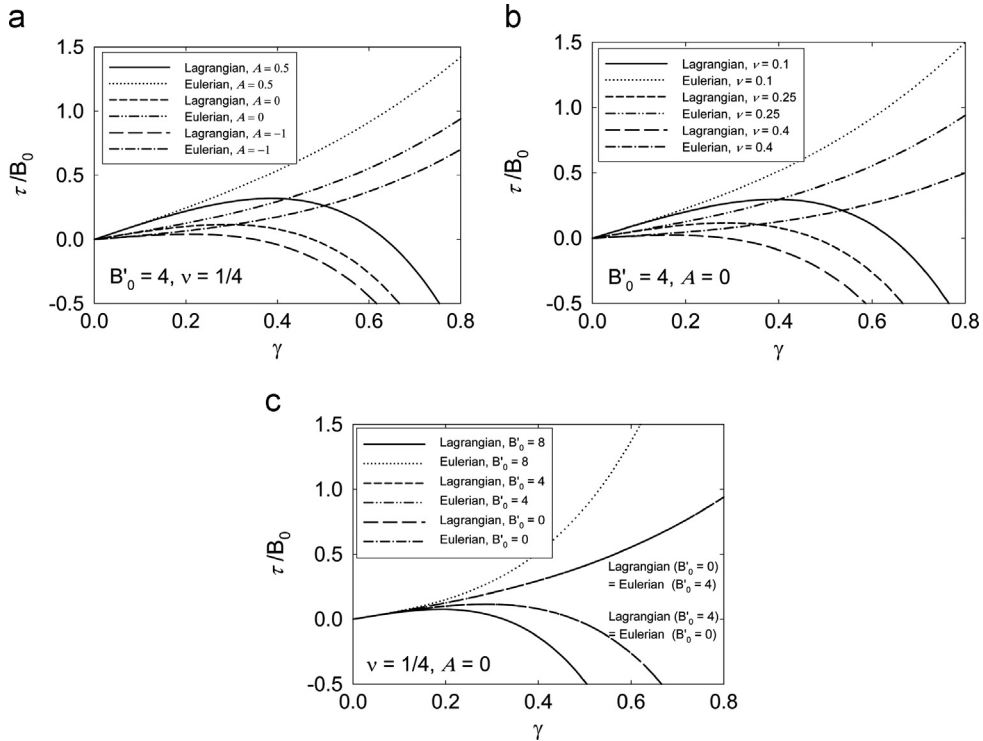


Fig. 7. Normalized shear stress for (a) variable A , (b) variable ν and (c) variable B'_0 .

Table 3

Stable domains for uniaxial strain over property ranges $0 \leq B'_0 \leq 8$, $\frac{1}{10} \leq \nu \leq \frac{2}{5}$, and $-1 \leq A \leq \frac{1}{2}$.

Theory	$\det[\mathbf{A}] > 0$	$\det[\mathbf{B}] > 0$
Lagrangian	$\gamma < 0.05$	$\gamma < 0.05$
	$\tau/B_0 < 4.8 \times 10^{-3}$	$\tau/B_0 < 4.8 \times 10^{-3}$
Eulerian	$\gamma < 0.09$	$\gamma < 0.09$
	$\tau/B_0 < 7.8 \times 10^{-3}$	$\tau/B_0 < 7.8 \times 10^{-3}$

corresponding to lowest shear modulus C_{44} . Eulerian theory is intrinsically stable to $\gamma \approx 0.09$ with either criteria, compared to the significantly smaller stable domain of Lagrangian theory ($\gamma \lesssim 0.05$).

3.5. Summary of analytical results and discussion

Key aspects of results in Sections 3.2–3.4 are summarized as follows. For hydrostatic compression, for a physically characteristic value $B'_0 \approx 4$, Eulerian theory appears more realistic than Lagrangian theory, giving a pressure response closer to the Murnaghan EOS, while Lagrangian theory fails to predict a rapidly increasing pressure at very large compression. Similar observations have been made elsewhere (Birch, 1947, 1978; Jeanloz, 1989). For uniaxial compression, with $B'_0 \approx 4$, Eulerian theory again offers a more physically realistic representation; however, when $B'_0 = 0$, Eulerian theory can produce negative strain energy at large compression. For simple shear, Eulerian theory is generally more stable and provides physically reasonable behavior (e.g., monotonically increasing energy with increasing shear strain) for $B' \geq 4$, while Lagrangian theory predicts decreasing shear stress and strain energy at large shear for $B' \geq 4$. The above statements apply for an ideal cubic crystal with highly symmetric anharmonic properties. Deviations may be expected for highly anisotropic materials, as shown in Section 4.

This work is focused primarily on comparison of only two theories based on two strain measures $\mathbf{E}$ and $\mathbf{D}$. Lagrangian $\mathbf{E}$ -based theory is considered because, historically, it is the most common measure used for anisotropic crystal hyperelasticity. Eulerian $\mathbf{D}$ -based theory is considered because, as shown already, it reduces to the successful Birch–Murnaghan EOS under hydrostatic compression, and because it has been demonstrated elsewhere to accurately predict the response of anisotropic crystals under pressure (Weaver, 1976; Perrin and Delannoy, 1978). The present work investigates, for the first time, potential accuracy of $\mathbf{D}$ -based theory for loading conditions involving deviatoric stress in addition to pressure.

An infinite number of possible strain measures exists for anisotropic hyperelasticity, e.g., constructions consisting of stretch $\mathbf{U}$ raised to various exponents are possible. A likely useful strain energy potential, not considered in this work, would depend on the logarithm of the right stretch, i.e., $W = W(\ln \mathbf{U})$. This logarithmic strain is of particular interest since its spatial counterpart, Hencky strain $\ln \mathbf{V}$, is useful for many isotropic solids under moderate to large deformation (Anand, 1979). For isotropic solids, the simple constitutive equality $\sigma = J^{-1} \partial W / \partial \ln \mathbf{V}$ holds, though $\mathbf{V}$ is not an appropriate state variable for anisotropic solids. In contrast, $W = W(\ln \mathbf{U})$ is appropriate for anisotropic hyperelasticity, and though not often encountered in the literature, was considered in Dlużewski (2000). In that work Dlużewski (2000), transformation formulae among third-order elastic constants for Green elasticity and logarithmic elasticity were derived, and it was shown that the latter tend to be smaller in magnitude for several cubic crystals, suggesting greater accuracy of polynomial energy functions depending on $\ln \mathbf{U}$ than $\mathbf{E}$ when truncated at a certain order. Whether or not $\ln \mathbf{U}$ -based theory is more accurate than $\mathbf{D}$ -based theory remains an open question that may be answered in future work; superiority of one measure over another likely will depend on particular material and loading regime. Since both $\ln \mathbf{U}$ and $\mathbf{D}$ increase rapidly in magnitude with increasing compression, a polynomial series for strain energy in either strain measure should account well for the rapid increase in energy, pressure, and stiffness observed in most solids at large compression. Computation of $\ln \mathbf{U}$, for example via usual algorithms requiring matrix diagonalization, is generally more cumbersome than $\mathbf{D}$, which requires only inversion of $\mathbf{F}$. Computation of derivatives such as $\partial \ln \mathbf{U} / \partial \mathbf{F}$ needed for stress, tangent stiffness, and various thermodynamic identities, is possible but generally tedious (Jog, 2009).

4. Shock compression of low-symmetry crystals

Considered in what follows next is the material response under loading by an ideal planar shock wave. Crystals with homogeneous properties but of arbitrary anisotropy are addressed, i.e., simplifying assumptions made in Section 3.1 on material symmetry are removed. Generic analytical solutions using nonlinear elastic theories based on strain measures $\mathbf{E}$ (Lagrangian) and $\mathbf{D}$ (Eulerian) are derived in Section 4.1. Specific materials—quartz, sapphire, and diamond—towards which the theories are applied, and requisite thermoelastic properties are presented in Section 4.2. Results of the model as applied to these materials are discussed in Section 4.3, with additional new developments in Section 4.4.

4.1. General 1-D solutions

A shock wave is represented mathematically as a propagating surface across which there may exist jump discontinuities in mass density, particle velocity, strain, stress, entropy, temperature, and internal energy. Considered here are 1-D (i.e., normal or longitudinal) shocks. Quantities associated with material ahead of the shock are labeled with superscript +, with material behind superscript −. Material ahead of the shock is assumed to be at rest, undeformed, unstressed, and at ambient reference temperature θ_0 . The jump in an arbitrary quantity $(\cdot)$ across the shock is written as

$$[(\cdot)] = (\cdot)^- - (\cdot)^+. \quad (4.1)$$

In derivations that follow, the shock moves at steady natural velocity $\mathfrak{D}$ in the $X = X_1$ direction. The deformation gradient is uniaxial strain of the form

$$\mathbf{F}^- = [F_{ij}]^- = \begin{bmatrix} F & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 + \xi & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}; \quad \mathbf{F}^+ = \mathbf{1}. \quad (4.2)$$

Behind the shock, with $x = x_1^-$ and $u = u_1^-$ the longitudinal particle coordinate and displacement,

$$F = \frac{\partial x}{\partial X} = 1 + \frac{\partial u}{\partial X} = 1 + \xi = J^- = \frac{V^-}{V_0} = \frac{\rho_0}{\rho^-}, \quad \xi = \partial u / \partial X. \quad (4.3)$$

In the present work attention is restricted to compressive shocks, for which $0 < F \leq 1$ and $-1 < \xi \leq 0$, moving with positive velocity $\mathfrak{D} > 0$. The only nonzero components of Lagrangian and Eulerian strain are, respectively,

$$E = E_{11}^- = \frac{1}{2}(F^2 - 1) = \xi \left(1 + \frac{1}{2}\xi \right), \quad D = D_{11}^- = \frac{1}{2}(1 - F^{-2}) = \frac{1}{2} \left[1 - \frac{1}{(1 + \xi)^2} \right]. \quad (4.4)$$

Longitudinal force per unit reference area (or equivalently, current area under uniaxial strain) behind the shock is, positive in compression,

$$P = -P_{11}^- = -J(F_{1k}^{-1} \sigma_{1k})^- = -\sigma_{11}^-. \quad (4.5)$$

Though often referred to as “Hugoniot pressure”, stress P is generally not equal to hydrostatic pressure $p = -\frac{1}{3} \sigma_{kk}$ in a solid with shear strength.

Let $\rho = \rho^-$ and $v = v_1^-$ denote mass density and particle velocity in the shocked state. Conservation laws for mass, linear momentum, and energy—often referred to as Rankine–Hugoniot equations—can be written, respectively, as (Thurston, 1974;

McQueen et al., 1970)

$$\rho_0 \mathfrak{D} = \rho(\mathfrak{D} - v) \Leftrightarrow \xi = -v / \mathfrak{D}, \quad (4.6)$$

$$P = \rho_0 \mathfrak{D} v \Rightarrow \rho_0 \mathfrak{D}^2 = -P / \xi \Leftrightarrow \rho_0 v^2 = -P \xi, \quad (4.7)$$

$$Pv = \mathfrak{D} \left(\frac{1}{2} \rho_0 v^2 + \llbracket U \rrbracket \right) \Rightarrow \llbracket U \rrbracket = \frac{1}{2} \rho_0 v^2. \quad (4.8)$$

From (4.6), requiring $1 \geq j > 0$ leads to constraints $\mathfrak{D} > v \geq 0$. In energy balance (4.8), the usual adiabatic assumption of null heat conduction has been used, which is thought appropriate for elastic materials (Thurston, 1974) as well as relatively weak shocks in elastic–plastic solids (Perrin and Delannoy-Coutiris, 1983), but may not be valid for overdriven shocks in elastic–plastic materials (Wallace, 1981). The shock process is neither isothermal nor isentropic; the entropy inequality can be written as (Germain and Lee, 1973)

$$\llbracket \eta / \rho_0 \rrbracket \geq 0 \Rightarrow \llbracket \eta \rrbracket \geq 0. \quad (4.9)$$

Subsequent derivations rely on internal energy-based constitutive models $\bar{U}(\mathbf{E}, \eta)$ and $\hat{U}(\mathbf{D}, \eta)$ of (2.72) and (2.73). Derivatives of these functions with respect to strain depend only on entropy changes $\Delta \eta$ from the reference state and hence are independent of $\eta_0 = \eta^+$. Furthermore, stress and temperature depend only on derivatives of internal energy with respect to strain and entropy, and hence are independent of U_0 . Therefore, to simplify forthcoming derivations, let

$$U_0 = U^+ = 0, \quad \eta_0 = \eta^+ = 0 \Rightarrow \llbracket U \rrbracket = U^- = U, \quad \llbracket \eta \rrbracket = \eta^- = \Delta \eta = \eta; \quad (4.10)$$

$$\theta^+ = (\partial U / \partial \eta)^+ = \theta_0, \quad \theta^- = (\partial U / \partial \eta)^- = \theta \Rightarrow \llbracket \theta \rrbracket = \theta^- - \theta^+ = \theta - \theta_0 = \Delta \theta. \quad (4.11)$$

Stress components thermodynamically conjugate to E or D are related to P via

$$P = -F_{1j} \bar{S}_{j1} = -F \bar{S} = -(1 + \xi) \bar{S}, \quad \bar{S} = \bar{S}_{11} = \partial \bar{U} / \partial E_{11} = \partial \bar{U} / \partial E; \quad (4.12)$$

$$P = -J^{-1} F_{11}^{-1} F_{1j}^{-1} \hat{S}_{j1} = -F^{-3} \hat{S} = -(1 + \xi)^{-3} \hat{S}, \quad \hat{S} = \hat{S}_{11} = \partial \hat{U} / \partial D_{11} = \partial \hat{U} / \partial D; \quad (4.13)$$

where all quantities are evaluated in the material behind the shock.

The following binomial series (Spiegel and Liu, 1999) proves useful, where a is a non-negative constant:

$$(a + f)^n = a^n + na^{n-1}f + \frac{n(n-1)}{2!}a^{n-2}f^2 + \frac{n(n-1)(n-2)}{3!}a^{n-3}f^3 + \frac{n(n-1)(n-2)(n-3)}{4!}a^{n-4}f^4 + \frac{n(n-1)(n-2)(n-3)(n-4)}{5!}a^{n-5}f^5 + \dots \quad (4.14)$$

Let $a=1$. From (4.4), selecting roots corresponding to $\xi=0$ at $E=D=0$,

$$\xi = -1 + (1 + 2E)^{1/2} = -1 + (1 - 2D)^{-1/2}. \quad (4.15)$$

From (4.14), with $n = \frac{1}{2}$ and $f = 2E$, the displacement gradient in the shocked state is

$$\xi = E - \frac{1}{2}E^2 + \frac{1}{2}E^3 - \frac{5}{8}E^4 + \frac{7}{8}E^5 - \dots \quad (4.16)$$

Similarly, letting $n = -\frac{1}{2}$ and $f = -2D$,

$$\xi = D + \frac{3}{2}D^2 + \frac{5}{2}D^3 + \frac{35}{8}D^4 + \frac{63}{8}D^5 + \dots \quad (4.17)$$

Finally, letting $n = \frac{3}{2}$ and $f = -2D$,

$$(1 + \xi)^{-3} = (1 - 2D)^{3/2} = 1 - 3D + \frac{3}{2}D^2 + \frac{1}{2}D^3 + \frac{3}{8}D^4 + \frac{3}{8}D^5 + \dots \quad (4.18)$$

The above series are valid for $-1 < f \leq 1$, which correspond to $0.7 \lesssim V/V_0 \lesssim 1.7$. Using (4.7), (4.10), (4.12), and (4.16), the second of (4.8) becomes, in terms of E ,

$$U = -\frac{1}{2}P\xi = \frac{1}{2}\bar{S}\xi(1 + \xi) = \frac{1}{2}\bar{S}(E + \frac{1}{2}E^2 - \frac{1}{2}E^3 + \frac{5}{8}E^4 - \frac{7}{8}E^5 + \dots). \quad (4.19)$$

Using (4.7), (4.10), (4.13), (4.17), and (4.18), the second of (4.8) becomes, alternatively in terms of D ,

$$U = -\frac{1}{2}P\xi = \frac{1}{2}\hat{S}\xi(1 + \xi)^{-3} = \frac{1}{2}\hat{S}(D - \frac{3}{2}D^2 - \frac{1}{2}D^3 - \frac{3}{8}D^4 - \frac{3}{8}D^5 - \dots). \quad (4.20)$$

Internal energy functions (2.72) and (2.73)–using (2.81) and specialized to the present uniaxial strain conditions with (2.74), (2.77), and (4.10), and extended to fourth order in strain and second order in entropy–are

$$\bar{U}(E, \eta) = \frac{1}{2}C_{11}E^2 + \frac{1}{6}\bar{C}_{111}E^3 + \frac{1}{24}\bar{C}_{1111}E^4 - \theta_0 \left(\Gamma_1 E \eta + \frac{1}{2}\Gamma'_1 E \eta^2 + \frac{1}{2}\bar{\Gamma}_{11} E^2 \eta \right) + \theta_0 \eta \left(1 + \frac{1}{2c_0} \eta \right), \quad (4.21)$$

$$\hat{U}(D, \eta) = \frac{1}{2}C_{11}D^2 + \frac{1}{6}\hat{C}_{111}D^3 + \frac{1}{24}\hat{C}_{1111}D^4 - \theta_0 \left(\Gamma_1 D \eta + \frac{1}{2}\Gamma'_1 D \eta^2 + \frac{1}{2}\hat{\Gamma}_{11} D^2 \eta \right) + \theta_0 \eta \left(1 + \frac{1}{2c_0} \eta \right). \quad (4.22)$$

Elastic constants in (4.21) and (4.22) are isentropic, and Voigt notation is used. The following simplified notation has been used for material constants referred to the reference state, upon consideration of (B.3) and (B.2),

$$C_{11} = \bar{C}_{011}^\eta = \hat{C}_{011}^\eta, \quad \Gamma_1 = \bar{\Gamma}_{01} = \hat{\Gamma}_{01}, \quad \Gamma'_1 = \bar{\Gamma}'_{01} = \hat{\Gamma}'_{01}. \quad (4.23)$$

Third- and fourth-order isentropic elastic constants with respect to strain measures $\mathbf{E}$ and $\mathbf{D}$ are written as

$$\bar{C}_{111} = \bar{C}_{0111}^\eta, \quad \bar{C}_{1111} = \bar{C}_{01111}^\eta; \quad \hat{C}_{111} = \hat{C}_{0111}^\eta, \quad \hat{C}_{1111} = \hat{C}_{01111}^\eta. \quad (4.24)$$

From (B.5), (B.10), and a similar derivation applied to fourth-order elastic constants, higher-order longitudinal constants are related by

$$\hat{\Gamma}_{11} = \bar{\Gamma}_{11} + 4\Gamma_1, \quad \hat{C}_{111} = \bar{C}_{111} + 12C_{11}, \quad \hat{C}_{1111} = \bar{C}_{1111} - 18\bar{C}_{111} - 318\bar{C}_{11}. \quad (4.25)$$

Longitudinal stress and temperature in the shocked state are, for Lagrangian theory,

$$\bar{S} = \partial \bar{U} / \partial E = C_{11}E + \frac{1}{2} \bar{C}_{111}E^2 + \frac{1}{6} \bar{C}_{1111}E^3 - \theta_0\eta(\Gamma_1 + \bar{\Gamma}_{11}E + \frac{1}{2}\Gamma'_1\eta), \quad (4.26)$$

$$\theta = \partial \bar{U} / \partial \eta = \theta_0(1 + \eta/c_0 - \Gamma_1E - \Gamma'_1\eta - \frac{1}{2}\bar{\Gamma}_{11}E^2); \quad (4.27)$$

and for Eulerian theory

$$\hat{S} = \partial \hat{U} / \partial D = C_{11}D + \frac{1}{2} \hat{C}_{111}D^2 + \frac{1}{6} \hat{C}_{1111}D^3 - \theta_0\eta(\Gamma_1 + \hat{\Gamma}_{11}D + \frac{1}{2}\Gamma'_1\eta), \quad (4.28)$$

$$\theta = \partial \hat{U} / \partial \eta = \theta_0(1 + \eta/c_0 - \Gamma_1D - \Gamma'_1\eta - \frac{1}{2}\hat{\Gamma}_{11}D^2). \quad (4.29)$$

Consider Lagrangian theory. Substitution of (4.26) into (4.19), with $U = \bar{U}$, gives

$$\begin{aligned} \bar{U} = & -\frac{1}{2} \{ \theta_0\eta(\Gamma_1 + \frac{1}{2}\Gamma'_1\eta) \} E + \frac{1}{2} \{ C_{11} - \theta_0\eta[\frac{1}{2}(\Gamma_1 + \frac{1}{2}\Gamma'_1\eta) + \bar{\Gamma}_{11}] \} E^2 + \frac{1}{4} \{ C_{11} + \bar{C}_{111} + \theta_0\eta[(\Gamma_1 + \frac{1}{2}\Gamma'_1\eta) - \bar{\Gamma}_{11}] \} E^3 \\ & + \frac{1}{24} \{ -6C_{11} + 3\bar{C}_{111} + 2\bar{C}_{1111} - \theta_0\eta[\frac{15}{2}(\Gamma_1 + \frac{1}{2}\Gamma'_1\eta) - 6\bar{\Gamma}_{11}] \} E^4 \\ & + \frac{1}{48} \{ 15C_{11} - 6\bar{C}_{111} + 2\bar{C}_{1111} + \theta_0\eta[21(\Gamma_1 + \frac{1}{2}\Gamma'_1\eta) - 15\bar{\Gamma}_{11}] \} E^5 + \dots \end{aligned} \quad (4.30)$$

Eqs. (4.21) and (4.30) can be treated as two equations in two unknowns U and η , and can, in principle, yield a solution for entropy jump $[\eta] = \eta^- = \eta$ in terms of strain, i.e., $\eta = \eta(E)$. For the strain energy function $\bar{U}$ in (4.21) that is quadratic in entropy, such a solution for η can most readily be obtained using numerical methods when $\xi = (V - V_0)/V_0$ is prescribed. With η so obtained, longitudinal stresses $\bar{S}$ and P can then be acquired immediately using (4.26) and (4.12), noting that $F = 1 + \xi = (1 + 2E)^{1/2}$.

When $\bar{U}$ is a linear function of entropy, then a solution for $\eta(E)$ can be obtained analytically in closed form (Thurston, 1974). In this simplified case, most valid for $(c_0^{-1} - \Gamma'_1E)\eta \ll 2$, (4.21) and (4.30) reduce to

$$\bar{U} = \frac{1}{2} C_{11}E^2 + \frac{1}{6} \bar{C}_{111}E^3 + \frac{1}{24} \bar{C}_{1111}E^4 - \theta_0(\Gamma_1E + \frac{1}{2}\bar{\Gamma}_{11}E^2)\eta + \theta_0\eta \quad (4.31)$$

and

$$\begin{aligned} \bar{U} = & -\frac{1}{2} \{ \theta_0\Gamma_1\eta \} E + \frac{1}{2} \{ C_{11} - \theta_0\eta[\frac{1}{2}(\Gamma_1 + \bar{\Gamma}_{11})] \} E^2 + \frac{1}{4} \{ C_{11} + \bar{C}_{111} + \theta_0\eta[\Gamma_1 - \bar{\Gamma}_{11}] \} E^3 \\ & + \frac{1}{24} \{ -6C_{11} + 3\bar{C}_{111} + 2\bar{C}_{1111} - \theta_0\eta[\frac{15}{2}\Gamma_1 - 6\bar{\Gamma}_{11}] \} E^4 + \frac{1}{48} \{ 15C_{11} - 6\bar{C}_{111} + 2\bar{C}_{1111} + \theta_0\eta[21\Gamma_1 - 15\bar{\Gamma}_{11}] \} E^5 + \dots \end{aligned} \quad (4.32)$$

Writing $\eta(E)$ as a polynomial with constant coefficients $a_0, a_1, a_2, \dots$,

$$\eta = a_0 + a_1E + a_2E^2 + a_3E^3 + a_4E^4 + a_5E^5 + \dots \quad (4.33)$$

Substituting (4.33) into (4.31) and (4.32), equating coefficients of like powers of E up to order 5, and noting that $\eta_0 = \eta(0) = 0$ from convention (4.10),

$$a_0 = a_1 = a_2 = 0, \quad a_3 = \frac{1}{12}\theta_0^{-1}(3C_{11} + \bar{C}_{111}), \quad (4.34)$$

$$a_4 = \frac{1}{24}\theta_0^{-1}[-6C_{11} + 3\bar{C}_{111} + \bar{C}_{1111} + \Gamma_1(3C_{11} + \bar{C}_{111})], \quad (4.35)$$

$$a_5 = \frac{1}{48}\theta_0^{-1}[15C_{11} - 6\bar{C}_{111} + 2\bar{C}_{1111} + \Gamma_1(-9C_{11} + 2\bar{C}_{111} + \bar{C}_{1111}) + \Gamma_1^2(3C_{11} + \bar{C}_{111})]. \quad (4.36)$$

Substitution of entropy jump $\eta(E) = [\eta]$, now known to fifth order in strain, into (4.26), (4.27), (4.12), and Hugoniot equations (4.6)–(4.8) then gives the longitudinal stresses, internal energy jump, particle velocity, shock velocity, and temperature completely in terms of E :

$$\bar{S} = C_{11}E + \frac{1}{2} \bar{C}_{111}E^2 + (\frac{1}{6}\bar{C}_{1111} - \theta_0\Gamma_1a_3)E^3 - \theta_0(\Gamma_1a_4 + \bar{\Gamma}_{11}a_3)E^4 - \theta_0(\Gamma_1a_5 + \bar{\Gamma}_{11}a_4)E^5, \quad (4.37)$$

$$P = -(1 + 2E)^{1/2}\bar{S}, \quad [U] = \frac{1}{2}\bar{S}[(1 + 2E) - (1 + 2E)^{1/2}], \quad (4.38)$$

$$v = \{(\bar{S}/\rho_0)[(1 + 2E) - (1 + 2E)^{1/2}]\}^{1/2}, \quad (4.39)$$

$$\mathfrak{D} = \{(\bar{S}/\rho_0)[(1+2E)-(1+2E)^{1/2}]\}^{1/2}[1-(1+2E)^{1/2}]^{-1}, \quad (4.40)$$

$$\theta = \theta_0(1 - \Gamma_1 E - \frac{1}{2}\bar{\Gamma}_{11} E^2). \quad (4.41)$$

Now consider Eulerian theory. Substitution of (4.28) into (4.20), with $U = \hat{U}$, gives

$$\begin{aligned} \hat{U} = & -\frac{1}{2}\{\theta_0\eta(\Gamma_1 + \frac{1}{2}\Gamma'_1\eta)\}D + \frac{1}{2}\{C_{11} + \theta_0\eta[\frac{3}{2}(\Gamma_1 + \frac{1}{2}\Gamma'_1\eta) - \hat{\Gamma}_{11}]\}D^2 + \frac{1}{4}\{-3C_{11} + \hat{C}_{111} + \theta_0\eta[\Gamma_1 + \frac{1}{2}\Gamma'_1\eta + 3\hat{\Gamma}_{11}]\}D^3 \\ & + \frac{1}{24}\{-6C_{11} - 9\hat{C}_{111} + 2\hat{C}_{1111} + \theta_0\eta[\frac{9}{2}(\Gamma_1 + \frac{1}{2}\Gamma'_1\eta) + 6\hat{\Gamma}_{11}]\}D^4 + \frac{1}{48}\{-9C_{11} - 6\hat{C}_{111} - 6\hat{C}_{1111} + \theta_0\eta[9(\Gamma_1 + \frac{1}{2}\Gamma'_1\eta) + 9\hat{\Gamma}_{11}]\}D^5 + \dots \end{aligned} \quad (4.42)$$

Eqs. (4.22) and (4.42) are two equations in two unknowns U and η , and can yield a solution for entropy jump $\eta = \eta(D)$. For $\hat{U}$ in (4.22) that is quadratic in entropy, such a solution can most readily be obtained using numerical methods when ξ is prescribed. Longitudinal stresses $\hat{S}$ and P can then be acquired immediately using (4.22) and (4.42), noting that $F = 1 + \xi = (1 - 2D)^{-1/2}$.

When $\hat{U}$ is a linear function of entropy, then a solution for $\eta(D)$ can be obtained analytically in closed form. In this simplified case, most valid for $(c_0^{-1} - \Gamma'_1 D)\eta \ll 2$, (4.22) and (4.42) reduce to

$$\hat{U} = \frac{1}{2}C_{11}D^2 + \frac{1}{6}\hat{C}_{111}D^3 + \frac{1}{24}\hat{C}_{1111}D^4 - \theta_0(\Gamma_1 D + \frac{1}{2}\hat{\Gamma}_{11}D^2)\eta + \theta_0\eta \quad (4.43)$$

and

$$\begin{aligned} \hat{U} = & -\frac{1}{2}\{\theta_0\eta\Gamma_1\}D + \frac{1}{2}\{C_{11} + \theta_0\eta[\frac{3}{2}\Gamma_1 - \hat{\Gamma}_{11}]\}D^2 + \frac{1}{4}\{-3C_{11} + \hat{C}_{111} + \theta_0\eta[\Gamma_1 + 3\hat{\Gamma}_{11}]\}D^3 \\ & + \frac{1}{24}\{-6C_{11} - 9\hat{C}_{111} + 2\hat{C}_{1111} + \theta_0\eta[\frac{9}{2}\Gamma_1 + 6\hat{\Gamma}_{11}]\}D^4 + \frac{1}{48}\{-9C_{11} - 6\hat{C}_{111} - 6\hat{C}_{1111} + \theta_0\eta[9\Gamma_1 + 9\hat{\Gamma}_{11}]\}D^5 + \dots \end{aligned} \quad (4.44)$$

Writing $\eta(D)$ as a polynomial with constant coefficients $b_0, b_1, b_2, \dots$,

$$\eta = b_0 + b_1D + b_2D^2 + b_3D^3 + b_4D^4 + b_5D^5 + \dots \quad (4.45)$$

Substituting (4.45) into (4.43) and (4.44), equating coefficients of like powers of D up to order 5, and noting that $\eta_0 = \eta(0) = 0$ from convention (4.10),

$$b_0 = b_1 = b_2 = 0, \quad b_3 = \frac{1}{12}\theta_0^{-1}(-9C_{11} + \hat{C}_{111}), \quad (4.46)$$

$$b_4 = \frac{1}{24}\theta_0^{-1}[-6C_{11} - 9\hat{C}_{111} + \hat{C}_{1111} + \Gamma_1(-9C_{11} + \hat{C}_{111})], \quad (4.47)$$

$$b_5 = \frac{1}{48}\theta_0^{-1}[-9C_{11} - 6\hat{C}_{111} - 6\hat{C}_{1111} + \Gamma_1(-33C_{11} - 6\hat{C}_{111} + \hat{C}_{1111}) + \Gamma_1^2(-9C_{11} + \hat{C}_{111})]. \quad (4.48)$$

Notice that $a_3 = b_3$. Substitution of entropy jump $\eta(D) = [\eta]$, now known to fifth order in strain, into (4.28), (4.29), (4.13), and Hugoniot equations (4.6)–(4.8) then gives the longitudinal stresses, internal energy jump, particle velocity, shock velocity, and temperature completely in terms of D :

$$\hat{S} = C_{11}D + \frac{1}{2}\hat{C}_{111}D^2 + (\frac{1}{6}\hat{C}_{1111} - \theta_0\Gamma_1b_3)D^3 - \theta_0(\Gamma_1b_4 + \hat{\Gamma}_{11}b_3)D^4 - \theta_0(\Gamma_1b_5 + \hat{\Gamma}_{11}b_4)D^5, \quad (4.49)$$

$$P = -(1 - 2D)^{3/2}\hat{S}, \quad [U] = \frac{1}{2}\hat{S}[(1 - 2D) - (1 - 2D)^{3/2}], \quad (4.50)$$

$$v = \{(\hat{S}/\rho_0)[(1 - 2D) - (1 - 2D)^{3/2}]\}^{1/2}, \quad (4.51)$$

$$\mathfrak{D} = \{(\hat{S}/\rho_0)[(1 - 2D) - (1 - 2D)^{3/2}]\}^{1/2}[1 - (1 - 2D)^{-1/2}]^{-1}, \quad (4.52)$$

$$\theta = \theta_0(1 - \Gamma_1 D - \frac{1}{2}\hat{\Gamma}_{11}D^2). \quad (4.53)$$

From (4.37) and (4.49), contributions to stresses $\bar{S}$ and $\hat{S}$ from entropy production are $O(E^3)$ and $O(D^3)$, respectively. The foregoing analytical solution for the elastic shock response in Lagrangian theory was derived by Thurston (1974); the analogous full and detailed derivation for Eulerian theory has not appeared elsewhere, to the author's knowledge.

In order to apply the above solutions to particular materials, the following six independent constants are needed at the unstressed ambient state at temperature θ_0 : isentropic elastic constants $C_{11}, \bar{C}_{111}, \bar{C}_{1111}$; Grüneisen parameters $\Gamma_1, \bar{\Gamma}_{11}$; and mass density ρ_0 . Higher-order constants in the Eulerian theory ($\hat{C}_{111}, \hat{C}_{1111}, \hat{\Gamma}_{11}$) can be obtained from those of Lagrangian theory via (4.25), or vice versa, or each set can be fit independently to material data.

In the application that follows in Section 4.2 in which Lagrangian and Eulerian elasticity theories are compared, greatest emphasis is placed on evaluation of the mechanical, rather than thermal, response, consistent with internal energy functions (4.31) and (4.43) quartic in strain but linear in entropy. Note from (2.37) that thermal expansion coefficients in the reference state are equivalent in Lagrangian and Eulerian theories:

$$\hat{\alpha}_{0j} = \bar{\alpha}_{0j} = \alpha_j \leftrightarrow \hat{\alpha}_{0\alpha} = \bar{\alpha}_{0\alpha} = \alpha_\alpha. \quad (4.54)$$

Perhaps most often measured is specific heat at constant stress/pressure $c_0^S = c^S(\mathbf{0}, \theta_0)$, which can be used in (2.43) to obtain $c_0 = c(\mathbf{0}, \theta_0)$:

$$c_0 = c_0^S - \theta_0 \alpha_\alpha \alpha_\beta C_{0\alpha\beta}^\theta, \quad C_{0\alpha\beta}^\theta = C_{\alpha\beta} - (\theta_0/c_0) \beta_{0\alpha} \beta_{0\beta}, \quad (4.55)$$

where second-order isothermal elastic constants are obtained from isentropic constants $C_{\alpha\beta}$ via (2.46). Grüneisen parameters can be calculated from second-order elastic constants, specific heat, and thermal expansion coefficients (Thurston, 1974; Clayton, 2011a):

$$\Gamma_\alpha = \beta_{0\alpha}/c_0 = C_{0\alpha\beta}^\theta \alpha_\beta / c_0 = C_{\alpha\beta} \alpha_\beta / c_0^S. \quad (4.56)$$

Experimental measurements of higher-order Grüneisen parameters are scarce. A typical assumption (Wallace, 1980) for weak shocks in crystals is $\rho \bar{T}_{ij} \approx \rho_0 \Gamma_{0ij}$, which yields

$$\begin{aligned} J^{-1} \bar{T}_{ij} = \text{constant} &\Rightarrow \partial \bar{T}_{ij} / \partial E_{KL} = -J \bar{T}_{ij} (\partial J^{-1} / \partial E_{KL}) = F_{iK}^{-1} F_{jL}^{-1} \bar{T}_{ij} \\ &\Rightarrow \bar{T}_{ijkl} = \frac{1}{2} (\partial \bar{T}_{ij} / \partial E_{KL} + \partial \bar{T}_{KL} / \partial E_{ij})|_0 \approx \frac{1}{2} (\Gamma_{0ij} \delta_{KL} + \Gamma_{0KL} \delta_{ij}). \end{aligned} \quad (4.57)$$

For constant specific heat, positive $\bar{T}_{\alpha\beta}$ correlates decreasing second-order elastic coefficients with increasing temperature. For a cubic crystal with scalar Grüneisen parameter $\bar{T} = \frac{1}{3} \bar{T}_{KK}$, this assumption corresponds to $(\partial \ln \bar{T} / \partial \ln V)|_0 = 1$. Isentropic third-order constants $\bar{C}_{\alpha\beta\gamma}$ can be computed at the reference state from mixed third-order constants $\bar{C}_{\alpha\beta\gamma}^{\eta, \theta}$ measured in ultrasonic experiments using the relation (Brugger, 1964)

$$\bar{C}_{\alpha\beta\gamma} = \bar{C}_{\alpha\beta\gamma}^{\eta, \theta} + \theta_0 \Gamma_\gamma [\bar{C}_{\alpha\beta\delta}^{\eta, \theta} - (\partial \bar{C}_{\alpha\beta}^\eta / \partial \theta)|_0]. \quad (4.58)$$

The difference between isentropic and mixed coefficients is often smaller than uncertainty in experimental measurements of either. In summary, the five parameters C_{11} , $\bar{C}_{111}$, $\bar{C}_{1111}$, Γ_1 , $\bar{T}_{11}$ can be calculated for a material of arbitrary symmetry using the above relations given $C_{1\beta}$ and α_β (where $\beta = 1, 2, \dots, 6$), c_0^S , $\partial \bar{C}_{11}^\eta / \partial \theta$, $\bar{C}_{111}^{\eta, \theta}$, and $\bar{C}_{1111}$. Experimental values exist for a number of crystals for all parameters except $\bar{C}_{1111}$; reported measurements of the latter are scarce.

4.2. Materials

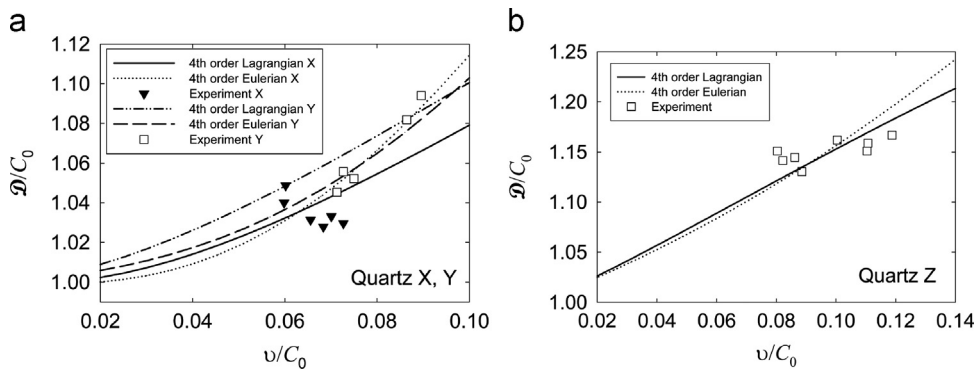
The theory and analytical solutions derived in Section 4.1 are applied to analyze shock compression behavior of single crystals of three hard minerals: quartz (α -SiO₂), sapphire (α -Al₂O₃ or corundum), and diamond (C). These materials are considered because their ratios of Hugoniot Elastic Limit (HEL) to longitudinal elastic moduli are relatively large, meaning that elastic deformations in excess of several percent volumetric compression can be achieved in uniaxial compression prior to activation of any inelastic deformation mechanisms that could render the analysis of Section 4.1 physically unrealistic. In contrast, the nonlinear elastic analysis of Section 4.1 could be applied to more ductile materials with a lower HEL—e.g., metals that undergo plastic slip or deformation twinning—but would be physically realistic only at smaller compressions where effects of higher-order moduli may be less evident. Above the HEL, closed-form analytical solutions for anisotropic solids become intractable because neither elastic nor plastic deformation are one-dimensional, and entropy production from inelasticity can be substantial. Quartz, sapphire, and diamond also belong to the limited set of anisotropic crystals whose third- and fourth-order elastic constants have been reported.

Specifically, analytical solutions are compared for anisotropic nonlinear elastic uniaxial shock compression involving internal energy functions (4.31) and (4.43) (Lagrangian and Eulerian theories, respectively) incorporating elastic constants up to fourth order. Quartz and sapphire have trigonal (i.e., rhombohedral) symmetry. Quartz is analyzed for compression along the a -axis (X-cut, $[\bar{1}2\bar{1}0]$), b -axis (Y-cut, $[\bar{1}010]$) and c -axis (Z-cut, $[0001]$); sapphire is analyzed for compression along the a -axis (X-cut) and c -axis (Z-cut). Diamond is cubic and is analyzed for compression along a cube axis (X-cut, $[100]$). Elastic constants are interchanged as needed for consistency with notation of Section 4.1. For example, for c -axis (i.e., Z-cut) uniaxial shock compression, the analysis of Section 4.1 remains valid with C_{11} replaced by C_{33} , C_{111} by C_{333} , Γ_1 by Γ_3 , etc.

Requisite material properties are listed in Table 4 corresponding to an ambient temperature of 295 K. Isentropic second-order elastic constants for all three materials are obtained from experiment (McSkimin et al., 1965, 1972; Hankey and Schuele, 1970), mixed third-order constants are obtained for quartz and sapphire from experiment (Thurston et al., 1966; Hankey and Schuele, 1970) and then converted to isentropic constants using (4.58). Fourth-order Lagrangian constants shown for quartz and sapphire are reported from fits to shock compression experiments (Fowles, 1967; Graham, 1972a) and are inherently adiabatic. Quartz is piezoelectric; constants listed correspond to open-circuit conditions (i.e., constant electric displacement). For diamond, third- and fourth-order constants are obtained verbatim from quantum mechanical calculations (Nielsen, 1986); no attempt is made to adjust these for finite temperature. Grüneisen parameters are calculated via (4.56) and (4.57) using experimentally determined specific heats at constant pressure (McSkimin et al., 1965; Furukawa et al., 1956; DeSorbo, 1953), linear thermal expansion coefficients (McSkimin et al., 1965; Burghartz and Schulz, 1994; Slack and Bartram, 1975), and isentropic second-order elastic constants. For quartz and sapphire, third-order Eulerian coefficients $\hat{C}_{111}$ are obtained using conversion (4.25). As discussed later in Section 4.3, fourth-order Eulerian constants $\hat{C}_{1111}$ for quartz and sapphire are fit to shock velocity versus particle velocity data (Fowles, 1967; Graham and Brooks, 1971) keeping third-order elastic constants fixed, following the same procedure used for $\bar{C}_{1111}$. Fitting this constant independently rather than using the last of (4.25) provides for the most fair comparison of fourth-order Lagrangian and Eulerian theories. For diamond,

Table 4Physical properties of single crystals ($\theta_0 = 295$ K; ρ_0 in g/cm³; $C_{\alpha\beta\gamma\dots}$ in GPa).

Property	Quartz (X)	Quartz (Y)	Quartz (Z)	Sapphire (X)	Sapphire (Z)	Diamond (X)
C_{11}	87.6	87.6	106	497	498	1079
$\bar{C}_{111}$	−211	−333	−814	−3870	−3340	−6300
$\hat{C}_{111}$	840	718	455	2090	2640	5570
$\bar{C}_{1111}$	15 930	15 930	18 490	50 000	50 000	43 600
$\hat{C}_{1111}$	15 000	10 500	6500	10 000	20 000	16 300
$r_1 = \bar{r}_{11}$	0.74	0.74	0.58	1.29	1.29	0.81
$\hat{r}_{11}$	3.70	3.70	2.90	6.43	6.46	4.04
P_{HEL}/C_{11}	0.10	0.10	0.15	0.05	0.05	0.08
ρ_0	2.65			3.98		3.51
B'_0	6.3			4.2		4.0

**Fig. 8.** Predicted and experimental (Fowles, 1967) shock velocity versus particle velocity for quartz, normalized by linear elastic wave speed C_0 : (a) X- and Y-cut and (b) Z-cut.

Eulerian higher-order constants $\hat{C}_{111}$ and $\hat{C}_{1111}$ are again taken verbatim from Nielsen (1986), where they have been obtained by fitting numerical data directly rather than using (4.25). For each material, pressure derivatives of bulk modulus B'_0 (Thurston et al., 1966; Nielsen, 1986; Clayton, 2009) are also listed. Finally, maximum HEL stresses P_{HEL} from shock experiments (Wackerle, 1962; Fowles, 1967; Graham, 1972b; Lang and Gupta, 2010) are shown for reference, normalized by second-order moduli for shocks in corresponding directions. The domain of validity of elastic analysis can be estimated as $V/V_0 \gtrsim (C_{11} - P_{\text{HEL}})/C_{11}$.

4.3. Results and discussion

Predicted shock velocity $\mathfrak{D}$ versus particle velocity v is compared with experimental shock compression data of Fowles (1967) in Fig. 8 for X-, Y-, and Z-cut quartz specimens. Experimental data are obtained from plane-wave explosive loading tests in which two-wave structures were often recorded (Fowles, 1967). Data considered here correspond only to the first, elastic shock wave in such tests. Velocities are normalized by longitudinal linear elastic wave speed

$$C_0 = (C_{11}/\rho_0)^{1/2}. \quad (4.59)$$

Lagrangian fourth-order constant $\bar{C}_{1111}$ for each orientation (Table 4) was fit to the data in Fowles (1967). Eulerian fourth-order constant $\hat{C}_{1111}$ in Table 4 has been fit to this same data in an analogous fashion here. Both Lagrangian and Eulerian fits are considered adequate for each orientation. The unusual nonlinearity (i.e., curvature) in the $\mathfrak{D}-v$ data was noted in Fowles (1967); Eulerian theory predicts relationships with greater curvature. Hugoniot stress (i.e., P) normalized by C_{11} is shown for each orientation in Fig. 9, along with experimental data (Fowles, 1967). Predictions marked “4th order” are obtained using complete solutions and all material constants. Predictions marked “3rd order” assume $\bar{C}_{1111} = 0$ or $\hat{C}_{1111} = 0$. Predictions marked “2nd order” assume $\bar{C}_{111} = \bar{C}_{1111} = 0$ or $\hat{C}_{111} = \hat{C}_{1111} = 0$. These designations apply for respective Lagrangian or Eulerian solutions. Predictions marked “2nd order mixed” are discussed later in Section 4.4. For each orientation, 4th order theories are required to accurately match the experimental Hugoniot data; 2nd and 3rd order models are insufficient.

Predicted shock velocity $\mathfrak{D}$ versus particle velocity v is compared with experimental shock compression data of Graham and Brooks (1971) in Fig. 10 for X- and Z-cut sapphire. Experimental data are obtained from flyer-plate and plane-wave explosive loading configurations; in the latter, two-wave structures were sometimes generated (Graham and Brooks, 1971). Data considered here correspond only to the elastic shock, with the secondary, slower “plastic” wave in which the HEL was

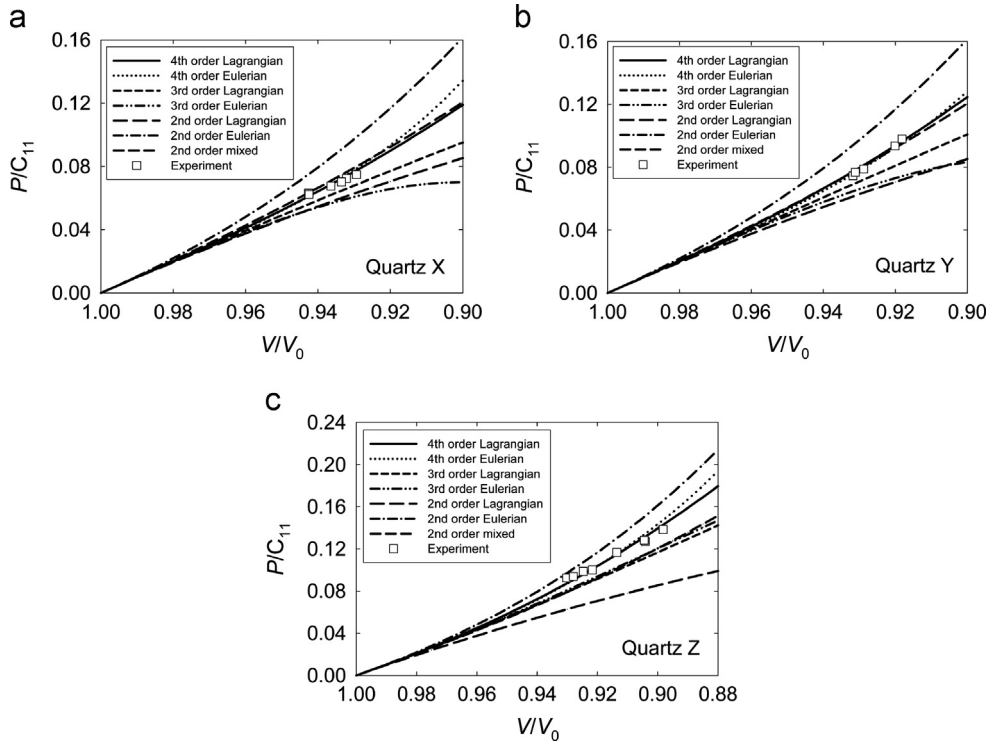


Fig. 9. Predicted and experimental (Fowles, 1967) Hugoniot stress for quartz, normalized by longitudinal second-order elastic constant C_{11} : (a) X-cut, (b) Y-cut and (c) Z-cut.

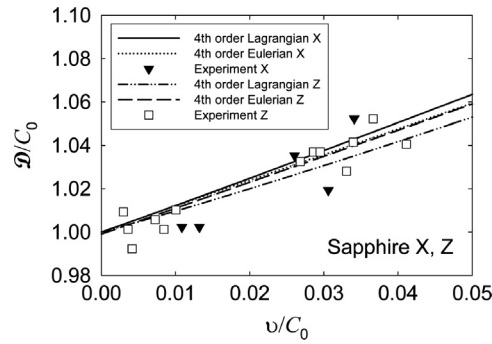


Fig. 10. Predicted and experimental (Graham and Brooks, 1971) shock velocity versus particle velocity for sapphire, normalized by linear elastic wave speed C_0 .

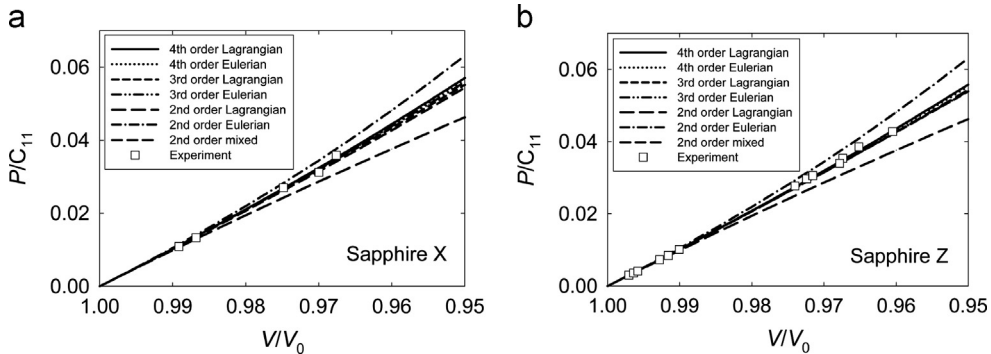


Fig. 11. Predicted and experimental (Graham and Brooks, 1971) Hugoniot stress for sapphire, normalized by longitudinal second-order elastic constant C_{11} : (a) X-cut and (b) Z-cut.

exceeded not addressed. Velocities are normalized by wave speed (4.59). Lagrangian fourth-order constant $\bar{C}_{1111}$ for each orientation (Table 4) was fit to this experimental data in Graham (1972a). Eulerian fourth-order constant $\hat{C}_{1111}$ in Table 4 has been fit to this same data here. Considering scatter in the data, both Lagrangian and Eulerian fits are adequate for each orientation, giving nearly linear $\mathfrak{D}$ - v curves over the relatively small compression range for which sapphire remains elastic ($V/V_0 \geq 0.95$). Hugoniot stress (i.e., P) normalized by C_{11} is shown for each orientation in Fig. 11, along with experimental data (Graham and Brooks, 1971). For each orientation, 3rd and 4th order Lagrangian and Eulerian theories are all capable of accurately matching the experimental stress data. Sufficiency of 3rd order Lagrangian theory was also noted in previous work (Clayton, 2009). Second-order elastic models are inaccurate, with 2nd order Eulerian theory too stiff and 2nd order Lagrangian theory too compliant.

For predictions of the shock response of diamond, all higher-order elastic constants in Table 4 have been taken directly from the quantum mechanical results of Nielsen (1986) since experimental measurements of third-order constants of diamond apparently have not been reported. Predictions of normalized shock velocity and Hugoniot stress are given in Fig. 12(a) and (b), respectively, compared with experimental data of Lang and Gupta (2010). These data, obtained from flyer-plate experiments, consist of five tests for which a high HEL was observed (peak shock pressures of ≈ 90 GPa) and six corresponding to peak shock pressures in excess of ≈ 115 GPa, which demonstrated a marked reduction in HEL strength (Lang and Gupta, 2010). No fitting or adjustment of third- or fourth-order Lagrangian or Eulerian constants has been undertaken, so the comparison of results can be deemed as much a confirmation of accuracy of atomic calculations as a test of relative merits of Lagrangian and Eulerian theories of various orders. From Fig. 12(a), 4th order Lagrangian theory provides a better fit to shock velocity than 4th order Eulerian theory at larger particle velocities corresponding to the higher HEL, with 4th order Eulerian theory tending to overestimate $\mathfrak{D}$. Conversely, at smaller particle velocities corresponding to the lower HEL, 4th order Eulerian

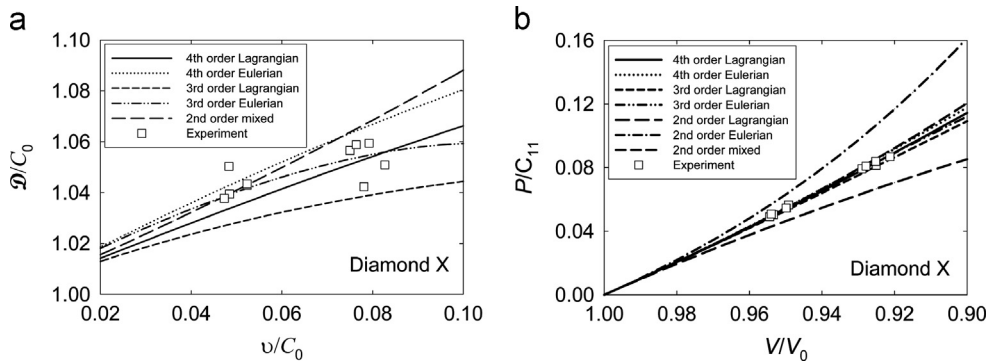


Fig. 12. Predicted and experimental (Lang and Gupta, 2010): (a) shock velocity versus particle velocity, normalized by linear elastic wave speed C_0 and (b) Hugoniot stress, normalized by longitudinal second-order elastic constant C_{11} .

Table 5
Thermodynamic predictions.

Material	Shock direction	V/V_0	θ/θ_0 Lagrangian	θ/θ_0 Eulerian	η/c_0^S Lagrangian	η/c_0^S Eulerian	P/P^i Lagrangian	P/P^i Eulerian
Quartz	X	0.96	1.028	1.028	0.002	0.002	1.0002	1.0002
		0.92	1.055	1.052	0.030	0.050	1.0013	1.0024
		0.88	1.079	1.069	0.133	0.418	1.0032	1.0039
	Y	0.96	1.028	1.028	0.003	0.002	1.0002	1.0002
		0.92	1.055	1.052	0.036	0.039	1.0016	1.0019
		0.88	1.079	1.069	0.153	0.300	1.0036	1.0079
	Z	0.96	1.022	1.022	0.007	0.006	1.0004	1.0004
		0.92	1.043	1.041	0.066	0.071	1.0017	1.0017
		0.88	1.062	1.054	0.246	0.373	1.0033	1.0042
Sapphire	X	0.96	1.049	1.049	0.016	0.015	1.0008	1.0007
		0.92	1.095	1.091	0.141	0.135	1.0028	1.0024
		0.88	1.137	1.119	0.483	0.531	1.0053	1.0055
	Z	0.96	1.050	1.049	0.014	0.012	1.0007	1.0006
		0.92	1.095	1.091	0.122	0.121	1.0025	1.0024
		0.88	1.137	1.120	0.430	0.578	1.0049	1.0071
Diamond	X	0.96	1.031	1.031	0.033	0.042	1.0003	1.0003
		0.92	1.060	1.057	0.255	0.311	1.0009	1.0010
		0.88	1.086	1.075	0.811	0.987	1.0017	1.0024

theory better represents experimental shock velocities, with Lagrangian theory yielding too-low values of $\mathfrak{D}$. For both clusters of experimental shock velocity data, 3rd order Eulerian theory provides a better fit than 3rd order Lagrangian theory. As shown in Fig. 12(b), all 4th order and all 3rd order models provide a reasonable prediction of longitudinal shock stress, though 3rd order Lagrangian theory might be considered overly compliant for $V/V_0 < 0.95$. Second-order elastic models do not accurately predict Hugoniot stress, with 2nd order Eulerian theory too stiff and 2nd order Lagrangian theory too compliant.

Considering key findings reported in Section 3.5 and that quartz, sapphire, and diamond all have $B'_0 \geq 4$, the lack of definitively greater accuracy of Eulerian theory relative to Lagrangian theory is somewhat unexpected. However, quartz and sapphire are not cubic and have directionally dependent covalent and ionic bonding, so trends from the ideal model of Section 3 that enforces Cauchy relations and isotropic symmetry for third-order constants may not apply. Diamond has strong covalent bonding (unlike the noble metals for which anharmonic properties are more symmetric, Hiki and Granato, 1966), and examination of all third-order constants in Nielsen (1986) shows that (3.13) and (3.16) are not well respected. Nielsen (1986) reported that 4th order Eulerian theory was better able than Lagrangian theory to collectively fit atomic simulation results for spherical deformation and straining along [100], [110], and [111] in diamond.

Predictions of fourth-order Lagrangian and Eulerian theories for temperature rise θ (normalized by reference temperature θ_0), entropy jump across the shock η (normalized by specific heat at constant pressure c_S^0), and Hugoniot stress P (normalized by uniaxial isentropic stress P^η) are listed in Table 5. Isentropes are computed as

$$P^\eta = -J(C_{11}E + \frac{1}{2}\bar{C}_{111}E^2 + \frac{1}{6}\bar{C}_{1111}E^3), \quad (\text{Lagrangian}) \quad (4.60)$$

$$P^\eta = -J^{-3}(C_{11}D + \frac{1}{2}\hat{C}_{111}D^2 + \frac{1}{6}\hat{C}_{1111}D^3). \quad (\text{Eulerian}) \quad (4.61)$$

Predicted temperatures are similar for Lagrangian and Eulerian theories, with temperature rise slightly smaller in the latter at large compression. Predicted entropy production is positive in agreement with (4.9) and is of the same order of magnitude among theories, with larger η predicted by Eulerian theory at large compression. Recall from Section 4.1 that the present analytical solutions have assumed a simple form of specific heat wherein the contribution to internal energy from entropy is linear, i.e., (4.31) and (4.43). When higher-order Grüneisen parameter $\Gamma'_1 = 0$ and $c_0 \approx c_0^S$, these approximations are most accurate for $\eta \ll 2c_0^S$. From Table 5, such conditions hold for $V/V_0 \geq 0.92$. But for very large compression (i.e., $V/V_0 = 0.88$), entropy production (especially in diamond) is large enough that a higher-order representation of entropy, e.g., (4.21) or (4.22), may be prudent. Examination of stresses in Table 5 shows that $P/P^\eta < 1.01$ in all cases, justifying isentropic assumptions used in previous stress analyses (Fowles, 1967; Clayton, 2009).

Upon examination of HEL stresses in Table 4, results in Table 5 are deemed valid for Z-cut quartz to $V/V_0 = 0.88$. However, for X- and Y-cut quartz and for diamond, the HEL is exceeded at $V/V_0 = 0.88$, and results are most valid only for $V/V_0 \geq 0.92$. For sapphire, the elastic range is even smaller and compression, in experiments, is elastic only for $V/V_0 = 0.96$. Values listed in Table 5 can be considered extrapolations when compression exceeds the HEL. Above the HEL, a nonlinear theory incorporating dislocation slip/twinning (Clayton, 2009, 2010b; Clayton and Knap, 2011a, 2011b) and cleavage fracture (Clayton, 2006, 2010a, 2011b) may be needed, accounting for anisotropic inelastic deformation mechanisms and their contributions to entropy production and temperature. If large densities of lattice defects are generated at shock pressures at or above the HEL, consideration of their effects on dilatation (Clayton, 2009, 2011a; Clayton and Bammann, 2009) and tangent elastic moduli (Clayton and Chung, 2006) may be worthwhile.

4.4. An alternative lower-order theory

Purely Lagrangian and Eulerian theories have been formulated using respective strain measures $\mathbf{E}$ and $\mathbf{D}$. These tensors are not the only possibilities for use in thermoelastic potentials. For example, a generic symmetric strain, in material coordinates, that vanishes when $\mathbf{F} = \mathbf{1}$, can be defined as a linear combination of $\mathbf{E}$ and $\mathbf{D}$:

$$\mathbf{G} = (1-\chi)\mathbf{E} + \chi\mathbf{D}, \quad 0 \leq \chi \leq 1. \quad (4.62)$$

Lagrangian (Eulerian) theory is recovered when $\chi = 0$ ($\chi = 1$). In what follows, take $\chi = \frac{1}{2}$, giving⁵

$$\mathbf{G} = \frac{1}{2}(\mathbf{E} + \mathbf{D}) = \frac{1}{4}(\mathbf{F}^T \mathbf{F} - \mathbf{F}^{-1} \mathbf{F}^{-T}) = \frac{1}{4}(\mathbf{U}^2 - \mathbf{U}^{-2}), \quad (4.63)$$

where $\mathbf{U} = \mathbf{R}^T \mathbf{F}$ is the right stretch tensor. Free and internal energy densities per unit reference volume are

$$\psi = \tilde{\psi}(\mathbf{G}, \theta), \quad U = \tilde{U}(\mathbf{G}, \eta). \quad (4.64)$$

Thermodynamic stress, entropy, and temperature obey

$$\tilde{\mathbf{S}} = \partial \tilde{\psi} / \partial \mathbf{G} = \partial \tilde{U} / \partial \mathbf{G} = \tilde{\mathbf{S}}^T, \quad \eta = -\partial \tilde{\psi} / \partial \theta, \quad \theta = \partial \tilde{U} / \partial \eta. \quad (4.65)$$

⁵ The author is grateful to M. Ortiz for suggesting, before calculations in the present work were undertaken, the possible utility of a strain such as (4.63).

Components of first Piola–Kirchhoff stress are obtained from chain rule differentiation:

$$P_{kl} = \frac{\partial \tilde{U}}{\partial F_{kl}} = \frac{\partial \tilde{U}}{\partial G_{ij}} \frac{\partial G_{ij}}{\partial F_{kl}} = \frac{1}{2} \tilde{S}_{ij} (\delta_{il} F_{kj} + F_{lk}^{-1} F_{jm}^{-1} F_{lm}^{-1}), \quad (4.66)$$

where $\tilde{U}$ can also be replaced with $\tilde{\Psi}$. Isentropic second-order elastic moduli are defined, in Voigt notation, as

$$\tilde{C}_{\alpha\beta}^{\eta} = \partial^2 \tilde{U} / \partial G_{\alpha} \partial G_{\beta}. \quad (4.67)$$

A complete three-dimensional thermomechanical theory of nonlinear elasticity can be formulated in terms of $\mathbf{G}$ paralleling steps taken in Section 2. For modeling 1-D shock compression, a scalar theory along the lines of those in terms of E and D in Section 4.1 is sufficient. For compression parallel to the $X = X_1$ direction, scalar uniaxial strain is

$$G = G_{11} = \frac{1}{2} (E_{11} + D_{11}) = \frac{1}{4} (F^2 - F^{-2}) = \frac{1}{4} J^{-2} (J^4 - 1). \quad (4.68)$$

For the present purpose, the following lower-order thermodynamic potentials suffice:

$$\tilde{U} = \frac{1}{2} C_{11} G^2 + \theta_0 \eta, \quad \tilde{\Psi} = \frac{1}{2} C_{11} G^2. \quad (4.69)$$

In this representation, temperature is constant, thermoelastic coupling is omitted, and isothermal and isentropic second-order elastic constants are indistinguishable and are both represented by C_{11} . Following the same arguments used to arrive at (B.3), this second-order elastic constant can be considered equivalent to second-order constants of Lagrangian and Eulerian theories of Section 4.1. Hugoniot stress P is equivalent to the second-order elastic isentrope, and is calculated using (4.66) and (4.68) as

$$P = -P_{11} = -\frac{1}{2} (F + F^{-3}) \tilde{S} = -\frac{1}{2} J^{-3} (1 + J^4) \partial \tilde{U} / \partial G = -\frac{1}{2} J^{-3} (1 + J^4) G C_{11} = \frac{1}{8} J^{-5} (1 + J^4) (1 - J^4) C_{11}. \quad (4.70)$$

This relation has the physically appealing feature that $|P| \rightarrow \infty$ as $J \rightarrow 0, \infty$.

Predictions of (4.70) are labeled “2nd order mixed” in Figs. 9, 11, and 12. Hugoniot stresses predicted using this mixed Eulerian–Lagrangian theory are more accurate than those predicted using purely Eulerian or Lagrangian 3rd order models for X- and Y-cut quartz [Fig. 9(a) and (b)] and X- and Z-cut sapphire [Fig. 11(a) and (b)], and for these crystals and orientations are of comparable accuracy as 4th order theory. Predictions from (4.70) are of comparable accuracy as those of 3rd order Eulerian or Lagrangian approaches for Z-cut quartz and diamond [Figs. 9(c) and 12], but in these two cases are less accurate than 4th order theory. The apparent success of (4.70) is not surprising considering that 2nd order Eulerian and Lagrangian models tend to respectively over- and under-predict experimental Hugoniot stress data. As noted previously, for many, if not most, kinds of single crystals only second-order elastic constants have been measured, with third- and higher-order constants unknown. These findings suggest that, for a single crystal ceramic or mineral undergoing finite elastic compression, a best estimate of Hugoniot stress might be obtained using one-parameter equation (4.70) if only second-order constant C_{11} is available.

5. Conclusions

A comprehensive theory of Eulerian thermoelasticity has been formulated and compared with traditional Lagrangian theory. Analytical solutions have been compared for homogeneous spherical deformation, uniaxial strain, and simple shear, for cubic crystals with fully anisotropic linear properties (three independent second-order elastic constants) but directionally independent anharmonicity (one independent third-order constant). For a typical value of pressure derivative of the bulk modulus of four, Eulerian solutions tend to demonstrate more physically realistic behavior (i.e., rapidly increasing stress and energy at very large deformation) and greater stability (e.g., positive strain energy to very large deformation).

An analytical solution, accurate to fifth order in strain, has been derived for the uniaxial shock response in Eulerian thermoelasticity, paralleling a derivation for Lagrangian theory. Entropy production across the shock is minimally third order in strain for either theory. Both Eulerian and Lagrangian treatments provide sufficient accuracy when fourth-order elastic constants are incorporated, with neither theory demonstrating consistent or definitive advantages over the other in describing Hugoniot data for quartz, sapphire, or diamond. A second-order model incorporating a mixed strain tensor that is an average of Lagrangian and Eulerian strains has been shown to provide a reasonable approximation of the Hugoniot stress for each of these materials. This strain measure is recommended for predicting the uniaxial shock response of other hard anisotropic crystalline materials if higher-order elastic constants are unknown.

Appendix A. Kinematics

Let $\mathbf{x}$ and $\mathbf{X}$ denote spatial and initial material coordinates of an element of a solid body, related by sufficiently smooth, and one-to-one at any time $t \geq 0$, functions

$$\mathbf{x} = \mathbf{x}(\mathbf{X}, t), \quad \mathbf{X} = \mathbf{X}(\mathbf{x}, t). \quad (A.1)$$

The deformation gradient $\mathbf{F}(\mathbf{X}, t)$ is

$$\mathbf{F} = \nabla_0 \mathbf{x}; \quad F_{ij} = \partial x_i / \partial X_j = \partial_j x_i. \quad (\text{A.2})$$

The inverse deformation gradient $\mathbf{F}^{-1}(\mathbf{x}, t)$ is

$$\mathbf{F}^{-1} = \nabla \mathbf{X}; \quad F_{ij}^{-1} = \partial X_i / \partial x_j = \partial_j X_i. \quad (\text{A.3})$$

Partial coordinate differentiation at fixed t obeys $\partial_j(\cdot) = F_{ij} \partial_i(\cdot)$. The following identities (Clayton, 2011a) that follow from $\mathbf{F}\mathbf{F}^{-1} = \mathbf{1}$ and $\nabla_0 \mathbf{F} = \nabla_0 \nabla_0 \mathbf{x}$ are used later:

$$\partial F_{ij}^{-1} / \partial F_{kl} = -F_{ik}^{-1} F_{lj}^{-1}, \quad \partial_k F_{ij} = \partial_j F_{ik}. \quad (\text{A.4})$$

Current volume V and mass density ρ are related to initial volume V_0 and initial density ρ_0 of a material element by Jacobian determinant $J(\mathbf{X}, t)$:

$$\frac{V}{V_0} = \frac{\rho_0}{\rho} = J = \det \mathbf{F}. \quad (\text{A.5})$$

Lagrangian Green strain $\mathbf{E}(\mathbf{X}, t)$ is defined as

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^T \mathbf{F} - \mathbf{1}); \quad E_{ij} = \frac{1}{2}(\partial_i x_k \partial_j x_k - \delta_{ij}). \quad (\text{A.6})$$

Letting $\mathbf{u}(\mathbf{X}, t)$ denote displacement and $u_j = u_i \delta_{ij}$,

$$\nabla_0 \mathbf{u} = \mathbf{F} - \mathbf{1}; \quad \partial_j u_k = F_{kj} - \delta_{kj}; \quad E_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i + \partial_i u_k \partial_j u_k). \quad (\text{A.7})$$

The following identities apply (Clayton, 2011a):

$$\frac{\partial E_{ij}}{\partial F_{kl}} = \frac{1}{2}(\delta_{il} F_{kj} + \delta_{jl} F_{ki}), \quad \frac{\partial J}{\partial F_{kl}} = J F_{lk}^{-1}, \quad \frac{\partial J}{\partial E_{ij}} = J F_{ik}^{-1} F_{jk}^{-1}. \quad (\text{A.8})$$

Eulerian strain $\mathbf{D}(\mathbf{x}, t)$ is defined as

$$\mathbf{D} = \frac{1}{2}(\mathbf{1} - \mathbf{F}^{-1} \mathbf{F}^{-T}); \quad D_{ij} = \frac{1}{2}(\delta_{ij} - \partial_k X_i \partial_k X_j). \quad (\text{A.9})$$

Letting $\mathbf{u}(\mathbf{x}, t)$ denote displacement,

$$\nabla \mathbf{u} = \mathbf{1} - \mathbf{F}^{-1}; \quad \partial_j u_k = \delta_{jk} - \partial_j X_k; \quad D_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i - \partial_k u_i \partial_k u_j) \delta_{ij}. \quad (\text{A.10})$$

Comparing (A.7) and (A.10), and noting that

$$\partial_j u_k = \partial_i u_k (\delta_{ij} + \partial_j u_i) = \partial_i u_k \delta_{ij} + O(\|\nabla \mathbf{u}\|^2), \quad (\text{A.11})$$

it follows that $\mathbf{E}$ and $\mathbf{D}$ agree to first order in displacement gradients:

$$\mathbf{D} = \mathbf{E} + o(\|\nabla \mathbf{u}\|). \quad (\text{A.12})$$

From (A.4) and identity $\partial \det \mathbf{A} / \partial A_{ij} = A_{ji}^{-1} \det \mathbf{A}$,

$$\frac{\partial D_{ij}}{\partial F_{kl}} = \frac{1}{2} F_{lm}^{-1} (F_{ik}^{-1} F_{jm}^{-1} + F_{jk}^{-1} F_{lm}^{-1}), \quad \frac{\partial J}{\partial D_{ij}} = J F_{kl} F_{kj}. \quad (\text{A.13})$$

From definitions (A.6) and (A.9), for $\|\mathbf{E}\| < 1$ and $\|\mathbf{D}\| < 1$, the following series apply:

$$\mathbf{D} = \frac{1}{2}[\mathbf{1} - (\mathbf{1} + 2\mathbf{E})^{-1}] = \frac{1}{2}[\mathbf{1} - (\mathbf{1} - 2\mathbf{E} + 4\mathbf{E}^2 - 8\mathbf{E}^3 + \dots)] = \mathbf{E} - 2\mathbf{E}^2 + 4\mathbf{E}^3 - \dots, \quad (\text{A.14})$$

$$\mathbf{E} = \frac{1}{2}[(\mathbf{1} - 2\mathbf{D})^{-1} - \mathbf{1}] = \frac{1}{2}[(\mathbf{1} + 2\mathbf{D} + 4\mathbf{D}^2 + 8\mathbf{D}^3 + \dots) - \mathbf{1}] = \mathbf{D} + 2\mathbf{D}^2 + 4\mathbf{D}^3 + \dots. \quad (\text{A.15})$$

Consider the polar decomposition of $\mathbf{F}$:

$$\mathbf{F} = \mathbf{R}\mathbf{U} = \mathbf{V}\mathbf{R}, \quad \mathbf{R}\mathbf{R}^T = \mathbf{1}, \quad \mathbf{U} = \mathbf{U}^T, \quad \mathbf{V} = \mathbf{V}^T. \quad (\text{A.16})$$

Define the Eulerian Almansi strain $\mathbf{e}(\mathbf{x}, t)$ by

$$\mathbf{e} = \frac{1}{2}(\mathbf{1} - \mathbf{F}^{-T} \mathbf{F}^{-1}); \quad e_{ij} = \frac{1}{2}(\delta_{ij} - \partial_i X_k \partial_j X_k) = \frac{1}{2}(\partial_i u_j + \partial_j u_i - \partial_i u_k \partial_j u_k). \quad (\text{A.17})$$

When there is no rotation, $\mathbf{F} = \mathbf{F}^T$, $\partial_i X_j = \partial_k X_L \delta_{kj} \delta_{iL}$, and $\partial_k u_j = \partial_j u_k$, leading to $\mathbf{e} = \mathbf{D}$ under these conditions. From the polar decomposition (A.16), strain tensors can be expressed in terms of stretches as

$$\mathbf{E} = \frac{1}{2}(\mathbf{U}^2 - \mathbf{1}), \quad \mathbf{D} = \frac{1}{2}(\mathbf{1} - \mathbf{U}^{-2}), \quad \mathbf{e} = \frac{1}{2}(\mathbf{1} - \mathbf{V}^{-2}). \quad (\text{A.18})$$

Spatial velocity gradient $\mathbf{l}(\mathbf{x}, t)$ and its symmetric part $\mathbf{d}(\mathbf{x}, t)$ are

$$\mathbf{l} = \nabla \mathbf{v} = \dot{\mathbf{F}} \mathbf{F}^{-1}, \quad \mathbf{d} = \frac{1}{2}(\mathbf{l} + \mathbf{l}^T); \quad l_{ij} = \partial_j v_i = \partial_j \dot{x}_i, \quad d_{ij} = \frac{1}{2}(\partial_i \dot{x}_j + \partial_j \dot{x}_i). \quad (\text{A.19})$$

It follows that

$$\dot{\mathbf{E}} = \mathbf{F}^T \mathbf{d} \mathbf{F}, \quad \dot{\mathbf{D}} = \mathbf{F}^{-1} \mathbf{d} \mathbf{F}^{-T}. \quad (\text{A.20})$$

Of particular interest are situations in which deformation is spherical (isotropic):

$$\mathbf{F} = J^{1/3} \mathbf{1}, \quad \mathbf{F}^{-1} = J^{-1/3} \mathbf{1}; \quad \mathbf{E} = \frac{1}{2}(J^{2/3} - 1) \mathbf{1}, \quad \mathbf{D} = \frac{1}{2}(1 - J^{-2/3}) \mathbf{1}. \quad (\text{A.21})$$

In this case, the following limits apply as $J = V/V_0 \rightarrow 0$, where $\|\mathbf{A}\| = (\mathbf{A} : \mathbf{A})^{1/2}$:

$$\lim_{J \rightarrow 0} \|\mathbf{E}\| = \sqrt{3}/2; \quad \lim_{J \rightarrow 0} \|\mathbf{D}\| \rightarrow \infty. \quad (\text{A.22})$$

Appendix B. Thermomechanical derivations

Material coefficients defined as derivatives of free or internal energy with respect to $\mathbf{E}$ are related to those with respect to $\mathbf{D}$ as follows. First, consider thermal stress coefficients. Setting $F_{ij} = F_{ji}^{-1} = \delta_{ij}$ in the reference state, (2.27) yields

$$\bar{\beta}_{0\alpha} = \hat{\beta}_{0\alpha}, \quad \bar{\beta}'_{0\alpha} = (\partial \bar{\beta}_{0\alpha} / \partial \theta)|_0 = (\partial \hat{\beta}_{0\alpha} / \partial \theta)|_0 = \hat{\beta}'_{0\alpha}. \quad (\text{B.1})$$

Recalling that $\bar{c} = \hat{c}$, or using (2.36), it follows that Grüneisen parameters

$$\bar{T}_{0\alpha} = \bar{\beta}_{0\alpha} / c_0 = \hat{\beta}_{0\alpha} / c_0 = \hat{T}_{0\alpha}, \quad \bar{T}'_{0\alpha} = (\partial \bar{T}_{0\alpha} / \partial \eta)|_0 = (\partial \hat{T}_{0\alpha} / \partial \eta)|_0 = \hat{T}'_{0\alpha}. \quad (\text{B.2})$$

Now consider second-order elastic stiffness coefficients. From (2.52), noting also that $\mathbf{P} = \mathbf{0}$ in the reference state,

$$\bar{C}_{0\alpha\beta}^\theta = \hat{C}_{0\alpha\beta}^\theta, \quad \bar{C}_{0\alpha\beta}^\eta = \hat{C}_{0\alpha\beta}^\eta. \quad (\text{B.3})$$

It follows that for higher-order thermal stress coefficients $\beta_{0\alpha\beta} \leftrightarrow \beta_{0\beta\alpha}$,

$$\hat{\beta}_{0\beta\alpha} - \bar{\beta}_{0\beta\alpha} = -(\partial \hat{\beta}_{0\alpha} / \partial \theta)|_0 + (\partial \bar{\beta}_{0\alpha} / \partial \theta)|_0 = \bar{\beta}_{0\alpha\beta} \delta_{\beta\alpha} + \bar{\beta}_{0\alpha\beta} \delta_{\beta\alpha} + \bar{\beta}_{0\alpha\beta} \delta_{\beta\alpha} + \bar{\beta}_{0\alpha\beta} \delta_{\beta\alpha}. \quad (\text{B.4})$$

Similarly, for higher-order Grüneisen parameters $\Gamma_{0\alpha\beta} \leftrightarrow \Gamma_{0\beta\alpha}$,

$$\hat{\Gamma}_{0\beta\alpha} - \bar{\Gamma}_{0\beta\alpha} = -\theta_0^{-1} (\partial \hat{\Gamma}_{0\alpha} / \partial \theta)|_0 + \theta_0^{-1} (\partial \bar{\Gamma}_{0\alpha} / \partial \theta)|_0 = \bar{\Gamma}_{0\alpha\beta} \delta_{\beta\alpha} + \bar{\Gamma}_{0\alpha\beta} \delta_{\beta\alpha} + \bar{\Gamma}_{0\alpha\beta} \delta_{\beta\alpha} + \bar{\Gamma}_{0\alpha\beta} \delta_{\beta\alpha}. \quad (\text{B.5})$$

Note that by definition, $\bar{T}_{0\alpha\beta} = [\partial (\bar{\beta}_{0\alpha} / c) / \partial E_\beta]|_0$, and that $\bar{T}_{0\alpha\beta} \neq \bar{\beta}'_{0\alpha} / c$ in general, since c may depend on $\mathbf{E}$ when $\bar{\beta}'_{0\alpha} \neq 0$. A similar statement applies for $\hat{T}_{0\alpha\beta}$. Finally consider third-order elastic coefficients. Differentiating (2.50) with respect to $\mathbf{F}$ gives (Clayton, 2011a; Clayton and Bammann, 2009)

$$\begin{aligned} A_{ijklmn} &= \frac{\partial^3 W}{\partial F_{ij} \partial F_{kl} \partial F_{mn}} = \frac{\partial^2 P_{ij}}{\partial F_{mn} \partial F_{kl}} = \frac{\partial A_{ijkl}}{\partial F_{mn}} = \frac{\partial}{\partial F_{mn}} (F_{in} F_{km} \bar{C}_{NJML} + \delta_{ik} \bar{S}_{JL}) \\ &= F_{il} F_{kk} F_{mm} \bar{C}_{IJKLMN} + \delta_{im} F_{kk} \bar{C}_{JNKL} + \delta_{km} F_{il} \bar{C}_{IJNL} + \delta_{ik} F_{mm} \bar{C}_{JLNM} \\ &= F_{il} F_{kk} F_{mm} \bar{C}_{IJKLMN} + \delta_{im} F_{Jq}^{-1} A_{qNKL} + \delta_{km} F_{Nq}^{-1} A_{ijqL} + \delta_{ik} F_{Jn}^{-1} A_{mNnL} - (\delta_{im} F_{jk}^{-1} F_{Nq}^{-1} P_{qL} + \delta_{km} F_{Ni}^{-1} F_{Jq}^{-1} P_{qL} + \delta_{ik} F_{Jm}^{-1} F_{Nq}^{-1} P_{qL}). \end{aligned} \quad (\text{B.6})$$

Differentiating (2.51) with respect to $\mathbf{F}$ gives

$$\begin{aligned} A_{ijklmn} &= \frac{\partial}{\partial F_{mn}} (F_{Pi}^{-1} F_{Rk}^{-1} F_{Jr}^{-1} F_{Qr}^{-1} F_{Lt}^{-1} F_{St}^{-1} \hat{C}_{PQRS} - F_{Jk}^{-1} P_{iL} - F_{Li}^{-1} P_{kJ} - F_{Jm}^{-1} F_{Lm}^{-1} F_{kN} P_{iN}) \\ &= F_{Pi}^{-1} F_{Rk}^{-1} F_{Um}^{-1} F_{Jr}^{-1} F_{Qr}^{-1} F_{Lt}^{-1} F_{St}^{-1} F_{Nw}^{-1} F_{Vw}^{-1} \hat{C}_{PQRSUV} - (F_{Pm}^{-1} F_{Ni}^{-1} F_{Rk}^{-1} F_{Jr}^{-1} F_{Qr}^{-1} F_{Lt}^{-1} F_{St}^{-1} \hat{C}_{PQRS} + F_{Rm}^{-1} F_{Nk}^{-1} F_{Pi}^{-1} F_{Jr}^{-1} F_{Qr}^{-1} F_{Lt}^{-1} F_{St}^{-1} \hat{C}_{PQRS} \\ &\quad + F_{Jm}^{-1} F_{Ni}^{-1} F_{Rk}^{-1} F_{Qr}^{-1} F_{Lt}^{-1} F_{St}^{-1} \hat{C}_{PQRS} + F_{Qm}^{-1} F_{Nr}^{-1} F_{Pi}^{-1} F_{Rk}^{-1} F_{Jr}^{-1} F_{Lt}^{-1} F_{St}^{-1} \hat{C}_{PQRS} \\ &\quad + F_{Lm}^{-1} F_{Nt}^{-1} F_{Pi}^{-1} F_{Rk}^{-1} F_{Jr}^{-1} F_{Qr}^{-1} F_{St}^{-1} \hat{C}_{PQRS} + F_{Sm}^{-1} F_{Nt}^{-1} F_{Pi}^{-1} F_{Rk}^{-1} F_{Jr}^{-1} F_{Qr}^{-1} F_{Lt}^{-1} \hat{C}_{PQRS}) \\ &\quad - (F_{Jk}^{-1} A_{iLmN} + F_{Li}^{-1} A_{kjmN} + F_{Jq}^{-1} F_{Lq}^{-1} F_{kp} A_{iPmN} + \delta_{mk} F_{Jq}^{-1} F_{Lq}^{-1} P_{iN}) \\ &\quad + F_{Jm}^{-1} F_{Nk}^{-1} P_{iL} + F_{Lm}^{-1} F_{Ni}^{-1} P_{kJ} + F_{Jm}^{-1} F_{Nq}^{-1} F_{Lq}^{-1} F_{kp} P_{iP} + F_{Lm}^{-1} F_{Nq}^{-1} F_{Jq}^{-1} F_{kp} P_{iP}. \end{aligned} \quad (\text{B.7})$$

Equating (B.6) and (B.7) produces a relationship between third-order tangent elastic coefficients at any deformation:

$$\begin{aligned} \bar{C}_{IJKLMN} &= F_{ii}^{-1} F_{Pi}^{-1} F_{Jj}^{-1} F_{Qj}^{-1} F_{Kk}^{-1} F_{Rk}^{-1} F_{Ll}^{-1} F_{Sl}^{-1} F_{Mm}^{-1} F_{Tm}^{-1} F_{Nn}^{-1} F_{Un}^{-1} \hat{C}_{PQRSTU} \\ &\quad - (F_{ii}^{-1} F_{Ni}^{-1} F_{Kk}^{-1} F_{Rk}^{-1} F_{Mm}^{-1} F_{Pm}^{-1} F_{Jr}^{-1} F_{Qr}^{-1} F_{Lt}^{-1} F_{St}^{-1} \hat{C}_{PQRS} + F_{ii}^{-1} F_{Pi}^{-1} F_{Kk}^{-1} F_{Nk}^{-1} F_{Mm}^{-1} F_{Rm}^{-1} F_{Jr}^{-1} F_{Qr}^{-1} F_{Lt}^{-1} F_{St}^{-1} \hat{C}_{PQRS} \\ &\quad + F_{ii}^{-1} F_{Pi}^{-1} F_{Kk}^{-1} F_{Rk}^{-1} F_{Mm}^{-1} F_{Jm}^{-1} F_{Nr}^{-1} F_{Qr}^{-1} F_{Lt}^{-1} F_{St}^{-1} \hat{C}_{PQRS} + F_{ii}^{-1} F_{Pi}^{-1} F_{Kk}^{-1} F_{Rk}^{-1} F_{Mm}^{-1} F_{Qm}^{-1} F_{Nr}^{-1} F_{Jr}^{-1} F_{Lt}^{-1} F_{St}^{-1} \hat{C}_{PQRS} \\ &\quad + F_{ii}^{-1} F_{Pi}^{-1} F_{Kk}^{-1} F_{Rk}^{-1} F_{Mm}^{-1} F_{Lm}^{-1} F_{Nt}^{-1} F_{Jr}^{-1} F_{Qr}^{-1} \hat{C}_{PQRS} + F_{ii}^{-1} F_{Pi}^{-1} F_{Kk}^{-1} F_{Rk}^{-1} F_{Mm}^{-1} F_{Sm}^{-1} F_{Nt}^{-1} F_{Ll}^{-1} F_{Jr}^{-1} F_{Qr}^{-1} \hat{C}_{PQRS}) \\ &\quad - (F_{Jk}^{-1} F_{Kk}^{-1} F_{Li}^{-1} F_{Mm}^{-1} A_{iLmN} + F_{ii}^{-1} F_{Li}^{-1} F_{Kk}^{-1} F_{Mm}^{-1} A_{kjmN} + F_{Jq}^{-1} F_{Lq}^{-1} F_{ii}^{-1} F_{Mm}^{-1} A_{iKmn} \\ &\quad + F_{ii}^{-1} F_{Mi}^{-1} F_{Kk}^{-1} F_{Jq}^{-1} A_{qNKL} + F_{Mk}^{-1} F_{Kk}^{-1} F_{Li}^{-1} F_{Nq}^{-1} A_{ijqL} + F_{ii}^{-1} F_{Ki}^{-1} F_{Jq}^{-1} F_{Mm}^{-1} A_{mNqL}) \\ &\quad + F_{ii}^{-1} F_{Mi}^{-1} F_{Jk}^{-1} F_{Kk}^{-1} F_{Nq}^{-1} P_{qL} + F_{ii}^{-1} F_{Ni}^{-1} F_{Km}^{-1} F_{Mm}^{-1} F_{Jq}^{-1} P_{qL} + F_{Ik}^{-1} F_{Kk}^{-1} F_{Jm}^{-1} F_{Mm}^{-1} F_{Nq}^{-1} P_{qL} \\ &\quad + F_{Jm}^{-1} F_{Mm}^{-1} F_{Kk}^{-1} F_{Nk}^{-1} F_{Li}^{-1} P_{iL} + F_{Li}^{-1} F_{Ni}^{-1} F_{Lm}^{-1} F_{Mm}^{-1} F_{Kk}^{-1} P_{kJ} + F_{Jm}^{-1} F_{Lm}^{-1} F_{Lq}^{-1} F_{Nq}^{-1} F_{Pi}^{-1} P_{iK} \\ &\quad + F_{Jq}^{-1} F_{Nq}^{-1} F_{Lm}^{-1} F_{Mm}^{-1} P_{iK} - F_{Jq}^{-1} F_{Lq}^{-1} F_{Kk}^{-1} F_{Mk}^{-1} F_{Li}^{-1} P_{iN}). \end{aligned} \quad (\text{B.8})$$

This equation applies analogously for either isothermal ($\bar{C}_{IJKLMN}^\theta, \hat{C}_{IJKLMN}^\theta$) or isentropic ($\bar{C}_{IJKLMN}^\eta, \hat{C}_{IJKLMN}^\eta$) coefficients. In the undeformed stress free reference state, using (2.50) and (B.3), (B.8) yields the following relationship between third-order isothermal elastic constants:

$$\begin{aligned}\hat{C}_{OIJKLMN}^\theta = & \bar{C}_{OIJKLMN}^\theta + \delta_{IK}\bar{C}_{OJLMN}^\theta + \delta_{IL}\bar{C}_{OJKMN}^\theta + \delta_{IM}\bar{C}_{OKLJN}^\theta + \delta_{IN}\bar{C}_{OKLJM}^\theta \\ & + \delta_{JK}\bar{C}_{OILMN}^\theta + \delta_{JM}\bar{C}_{OINKL}^\theta + \delta_{JL}\bar{C}_{OIKMN}^\theta + \delta_{JN}\bar{C}_{OIMKL}^\theta + \delta_{KM}\bar{C}_{OIJLN}^\theta + \delta_{KN}\bar{C}_{OIJLM}^\theta + \delta_{LM}\bar{C}_{OIJKN}^\theta + \delta_{LN}\bar{C}_{OIJKM}^\theta.\end{aligned}\quad (\text{B.9})$$

Similarly, for isentropic constants,

$$\begin{aligned}\hat{C}_{OIJKLMN}^\eta = & \bar{C}_{OIJKLMN}^\eta + \delta_{IK}\bar{C}_{OJLMN}^\eta + \delta_{IL}\bar{C}_{OJKMN}^\eta + \delta_{IM}\bar{C}_{OKLJN}^\eta + \delta_{IN}\bar{C}_{OKLJM}^\eta \\ & + \delta_{JK}\bar{C}_{OILMN}^\eta + \delta_{JM}\bar{C}_{OINKL}^\eta + \delta_{JL}\bar{C}_{OIKMN}^\eta + \delta_{JN}\bar{C}_{OIMKL}^\eta + \delta_{KM}\bar{C}_{OIJLN}^\eta + \delta_{KN}\bar{C}_{OIJLM}^\eta + \delta_{LM}\bar{C}_{OIJKN}^\eta + \delta_{LN}\bar{C}_{OIJKM}^\eta.\end{aligned}\quad (\text{B.10})$$

These derivations—which effectively equate strain energies to third order in Taylor series with respect to $\mathbf{F}$ —lead to relations among third-order elastic coefficients equivalent to those derived elsewhere (Weaver, 1976; Perrin and Delannoy, 1978) by applying series approximations [e.g., (A.14)] and equating coefficients of like terms in Lagrangian and Eulerian energy potentials.

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(PDF) US ARMY RESEARCH LAB
RDRL CIO LL

1 GOVT PRINTG OFC
(PDF) A MALHOTRA

ABERDEEN PROVING GROUND

36 DIR USARL
(PDF) RDRL CIH C
P CHUNG
J KNAP
RDRL WM
B FORCH
J MCCAULEY
P PLOSTINS
RDRL WML B
I BATYREV
B RICE
D TAYLOR
N WEINGARTEN
RDRL WML H
B SCHUSTER
RDRL WMM
J BEATTY
RDRL WMM B
G GAZONAS
C RANDOW
T SANO
RDRL WMM E
J SWAB
RDRL WMM F
M TSCHOPP
RDRL WMM G
J ANDZELM
RDRL WMP
S SCHOENFELD
RDRL WMP B
C HOPPEL
D POWELL
S SATAPATHY
M SCHEIDLER
T WEERISOORIYA

NO. OF
COPIES ORGANIZATION

RDRL WMP C
R BECKER
S BILYK
T BJERKE
D CASEM
J CLAYTON
D DANDEKAR
M GREENFIELD
R LEAVY
M RAFTENBERG
S SEGLETES
C WILLIAMS
RDRL WMP D
R DONEY
RDRL WMP E
S BARTUS

INTENTIONALLY LEFT BLANK.