

A Reformulation of Nonlinear Anisotropic Elasticity for Impact Physics

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ARL-TR-6837

February 2014

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REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
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1. REPORT DATE (DD-MM-YYYY) February 2014		2. REPORT TYPE Final		3. DATES COVERED (From - To) October 2012–January 2014	
4. TITLE AND SUBTITLE A Reformulation of Nonlinear Anisotropic Elasticity for Impact Physics				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) John D. Clayton				5d. PROJECT NUMBER DRI13-WMR-019	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) U.S. Army Research Laboratory ATTN: RDRL-WMP-C Aberdeen Proving Ground MD, 21005				8. PERFORMING ORGANIZATION REPORT NUMBER ARL-TR-6837	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited.					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT A new anisotropic Eulerian theory of nonlinear thermoelasticity developed in the present work has been shown to provide superior accuracy and/or stability over existing Lagrangian thermoelasticity theory for large static compression and shear deformation of ideal cubic crystals and diamond, and for the shock response of three different metallic crystals. For the shock response of single crystals of quartz and sapphire, Eulerian and Lagrangian theories are of comparable accuracy, with fourth-order elastic constants (quartz) and third-order elastic constants (diamond) necessary for a best fit to published experimental shock-compression data. Superior accuracy of this Eulerian theory, which degenerates to a Birch-Murnaghan equation-of-state when deviatoric stresses are negligible, has been demonstrated for representing the shock-compression response of aluminum, copper, and magnesium.					
15. SUBJECT TERMS impact physics, shock compression, elasticity, plasticity					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	18. NUMBER OF PAGES 22	19a. NAME OF RESPONSIBLE PERSON John D. Clayton
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified			19b. TELEPHONE NUMBER (Include area code) 410-278-6146

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1. Objective

Accurate, efficient, stable, and thermodynamically consistent models for nonlinear anisotropic elasticity are needed for mesoscale modeling of metals and ceramics subjected to large stresses that occur under ballistic loading conditions. Nonlinear elasticity theory describes large deformation behavior of solid bodies subjected to stresses—including metals, ceramics, minerals, and energetic materials. The standard Lagrangian formulation (1–3) of nonlinear elasticity in Cartesian coordinates for anisotropic crystals incorporates right Cauchy-Green strain tensor

$$\mathbf{E}(\mathbf{X}) = \frac{1}{2}(\mathbf{F}^T \mathbf{F} - \mathbf{1}), \quad E_{IJ}(X_K) = \frac{1}{2}(F_{KI} F_{KJ} - \delta_{IJ}) \quad (1)$$

entering thermodynamic potentials, (e.g., internal energy U and Helmholtz free energy Ψ):

$$U = U(\mathbf{E}, S), \quad \Psi = \Psi(\mathbf{E}, T) \quad (2)$$

where S is entropy and T temperature. Deformation gradient $\mathbf{F}$ and volume ratio J are

$$F_{IJ}(X_K) = \partial x_i / \partial X_J = \delta_{IJ} + \partial u_i / \partial X_J, \quad J(\mathbf{X}) = \frac{V}{V_0} = \det \mathbf{F} = [\det(2\mathbf{E} + \mathbf{1})]^{1/2} \quad (3)$$

where $\mathbf{u}$ is the particle displacement that here depends on reference coordinates $\mathbf{X}$.

This Lagrangian approach, when elastic constants of up to third order are included, has been successful for modeling many materials under compression up to $V_0 - V \approx 0.05V_0$, but its accuracy degrades at larger compression that may arise in shock loading or in extreme ballistic events; for example, elastic constants of orders four and higher—very difficult to measure and unknown for most anisotropic materials—may be needed (3). Existing theory and one-dimensional research wave propagation codes that incorporate Lagrangian theory with higher-order constants suffer from numerical inefficiency and intrinsic material instability, particularly for conditions involving simultaneous shear and compression (4). Many finite-strain elastic-plastic models used in three-dimensional hydrocodes for design of armor and munitions incorporate hypoelastic stress updates that are legacies from the 1980s; when elastic strains are large, such approaches can give physically unrealistic and mathematically unsound results (5). Codes typically compute deviatoric and spherical stress components in a decoupled way inconsistent with thermodynamic and material symmetry requirements, especially for anisotropic materials. A few advanced models for anisotropic crystals available in hydrocodes propose stress-strain relationships directly in terms of logarithmic strain (6, 7), which provide apparent numerical stability but apparently do not ensure integrability of stress-strain-entropy relations to analytic thermodynamic potentials. Without existence of potentials, relationships among state variables and material constants (e.g., thermal expansion, specific heat, isothermal versus isentropic constants) must be posited by conjecture, since Maxwell's identities among cross derivatives of

state quantities do not necessarily apply. Furthermore, in the absence of an elastic potential, solutions to elastostatic problems need not reflect stationary points of the energy functional for the body.

The objective of the proposed work is construction and implementation of a new continuum theory to remedy these issues. Specifically, this research will fully develop a complete theory of nonlinear thermoelasticity incorporating the Eulerian material strain tensor:

$$\mathbf{D}(\mathbf{x}) = \frac{1}{2}(\mathbf{1} - \mathbf{F}^{-1}\mathbf{F}^{-T}), \quad D_{IJ}(x_i) = \frac{1}{2}(\delta_{IJ} - F_{Ik}^{-1}F_{Jk}^{-1}) \quad (4)$$

Indices of this strain tensor are referred to the material coordinate system, even though the strain tensor is “Eulerian” in sense that it is constructed from the inverse deformation gradient. Because $\mathbf{D}$ is symmetric and referred to material coordinates, the functional form of its thermoelastic potentials will be the same as that for a conventional potential based on $\mathbf{E}$. 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. Restricting attention to fixed S for illustrative purposes, assuming a stress-free reference configuration, and written explicitly with elastic constants up to fourth order in either strain variable:

$$U(\mathbf{E}) = \frac{1}{2!}C_{\alpha\beta}E_\alpha E_\beta + \frac{1}{3!}C_{\alpha\beta\gamma}E_\alpha E_\beta E_\gamma + \frac{1}{4!}C_{\alpha\beta\gamma\delta}E_\alpha E_\beta E_\gamma E_\delta + \dots \quad (5)$$

$$U(\mathbf{D}) = \frac{1}{2!}c_{\alpha\beta}D_\alpha D_\beta + \frac{1}{3!}c_{\alpha\beta\gamma}D_\alpha D_\beta D_\gamma + \frac{1}{4!}c_{\alpha\beta\gamma\delta}D_\alpha D_\beta D_\gamma D_\delta + \dots \quad (6)$$

Greek indices denote Voigt notation and span 1,2, ... 6. Equating equations 5 and 6, expanding $\mathbf{E}$ and $\mathbf{D}$ in powers of displacement gradients, and matching terms leads to mathematically consistent relationships among second-, third-, and higher-order elastic constants $C_{\alpha\beta}, C_{\alpha\beta\gamma}, \dots$ and $c_{\alpha\beta}, c_{\alpha\beta\gamma}, \dots$. Upon derivation of such transformation formulae, published values for Lagrangian constants entering equation 5 can be immediately converted to those in equation 6, without need for further experiments. An obvious advantage of equation 6 over 5 is that under spherical compression, $\lim_{V \rightarrow 0} \|\mathbf{D}\| \rightarrow \infty$ whereas $\lim_{V \rightarrow 0} \|\mathbf{E}\| \rightarrow \sqrt{\frac{3}{4}}$, so a potential incorporating $\mathbf{D}$ such as equation 6 would correctly tend towards infinite energy as the material shrinks to infinitesimal volume, whereas an energy function of $\mathbf{E}$ such as equation 5 truncated at reasonable order would unrealistically yield finite energy at zero volume.

Success of the $\mathbf{D}$ -based Eulerian theory will be gauged by its ability to describe stresses in ceramics and metals subjected to uniaxial strain as occurring in plate impact, with fewer constants than the usual $\mathbf{E}$ -based finite-strain theory. Associated tasks include incorporation of thermal effects (Grüneisen tensors), inelasticity (slip and twinning), and internal stability analyses, none of which have been reported for this kind of theory for general stress states and crystals of arbitrary symmetry. Recent work (4) has demonstrated that under finite shear, $\mathbf{E}$ -based theory is prone to intrinsic instability in terms of attainment of zero eigenvalue(s) of the incremental stiffness (8) with increasing magnitude of third-order elastic constants, regardless of

their sign. While certain materials such as quartz (9) and boron carbide (10–12) demonstrate true physical instabilities, in a model such instabilities should result from the constitutive laws rather than problems associated with extrapolation of the strain-based theory to large deformation.

Benefits of using Eulerian strain tensors for isotropic materials were perhaps first posited in the 1930s by Murnaghan (13), and were substantiated for cubic crystals under hydrostatic stress by Birch (14). Thermal effects for cubic crystals were considered later in an Eulerian formulation (15), and a mechanical theory for noncubic crystals was initiated in (16) and exercised soon thereafter (17). With the exception of (13, 14), these papers remain obscure, and theoretical derivations/predictions and comparisons with data are limited to hydrostatic pressure loading. Nonetheless, the Eulerian approach has demonstrated promise for hydrostatic compression of anisotropic materials, as shown in figure 1.

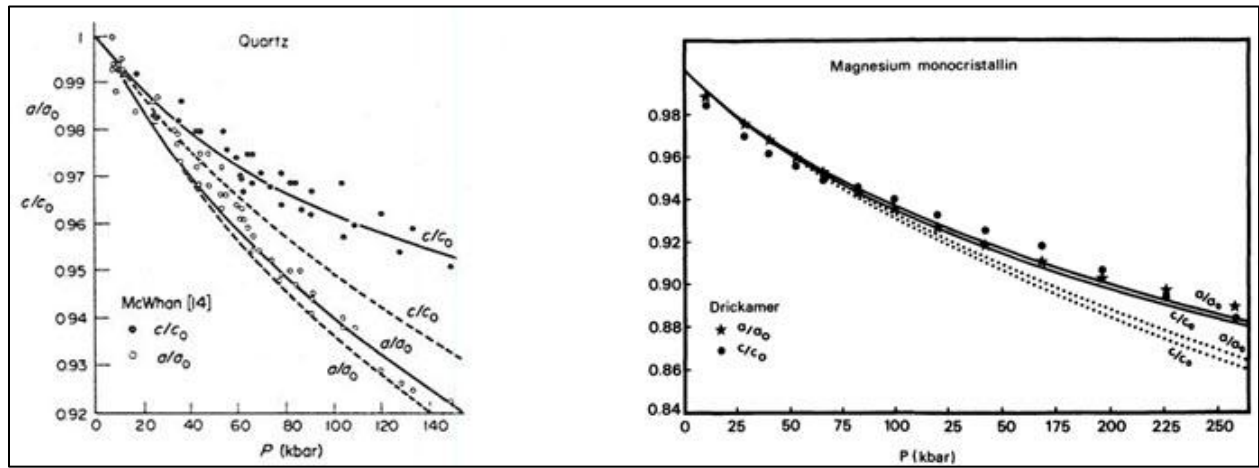


Figure 1. Comparison of accuracy of second- (—) and third- (---) order Eulerian models for hydrostatic compression of α -quartz (left [16]) and demonstration of superior accuracy of Eulerian (—) over Lagrangian (···) theory for hydrostatic compression of magnesium (right [17]).

Despite such promise, prior to the current work, Eulerian $\mathbf{D}$ -based theory had not been derived for solids of arbitrary anisotropy, and was untested for general stress states incorporating shear and compression. The theory had previously not been applied to dynamic or adiabatic conditions characteristic of shock or terminal ballistics. Use of such a model in numerical simulations appeared nonexistent, with algorithms unavailable in shock physics codes.

Formally, objectives of this proposal are to derive complete governing equations and assess accuracy and stability of this new Eulerian anisotropic finite-strain model. The intent is to prove, for materials of interest, that this approach offers greater accuracy with fewer higher-order constants, with less pathological (i.e., nonphysical) instability than Lagrangian theory.

2. Approach

Technical tasks for a two-year research program are discussed below. The first-year approach has focused on nonlinear elastic crystalline materials (i.e., pure or ideal crystals without defects or inelastic deformation mechanisms). Specifically, in Fiscal Year 2013 (FY13):

- Derivations have been completed for a fully anisotropic thermoelastic Eulerian formulation, including transformation rules among thermal and elastic material constants, for materials of arbitrary symmetry. Details are published (18), and key results will be highlighted later.
- New analytical solutions have been derived and studied for hydrostatic compression, uniaxial strain, and simple shear, for ideal crystals with cubic and Cauchy symmetry. These solutions, including stress-deformation responses and intrinsic stability criteria, have been evaluated over a realistic range of cubic elastic constants, and as a degenerate case include isotropic (polycrystalline) materials. Results, discussed more later, are published (18).
- A new analytical solution has been derived for the anisotropic shock response of single crystals, for an Eulerian internal energy potential quartic in strain and linear in entropy. This solution has been evaluated, and compared with available shock compression data, for single crystal quartz (trigonal symmetry), alumina (i.e., sapphire; trigonal symmetry), diamond (cubic symmetry), aluminum (cubic symmetry), copper (cubic symmetry), and magnesium (hexagonal symmetry). Comparison has been made with the analogous Lagrangian solution. Derivation of the solution and its evaluation for nonmetals have been published (18). Results for metals will be published (19) and are summarized later.

Work in FY13 has focused on behavior of ideal nonlinear elastic solids. Finite, purely elastic deformations of real crystals are generally possible under limited circumstances studied already: hydrostatic compression (in which shearing and tensile inelastic mechanisms are inhibited by the imposed stress state); uniaxial or shock compression of stiff crystals such as diamond, quartz, and sapphire below the yield point or Hugoniot Elastic Limit (HEL) (18); in very small volumes of ductile or brittle material amenable to atomic simulation of shock compression (19); or in the vicinity of defect cores (20). In ductile crystals—for example, metals and some minerals and organic crystals—inelastic deformation associated with dislocation glide, twinning, vacancy or void production, and/or fracture almost always accompanies (large) elastic deformation for loading conditions involving significant shear and/or tensile stress. Such complex loading conditions are inevitably encountered during ballistic impact problems pertinent to Army applications in Protection and Lethality, for example. Thus, technical tasks for FY14 will address the following:

- The fully anisotropic theoretical formulation will be extended to include plastic slip and twinning mechanisms that occur in more ductile materials and associated entropic temperature rise for shock loading.
 - New solutions for the elastic-plastic planar shock problem incorporating this more general elastic-plastic finite-strain theory will be sought.
 - The complete Eulerian theory will be implemented numerically in a finite-deformation wave propagation code accounting for dissipative inelastic mechanisms.
 - Accuracy of the new nonlinear elastic-plastic model(s) will be evaluated versus hydrostatic and shock compression data for ceramic and metallic single crystals of interest.
-

3. Results

In reference 18, a complete continuum thermoelastic theory for large deformation of crystals of arbitrary symmetry has been 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, written as $\mathbf{D}$ in equation 4. Thermodynamic identities and relationships among Eulerian and the usual Lagrangian material coefficients have been 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 have been studied over a prescribed range of elastic coefficients; stress states and intrinsic stability measures have been compared. For realistic coefficients, Eulerian theory has been shown to predict more physically realistic behavior than Lagrangian theory under large compression and shear. Analytical solutions for shock compression of anisotropic single crystals have been derived for internal energy functions quartic in Lagrangian or Eulerian strain and linear in entropy; results have been analyzed for quartz, sapphire (i.e., alumina), 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 provides a reasonable approximation of experimental data.

Some notable results are highlighted in what follows. Axial components of strains are compared for spherical and uniaxial deformations in figure 2. The magnitude of the axial component of $\mathbf{D}$ increases much more rapidly than the magnitude of the axial component of $\mathbf{E}$ under compression. Internal energy, stress/pressure, and stiffness of typical strong solids all tend to increase rapidly with large compression (14, 21). Therefore, Eulerian theory would logically be expected to converge faster, with fewer higher-order elastic constants needed, than Lagrangian theory.

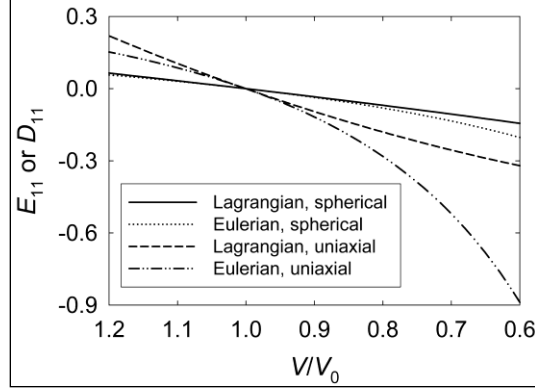


Figure 2. Lagrangian (E_{11}) and Eulerian (D_{11}) strains under spherical and uniaxial deformation (18).

Analytical results for pressure p under hydrostatic compression, axial stress P under uniaxial compression, and shear stress τ under simple shear are compared in figures 3a, b, and c, respectively. Stresses are normalized by ambient bulk modulus B_0 ; Poisson's ratio is ν . Stresses increase more rapidly with large strain for Eulerian theory than for Lagrangian theory, in general agreement with most data (14, 21) ($B'_0 \approx 4$), where B'_0 is the ambient pressure derivative of the tangent bulk modulus. The pressure-volume response of the Eulerian model similar is similar to the Murnaghan equation of state (figure 3a). Lagrangian theory is unstable for large shear strain as is evident from the softening with increasing shear strain γ in figure 3c. Evaluation of eigenmodes of incremental stiffness tensors showed that Eulerian theory is also more intrinsically stable than Lagrangian theory under compression.

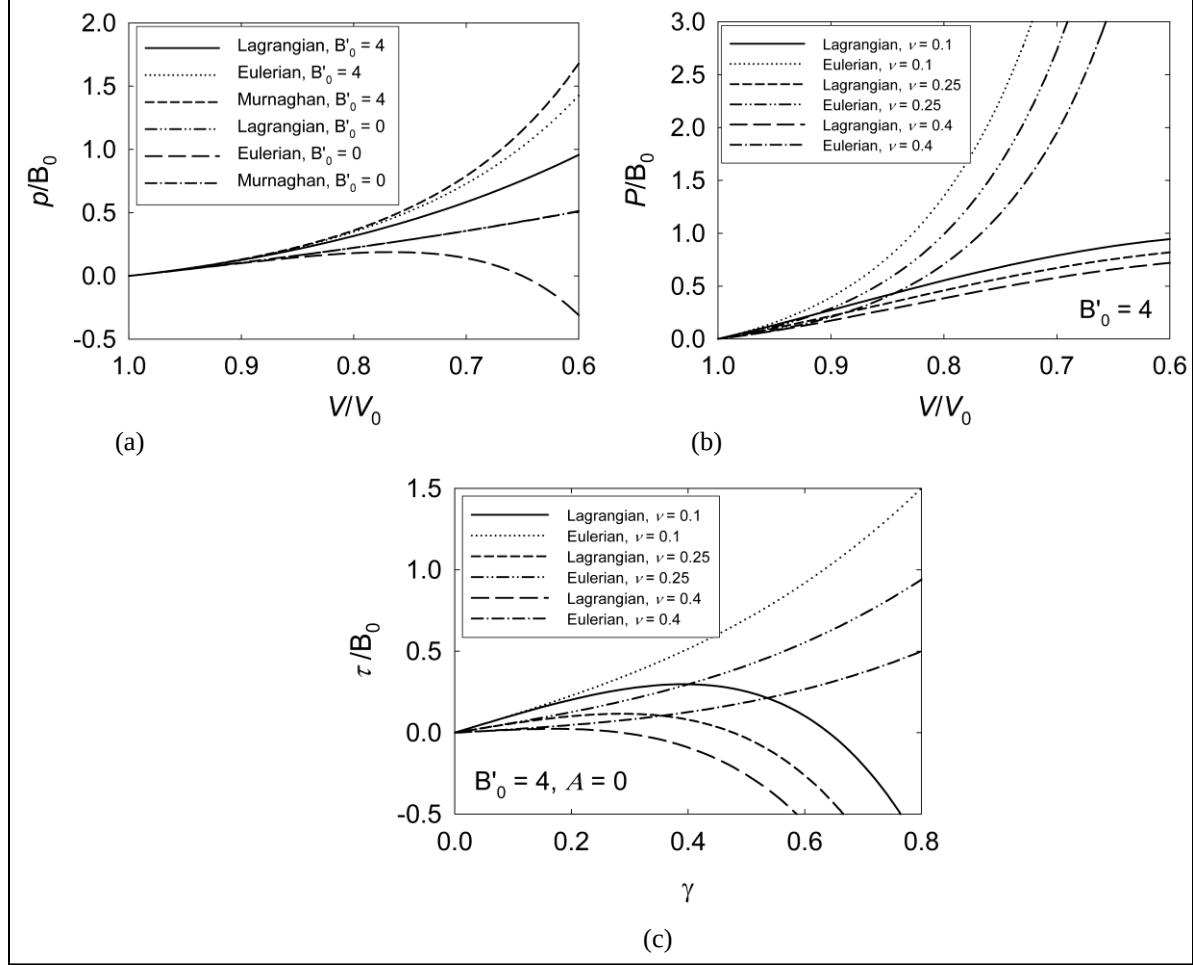


Figure 3. Analytical solutions (18) for normalized stress components: (a) hydrostatic compression; (b) uniaxial strain compression; (c) simple shear.

In reference 19, nonlinear elastic-plastic theory has been advanced for anisotropic solids incorporating an Eulerian strain measure, in locally unstressed material coordinates, that is a function of the inverse elastic deformation gradient and its transpose. A new general thermomechanical theory accounting for both elastic and plastic deformations has been briefly outlined in parallel with equations for usual Lagrangian finite-strain theory; however, a complete anisotropic Eulerian crystal elastic-plastic theory remains to be derived and numerically implemented in a wave propagation code in FY14. Idealized predictions of Eulerian and Lagrangian theories for elastic shock stress in single crystals of aluminum, copper, and magnesium have been compared, applicable for very small volumes of material without defects (i.e., no slip/twinning). Eulerian solutions demonstrate greater accuracy compared to published atomic simulation data for aluminum (22); see figure 4a, which shows shock pressure P in a [100]-oriented Al single crystal, normalized by isentropic second-order longitudinal stiffness C_{11} . For all three metals, Eulerian theory exhibits faster convergence than Lagrangian theory with increasing order of elastic constants entering internal energy. Such convergence is further verified by smaller magnitudes of all third- and fourth-order elastic constants of Eulerian theory

relative to those of Lagrangian theory for the same material. If strength can be neglected, Eulerian theory offers superior prediction of shock Hugoniot for all three metals; this is demonstrated for Al in figure 4b, which compares predicted pressure with shock data (23).

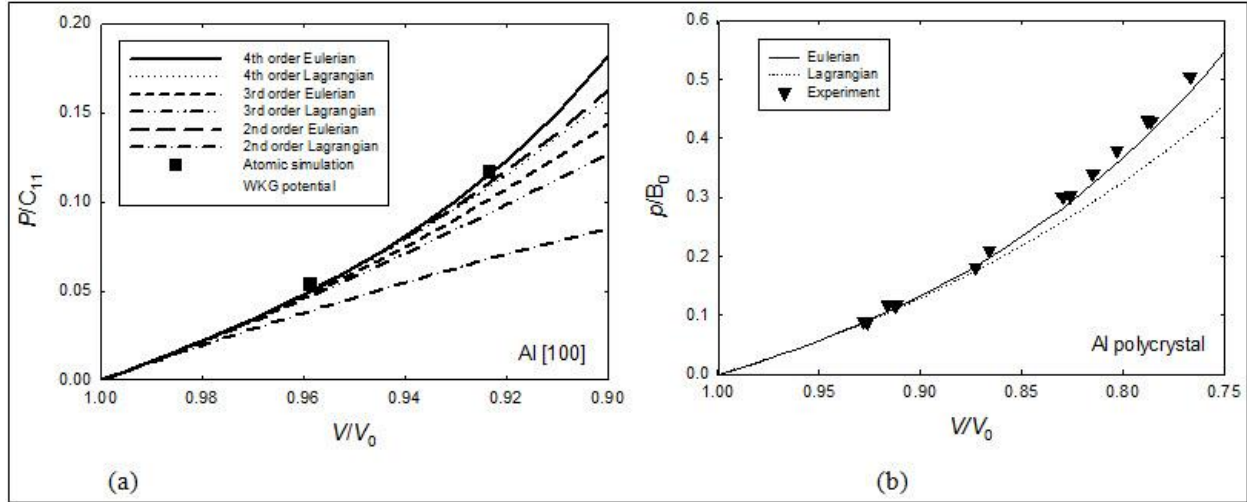


Figure 4. Analytical anisotropic thermoelastic solutions (19) for axial stress in shocked aluminum (Al) single crystals compared with atomic simulation data (22) (a); and analytical pressure solution for shocked Al polycrystals in the hydrodynamic limit compared with experimental data (23) (b).

Table 1 summarizes loading conditions, materials, and model performance studied in FY13, as discussed in detail in references (18, 19). Overall, the Eulerian nonlinear thermoelastic theory fully developed in Year 1 of this Director's Research Initiative (DRI) project appears superior to traditional Lagrangian theory, justifying ongoing research in FY14 and subsequent transition of the theory to the U.S. Army Research Laboratory (ARL) simulation codes used for development and analysis of armor and munitions.

Table 1. Summary of FY13 research results: finite-strain model evaluations.

Loading Protocol	Material	Best Model	Remarks	Ref.
Hydrostatic compression	Ideal cubic, $B'_0 = 4$	Eulerian	Eulerian more accurate p - V response	(18)
Uniaxial compression	Ideal cubic, $B'_0 = 4$	Eulerian	Eulerian more accurate and stable	(18)
Simple shear	Ideal cubic, $B'_0 = 4$	Eulerian	Eulerian more accurate and stable	(18)
Shock compression	α -Quartz	Either	Lagrangian & Eulerian equally valid	(18)
Shock compression	α -Alumina	Either	Lagrangian & Eulerian equally valid	(18)
Shock compression	Diamond	Eulerian	Eulerian more accurate overall	(18)
Shock compression	Aluminum	Eulerian	Eulerian best fit to atomic simulation	(19)
Shock compression	Copper	Eulerian	Eulerian faster convergence	(19)
Shock compression	Magnesium	Eulerian	Eulerian faster convergence	(19)

4. Conclusions

The new anisotropic Eulerian theory developed in the present work has been shown to provide superior accuracy and/or stability over existing Lagrangian theory for large static compression and shear deformation of ideal cubic crystals and diamond, and for the shock response of three different metallic crystals. For the shock response of single crystals of quartz and sapphire, Eulerian and Lagrangian theories are of comparable accuracy, with fourth-order elastic constants (quartz) and third-order elastic constants (diamond) necessary for a best fit to published experimental shock compression data. The second-year investigation will consider extension of the theory to finite-strain elastic-plastic behavior and numerical simulations of wave propagation.

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6. Transitions

Results of the current work are of high interest to modeling communities within the Department of Defense (DOD), Department of Energy (DOE), and the Materials in Extreme Dynamic Environments Collaborative Research Alliance (MEDE CRA). To date, research results have been transitioned via publications (18–20). Upon completion of Year 2 of this project, a plan will be formalized for implementation of the model into multiscale simulations of armor and munitions at ARL. Specifically, research developments from this DRI are expected to offer substantial improvements over prior analytical and computational studies of the finite-strain response of metals (24–32), ceramics (33–37), concrete and geologic materials (38, 39), and energetic molecular crystals (7). The nonlinear elastic model can also be directly implemented into phase-field simulations of microstructure (40–42). New developments in studies of lattice defects in electronic materials (43–45) and generic crystalline solids (46–54) are also foreseen.

List of Symbols, Abbreviations, and Acronyms

ARL	U.S. Army Research Laboratory
DOD	Department of Defense
DOE	Department of Energy
DRI	Director's Research Initiative
FY	Fiscal Year
HEL	Hugoniot Elastic Limit
MEDE CRA	Materials in Extreme Dynamic Environments Collaborative Research Alliance

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