



ARL-TR-9320 • SEP 2021



Thermodynamic Phase Field Models for Fracture and Inelasticity

by John D Clayton

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REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
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1. REPORT DATE (DD-MM-YYYY) September 2021		2. REPORT TYPE Technical Report		3. DATES COVERED (From - To) October 2020–September 2021	
4. TITLE AND SUBTITLE Thermodynamic Phase Field Models for Fracture and Inelasticity				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) John D Clayton				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) DEVCOM Army Research Laboratory ATTN: FCDD-RLW-TC Aberdeen Proving Ground, MD 21005-5066				8. PERFORMING ORGANIZATION REPORT NUMBER ARL-TR-9320	
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 is unlimited.					
13. SUPPLEMENTARY NOTES primary author's email: <john.d.clayton1.civ@mail.mil>.					
14. ABSTRACT A geometrically nonlinear phase field theory accounting for dissipation, rate effects, nonlinear thermoelasticity, fracture, and other structural changes is constructed in the context of continuum thermodynamics. Order parameters represent fractures, solid-solid phase transformations, deformation twinning, or slip of partial dislocations. Pressure-dependent strength commensurate with frictional resistance is enabled in novel kinetic equations for dynamic fracture with irreversibility constraints. Linearization suitable for moderate volume changes but small deviatoric elastic strain and rotation is undertaken. The theory is applied to study deformation and failure of polycrystalline boron carbide (B ₄ C), titanium diboride (TiB ₂), and a B ₄ C-TiB ₂ ceramic composite. Solutions are derived and evaluated numerically for uniaxial stress tension and compression, uniaxial strain compression, and planar shock compression. The latter analysis yields relationships among viscosity coefficients, gradient regularization lengths, and characteristics of steady waveforms. Results give new insight into high-rate deformation mechanisms in these materials. This report includes and enlarges content of a recent journal publication by the author.					
15. SUBJECT TERMS phase field, thermodynamics, crystals, fracture, slip, twinning, shock compression, nonlinear elasticity					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	18. NUMBER OF PAGES 155	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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Acknowledgments

The author acknowledges support of the US Army Combat Capabilities Development Army Research Laboratory.

This report encompasses and extends an original, but more terse, presentation by the author¹ first appearing in *Journal of the Mechanics and Physics of Solids* (“Non-linear thermodynamic phase field theory with application to fracture and dynamic inelastic phenomena in ceramic polycrystals”, vol. 157, 104633, 2021).

1. Introduction

The phase field method has been applied to numerous classes of problems in the physical sciences. Among general applications involving representation of diffuse interfaces in materials,² continuum and failure mechanics of solids have witnessed tremendous research activity on the subject of phase field-type modeling over the past two decades. Examples of phase field models, or their predecessors based on energy minimization principles, for fracture are widespread.^{3–11} As noted elsewhere,¹⁰ a variational treatment for minimization of energy functionals in the context of fracture mechanics builds on earlier work^{12,13} that analyzed similar functionals in the context of image segmentation.¹⁴ Examples of phase field models for solid-solid phase changes are also abundant.^{15–18} Phase field models of deformation twinning have been implemented as well.^{19–22} In some models, dislocation slip is resolved explicitly via phase field mechanics,^{23–25} while in others, a continuum elasto-plasticity accounts for numerous dislocations too small to resolve individually, and phase field mechanics addresses ductile fractures^{26–28} or deformation twins.²⁹

1.1 Background

Advantages of fundamental phase field models over conventional continuum mechanics models for plasticity and damage mechanics include the requirement of relatively few, if any, calibrated material parameters; regularized numerical solutions; and compatibility with standard numerical discretization schemes (e.g., standard finite elements or finite difference grids). No cumbersome changes in mesh topology needed for cohesive-zone finite element implementations^{30–33} are necessary with the phase field approach to modeling fractures or other localized damage in the material. Finally, Γ -convergence of certain phase field-type models based on energy minimization to the fundamental Griffith theory of fracture, with parallels to other historical models, can be demonstrated.¹⁰

Phase field-type models can be categorized in various ways. Geometrically linear (i.e., small deformation) theories are most typical, for example, those used for fracture^{4,6,8,11} and for deformation twinning.^{19,21} Geometrically nonlinear models for fracture exist,^{7,34–37} as do those for phase transformations^{18,38–40} and for deformation twinning.^{20,41} Linear models for fracture are sufficient for brittle solids (e.g., ceramics, concrete) under typical engineering loads, since failure ensues before deformations become severe. Linear models for phase changes and twinning have lim-

itations, as discussed elsewhere,^{42,43} whereby accuracy may be compromised for the case of large transformation strains or large twinning shears typical of many crystalline solids. Similar, but not identical, results were obtained in phase field simulations with linear and nonlinear models invoking twinning⁴³ or simultaneous twinning and fracture.⁴⁴ Furthermore, geometrically nonlinear formulations are necessary to properly address finite plastic strains in ductile failure problems.^{26,27} For brittle materials under combined shear and compression, enhancements to phase field fracture theory based on Mohr–Coulomb criteria have been enacted⁴⁵ to address effects of normal stress on shear strength due to frictional contact of microcrack faces in plastic zones, for example. Generalizations of phase field theory for geometrically enriched continua, intended to address physics at different length scales, have also been posited, including micromorphic²⁷ and Finsler-type^{46,47} internal degrees-of-freedom.

Models can be further characterized as quasi-static, fully dynamic, or mixed with regard to stress equilibrium and order parameter kinetics. Quasi-static models for order parameter equilibrium frequently invoke variational techniques in conjunction with incremental energy minimization. These classes of models are widely used for fracture,^{4,7,10,34,48} and less frequently, for twinning and coupled field problems.^{20,44} Fully dynamic approaches simultaneously address inertia (i.e., material acceleration and stress waves) as well as order parameter kinetics for phase field evolution. Models of this sort have been developed for fracture^{6,26,35,37,39,49} and for phase transformations and twinning.^{16,22,50} Finally, mixed approaches presume quasi-static equilibrium for the stress field but dynamic (i.e., time-dependent) evolution of phase field order parameter(s). Treatments of this type can account for phase transformations,⁵¹ twinning,^{19,21} and fracture.^{8,28}

Different prescription of contributions of order parameters, their spatial gradients, and their rates to stored versus dissipated energy will lead to different thermodynamic behaviors. A general treatment⁵¹ based on microforces permits order parameters, gradients, and rates to contribute in various ways, where under certain assumptions, the time-dependent Ginzburg–Landau (TDGL) equation for dissipative order parameter kinetics can be transparently derived. See also an earlier reference⁵² wherein balanced configurational forces are introduced in the context of solid-solid phase transformations. Standard models attribute spatial gradients of order parameters to energy storage, leading to natural definitions of surface energy in the vicinity

of fractures or phase/twin boundaries.^{10,11,20,38,40} Recent models for fracture have omitted the gradient contribution to free energy, such that there is no storage of energy due to inhomogeneous order parameter evolution, and dissipation from order parameter kinetics is ensured as non-negative via use of an auxiliary energy functional.^{26,28,35} While most phase field mechanics models for fracture have been restricted to isothermal problems, some advanced implementations have considered heat transfer.³⁵

1.2 Contributions of the Current Work

The current report extends prior works for fracture, deformation twinning, and solid-solid phase transformations,^{20,34,53} based on variational principles for quasi-static equilibrium, to the fully dynamic case. Balance equations and kinetic laws enable material inertia and rate-dependent order parameter evolution. Finite strains and temperature gradients in both time and space are admitted, as are stress waves. The most prominent novel theoretical contributions are the following:

- A new thermodynamically admissible, irreversible model for fracture kinetics enables accurate depiction of very different strengths of brittle materials under tension, unconfined compression, and shock uniaxial compression, as well as elastic-to-failure behavior and abrupt stress drop after peak load observed in real brittle solids.
- The phase field method is used, for the first time, to determine the structure of steady shock wave profiles in brittle materials,⁵⁴ as arising from plate impact or laser shock experiments, by integration of the conservation and regularized kinetic equations along Rayleigh lines. A novel method of extracting the viscosity parameters for order parameter kinetics from measured shock rise times is invoked. Results show that widths of moving interfaces are constrained by two regularization lengths—one from gradient regularization, the other from viscous regularization—and that neither can be chosen arbitrarily.
- A new, geometrically linearized version of the logarithmic elasticity model is derived that includes nonlinear thermoelastic contributions from density changes important for shock compression loading. This linearized model, with pressure correction, is more amenable to large-scale computations than its nonlinear counterpart since finite deformation configurational mappings and calculations of tensor logarithms are avoided. Accuracy of this model

is found to be comparable, in most cases, to the fully nonlinear theory for analysis of shock compression of ceramic materials.

The aforementioned linearized version omits nonlinearity in the elastic shearing response. This omission is often deemed appropriate for brittle materials that are unable to sustain large elastic shear strains without fracture and strength loss. The linearized model, while accurately accounting for moderate volumetric compression, is however subject to the usual accuracy constraints imposed by small-deformation limitations of classical linear elasticity and, as such, is not intended for solutions of problems involving large arbitrary strains or finite rotations.

Additional new theoretical contributions, while not as profound as the three listed previously include the following:

- A multiplicative decomposition of the deformation gradient is invoked, and a thermoelastic potential based on logarithmic thermoelastic strain referred to the locally unloaded intermediate configuration—shown to accurately depict the shock compression response of a number of ceramics and minerals^{55–57}—is used for the first time in the phase field method. This formulation differs from others^{26,27} that assume an additive decomposition of the total logarithmic strain and is not consistent with a multiplicative decomposition of deformation gradient. Logarithmic thermoelasticity and general curvilinear coordinates have been considered, however, in other treatments by the author with a basis in differential geometry^{47,58,59} that share some features with phase field mechanics.
- Derivations and analysis of problems (e.g., cylindrical symmetry) apply general curvilinear coordinates—including anholonomic curvilinear coordinates of the intermediate configuration—rather than Cartesian coordinates as ubiquitously invoked elsewhere in phase field analysis of fracture and solid-solid phase transformations.

Both the fully nonlinear model and the linearized model are evaluated for three classes of problems: uniaxial stress tension/compression, uniaxial strain compression, and planar shock compression. Three ceramic materials are considered: polycrystalline boron carbide (B_4C),^{60–63} polycrystalline titanium diboride (TiB_2),^{56,64–66}

and a polycrystalline B_4C - TiB_2 composite.^{67–70} In conjunction with experimental data, these problems and their solutions demonstrate parameter selection, accuracy and regimes of applicability of the theory, and new information on effects of evolving microstructure on thermo-mechanical response. Geometric extensions of phase field theory^{58,71,72} modeled shock compression of single crystals rather than polycrystals, and did not include order parameter kinetics or multiple order parameter fields (e.g., for simultaneous phase transformations, slip/twinning, and fracture) addressed herein. In those works,^{58,71} shocks were idealized as singular surfaces rather than structured steady waves of finite width. New information revealed, in the current work, about the physical response of the polycrystalline materials is summarized as follows:

- For B_4C , different time scales for kinetics of fracture versus amorphization enable the phase field method to reproduce different fracture and amorphization tendencies, or lack thereof, experimentally observed in dynamic Kolsky-bar compression,^{73,74} plate impact,^{60,75} and laser shock compression.⁶²
- For TiB_2 under shock compression, initial yield arises from fracture, while limited dislocation slip is a viable source of the second yield point in the Hugoniot.^{65,76} An accurate depiction of high shear strength maintained at large compression is afforded by pressure-dependent fracture kinetics, whereby viscosity from frictional mechanisms increases such that crack extension and comminution are suppressed at high pressures.
- Predicted temperature rises for shocks below the overdriven threshold do not approach melt in either monolithic material, and are insufficient to increase dislocation mobility or incur a brittle-to-ductile transition in the context of available static test data at high temperatures. In B_4C , an increasing tendency for amorphization due to adiabatic heating has been posited,^{63,77} but this mechanism is unconfirmed by the present results since temperatures are far below those for melting for the shock pressures considered.
- The ceramic composite demonstrates unusually rate sensitive behavior for a ceramic,^{67,78} which can be accurately represented using the present phase field fracture theory with viscous fracture kinetics. However, limited shock compression data⁶⁸ show anomalous high strength above the yield point that remains explained.

The primary objective, and most important original contribution, of this work is study of shock waves in the real materials mentioned previously. To address this class of problems via the phase field method, (1) nucleation of cracks in confined compression and (2) coupled fracture and transformation phenomena are necessarily modeled. These two aspects are open areas of research, and each warrants a more in-depth theoretical and numerical treatment in the future. The present models sufficiently address these topics to enable the objective of 1D shock wave modeling, but their performance in 2D and 3D problems remains unexplored. Models have been verified versus macroscopic data (which is historically the most readily available for shocked ceramics), whereby parameters have been obtained in a logical, physically motivated manner. Such parameters are now available for use in future numerical implementations to study other initial boundary value problems, including other localization phenomena.

The fully nonlinear theory is derived in Section 2. Linearization is undertaken in Section 3. Material modeling for the ceramics of interest is described in Section 4. Analysis of uniaxial stress problems is discussed in Section 5, followed by homogeneous uniaxial strain in Section 6. The planar shock compression problem for structured steady waveforms is studied in Section 7. Conclusions follow in Section 8. Direct tensor notation is used primarily, with vectors and higher-order tensors in bold italic font. When the index notation is invoked, summation is implied over repeated contravariant-covariant indices, where general curvilinear coordinates are admitted unless noted otherwise.

2. Nonlinear Theory

The geometrically nonlinear theory with time dependence is derived next. A solid body is considered with reference domain (i.e., initial volume) Ω_0 and boundary $\partial\Omega_0$. Let $\mathbf{X}$, with components X^K , denote position of a material particle and t denote time. The outward unit normal to $\partial\Omega_0$ is the vector $\mathbf{N}(\mathbf{X})$.

2.1 Order Parameter Definitions

Considered are two sets of order parameter fields $\eta^i(\mathbf{X}, t)$ and $\xi^j(\mathbf{X}, t)$. The former measure structural changes in the solid that do not involve formation of free surfaces or free volume, for example, solid-solid phase transformations or deformation twinning. The latter account for fracture, cavitation, or other “damage” mechanisms that physically introduce free surfaces or local displacement discontinuities, though in the continuum phase field approach, such discontinuities are smoothed by construction.

2.1.1 Structural Transformations

First consider structural change fields η^i , where $i = 1, \dots, k$, and the total number of phases or domains is $k + 1$. For example, in single crystals, k could correspond to the number of potential twin systems,^{20,79} or to the number of martensitic variants.^{38,40} Physical meanings are

$$\begin{aligned} \eta^i(\mathbf{X}, t) &= 0 \quad \forall i = 1, \dots, k : \text{parent elastic crystal or initial phase at } (\mathbf{X}, t), \\ \eta^i(\mathbf{X}, t) &= 1, \quad \eta^j(\mathbf{X}, t) = 0 \quad \forall j \neq i : \text{fully transformed or twinned state } i \text{ at } (\mathbf{X}, t), \\ \eta^i(\mathbf{X}, t) &\in (0, 1) \text{ for any } i = 1, \dots, k : \text{phase or twin boundary zone at } (\mathbf{X}, t). \end{aligned} \tag{1}$$

Bounds and constraints on the η^i are

$$\eta^i \in [0, 1] \quad \forall i, \quad \sum_{i=1}^k \eta^i(\mathbf{X}, t) \leq 1. \tag{2}$$

The latter constraint in Eq. 2 prevents the total, local volume fraction of all phases from exceeding unity when the η^i are physically identified with the referential volume fractions of each phase i . The local fraction of parent phase can be quantified by $\eta^0(\mathbf{X}, t) = 1 - \sum_{i=1}^k \eta^i(\mathbf{X}, t)$.

2.1.2 Fracture

Now consider fracture/damage fields ξ^j , where $j = 1, \dots, l$, and the total number of failure mechanisms is l . For example, in single crystals, fractures on multiple cleavage planes^{36,80,81} can be represented by l order parameters, where l is the number of potential failure planes. Physical meanings are

$$\begin{aligned} \xi^j(\mathbf{X}, t) &= 0 \forall j = 1, \dots, l : \text{fully intact material at } (\mathbf{X}, t), \\ \xi^j(\mathbf{X}, t) &= 1 \text{ for any } j = 1, \dots, l : \text{fully damaged or fractured state } j \text{ at } (\mathbf{X}, t), \\ \xi^j(\mathbf{X}, t) &> 0 \text{ for any } j = 1, \dots, l \text{ and} \\ \xi^i(\mathbf{X}, t) &< 1 \forall i = 1, \dots, l : \text{partially degraded state } j \text{ at } (\mathbf{X}, t). \end{aligned} \tag{3}$$

Bounds and constraints on the ξ^j are

$$\xi^j \in [0, 1] \forall j, \quad \sum_{j=1}^l \xi^j(\mathbf{X}, t) \leq l. \tag{4}$$

2.2 Kinematics

Denote by $\mathbf{x}$ with components x^k the spatial position of material points of the deformed body $\Omega(t)$, with boundary $\partial\Omega$ and unit outward normal $\mathbf{n}(\mathbf{x})$.

2.2.1 General Motions

Motions between reference and spatial configurations of the body are the following functions, at least twice differentiable:

$$\mathbf{x} = \boldsymbol{\phi}(\mathbf{X}, t), \quad \mathbf{X} = \boldsymbol{\Phi}(\mathbf{x}, t). \tag{5}$$

Components of metric tensors are $G_{IJ}(\mathbf{X}) = \partial_I \mathbf{X} \cdot \partial_J \mathbf{X} = \mathbf{G}_I \cdot \mathbf{G}_J$ and $g_{ij}(\mathbf{x}) = \partial_i \mathbf{x} \cdot \partial_j \mathbf{x} = \mathbf{g}_i \cdot \mathbf{g}_j$. Fields of natural basis vectors are $\mathbf{G}_I(\mathbf{X})$ and $\mathbf{g}_i(\mathbf{x})$. Partial coordinate differentiation is written $\partial_K(\cdot) = \partial(\cdot)/\partial X^K$ and $\partial_k(\cdot) = \partial(\cdot)/\partial x^k$. The deformation gradient and its inverse are

$$\mathbf{F} = \partial \boldsymbol{\phi} / \partial \mathbf{X}, \quad \mathbf{F}^{-1} = \partial \boldsymbol{\Phi} / \partial \mathbf{x}. \tag{6}$$

The Jacobian determinant relating positive volume elements $d\Omega$ and $d\Omega_0$ is

$$J = \sqrt{g/G} \det(F_J^i) = d\Omega/d\Omega_0 > 0; \quad g = \det(g_{ij}), \quad G = \det(G_{IJ}). \quad (7)$$

Denote $\dot{f}(\mathbf{X}, t) = \partial f(\mathbf{X}, t)/\partial t$ the material time derivative of a differentiable function f . Particle velocity and acceleration are the respective fields

$$\mathbf{v}(\mathbf{X}, t) = \dot{\mathbf{x}}(\mathbf{X}, t), \quad \dot{\mathbf{v}}(\mathbf{X}, t) = \ddot{\mathbf{x}}(\mathbf{X}, t). \quad (8)$$

Denote by $\nabla_0(\cdot)$ the covariant derivative with respect to $\mathbf{X}$, enacted by Levi–Civita connection coefficients from G_{IJ} . Denote by $\nabla(\cdot)$ the covariant derivative with respect to $\mathbf{x}$, enacted by Levi–Civita connection coefficients from g_{ij} . The spatial velocity gradient and its trace obey

$$\nabla \mathbf{v} = \dot{\mathbf{F}} \mathbf{F}^{-1}, \quad \dot{J}/J = \text{tr}(\nabla \mathbf{v}) = \nabla \cdot \mathbf{v}. \quad (9)$$

Pointwise integrability of $\mathbf{F}$ over Ω_0 , and of $\mathbf{F}^{-1}$ over Ω , leads to the following compatibility conditions⁸²:

$$\nabla_0 \times \mathbf{F} = \mathbf{0}, \quad \nabla_0 \cdot (J\mathbf{F}^{-1}) = \mathbf{0}; \quad \nabla \times \mathbf{F}^{-1} = \mathbf{0}, \quad \nabla \cdot (J^{-1}\mathbf{F}) = \mathbf{0}. \quad (10)$$

Conditions in Eq. 10, for a simply connected body, are consistent with the presumption of holonomic geometric spaces Ω_0 and Ω , with $\mathbf{F}$ and its inverse the corresponding tangent mappings between them.

2.2.2 Multiplicative Kinematics

Similar to constructions used for crystal plasticity theory^{79,83,84} and continuum elastic-twinning theory,^{85,86} a multiplicative decomposition of the total deformation gradient into a thermoelastic part $\mathbf{F}^E$ and an evolving microstructure-dependent part $\bar{\mathbf{F}}$ is invoked:

$$\mathbf{F}(\mathbf{X}, t) = \mathbf{F}^E(\mathbf{X}, t) \cdot \bar{\mathbf{F}}(\eta^i(\mathbf{X}, t), \xi^j(\mathbf{X}, t)). \quad (11)$$

The two-point tensor field $\bar{\mathbf{F}}$ is a state function of the order parameter fields. A more specific form invoked later presumes separability of contributions of mechanisms as follows:

$$\bar{\mathbf{F}}(\eta^i(\mathbf{X}, t), \xi^j(\mathbf{X}, t)) = \mathbf{F}^\xi(\xi^j(\mathbf{X}, t)) \cdot \mathbf{F}^\eta(\eta^i(\mathbf{X}, t)). \quad (12)$$

The sequence of mappings on the right side of Eq. 12 is somewhat arbitrary; the form used here may prove more convenient when damage follows after other structural changes, though no temporal order is mandated by Eq. 12 (i.e., fracture can precede phase changes during a local deformation history, or vice versa).

The decomposition in Eq. 11 implies existence of a local, thermoelastically unloaded intermediate configuration $\bar{\Omega}$, as shown in Fig. 1. A generic metric tensor on this configuration⁸⁷ is $\bar{g}_{\alpha\beta}(\mathbf{X}, t) = \bar{\mathbf{g}}_\alpha \cdot \bar{\mathbf{g}}_\beta$, with $\bar{g} = \det(\bar{g}_{\alpha\beta})$. Fields of anholonomic basis vectors^{82,88} are $\bar{\mathbf{g}}_\alpha(\mathbf{X}, t)$ ($\alpha = 1, 2, 3$). All mappings in Eqs. 11 and 12 have positive determinants and are continuously differentiable with respect to time and position.

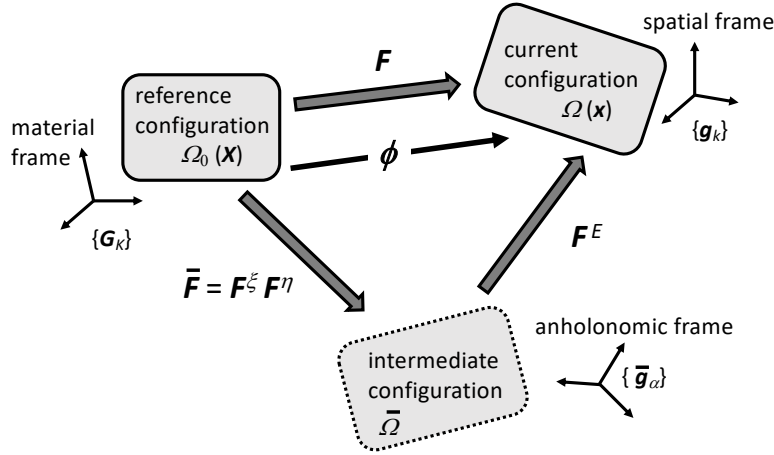


Fig. 1 Configurations, tangent mappings, and coordinate frames associated with Eqs. 5, 6, 11, and 12

Denote by $d\bar{\Omega}$ a local, intermediate configuration volume element. Jacobian determinants for thermoelasticity and structure changes enable the following relationships:

$$\begin{aligned} J^E &= \sqrt{g/\bar{g}} \det \mathbf{F}^E = d\Omega/d\bar{\Omega} > 0, & \bar{J} &= \sqrt{\bar{g}/G} \det \bar{\mathbf{F}} = d\bar{\Omega}/d\Omega_0 > 0; \\ J &= J^E \bar{J}. \end{aligned} \quad (13)$$

Define the following structure tensors:

$$\mathbf{A}_j^\xi = \partial \bar{\mathbf{F}} / \partial \xi^j, \quad \mathbf{A}_i^\eta = \partial \bar{\mathbf{F}} / \partial \eta^i. \quad (14)$$

The spatial velocity gradient Eq. 9 then obeys an additive decomposition:

$$\begin{aligned}\nabla \mathbf{v} &= \dot{\mathbf{F}}^E \mathbf{F}^{E-1} + \mathbf{F}^E \bar{\mathbf{L}} \mathbf{F}^{E-1}, \\ \bar{\mathbf{L}} = \dot{\bar{\mathbf{F}}} \bar{\mathbf{F}}^{-1} &= \sum_{j=1}^l \mathbf{A}_j^\xi \bar{\mathbf{F}}^{-1} \dot{\xi}^j + \sum_{i=1}^k \mathbf{A}_i^\eta \bar{\mathbf{F}}^{-1} \dot{\eta}^i = \mathbf{A}_j^\xi \bar{\mathbf{F}}^{-1} \dot{\xi}^j + \mathbf{A}_i^\eta \bar{\mathbf{F}}^{-1} \dot{\eta}^i,\end{aligned}\quad (15)$$

where summation over order parameters is implied by repeated indices in the right-most expression. The following identities hold for rates of thermoelastic and residual volume change⁸²:

$$\dot{J}^E / J^E = \text{tr}(\dot{\mathbf{F}}^E \mathbf{F}^{E-1}), \quad \dot{\bar{J}} / \bar{J} = \text{tr}(\bar{\mathbf{L}}). \quad (16)$$

From the first of Eq. 10 and Eq. 11, the following identity can be derived, newly extending a prior derivation⁸² via use of Eq. 14:

$$\begin{aligned}J^E (F^{E-1})_p^\alpha \epsilon^{pqr} \nabla_r (F^{E-1})_q^\beta &= \bar{J}^{-1} \bar{F}_P^\alpha \epsilon^{PQR} \nabla_{0R} \bar{F}_Q^\beta \\ &= \bar{J}^{-1} \bar{F}_P^\alpha \epsilon^{PQR} \left[(A_j^\xi)_Q^\beta \nabla_{0R} \xi^j + (A_i^\eta)_Q^\beta \nabla_{0R} \eta^i \right].\end{aligned}\quad (17)$$

Permutation tensors in spatial and reference frames are ϵ^{ijk} and ϵ^{IJK} . When both sides of Eq. 17 vanish identically over a simply connected body Ω_0 , then intermediate configuration $\bar{\Omega}$ becomes holonomic, and twice-differentiable coordinates $\bar{\mathbf{x}}(\mathbf{X}, t)$ exist such that $\bar{F}_K^\alpha = \partial_K \bar{x}^\alpha$ and $(F^{E-1})_k^\alpha = \partial_k \bar{x}^\alpha$. Otherwise, the right side of Eq. 17 is one measure of incompatibility of residual deformation, related to material gradients of order parameters. When structure changes manifest from plastic slip, this incompatibility can be related to a dislocation density tensor.^{79,83,84} For η^i describing deformation twinning, a similar interpretation may be possible in terms of dislocations at interfaces between parent and twin or among different twins.⁷⁹ This is consistent with the phase field concept that internal boundaries in microstructures are related to order parameter gradients.

2.2.3 Thermoelastic Strain

The symmetric thermoelastic deformation tensor, with covariant components referred to configuration $\bar{\Omega}$, is defined and related to thermoelastic volume change as

follows:

$$\mathbf{C}^E = (\mathbf{F}^E)^T \mathbf{F}^E, \quad C_{\alpha\beta}^E = (F^E)_\alpha^i g_{ij} (F^E)_\beta^j; \quad \det(C_{\alpha\beta}^E) = (J^E)^2 \bar{g}. \quad (18)$$

The symmetric logarithmic thermoelastic strain, likewise referred to $\bar{\Omega}$, is defined and related to volume change as^{55,61}

$$\mathbf{e}^E = \frac{1}{2} \ln(\mathbf{C}^E), \quad e_{\alpha\beta}^E = \frac{1}{2} (\ln C^E)_{\alpha\beta}; \quad \text{tr}(\mathbf{e}^E) = (e^E)_\alpha^\alpha = \ln(J^E). \quad (19)$$

Both $\mathbf{C}^E = C_{\alpha\beta}^E \bar{\mathbf{g}}^\alpha \otimes \bar{\mathbf{g}}^\beta$ and $\mathbf{e}^E = e_{\alpha\beta}^E \bar{\mathbf{g}}^\alpha \otimes \bar{\mathbf{g}}^\beta$ are invariant under rotations of the spatial coordinate system and thus are suitable for use in anisotropic constitutive models⁷² when their corresponding anholonomic basis vectors $\{\bar{\mathbf{g}}^\alpha, \bar{\mathbf{g}}_\alpha\}$ are invariant (see Section 4.4.3). The present logarithmic thermoelastic strain differs from that used by others,^{26,27} which assumes an additive decomposition of the total logarithmic strain $\frac{1}{2} \ln(\mathbf{F}^T \mathbf{F})$ into elastic and plastic parts, both referred to Ω_0 . The latter kinematic construction^{26,27} is inconsistent with a multiplicative decomposition of the form Eq. 11. Algorithms for computing the logarithm of a second-order tensor and $\mathbf{M}^E = 2\partial\mathbf{e}^E/\partial\mathbf{C}^E$ are available in the literature.^{55,89,90}

2.3 Balance Laws and Thermodynamics

Balance laws are derived under assumptions of no mass transport, no body forces at macroscopic or microscopic scales, and no point heat sources. The latter two (i.e., body forces and heat sources) can be added without any conceptual challenges.

2.3.1 Mass

Denote by $dm = \rho_0 d\Omega_0$ a differential mass element. Mass conservation is described by the following global and local equations that follow from Eq. 7:

$$\frac{d}{dt} \int_{\Omega_0} dm = \frac{d}{dt} \int_{\Omega_0} \rho_0 d\Omega_0 = \frac{d}{dt} \int_{\Omega} \rho d\Omega = 0 \quad \Rightarrow \quad \rho_0 = \rho J, \quad \dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0. \quad (20)$$

2.3.2 Momentum

The classical macroscopic linear momentum equations in global and local forms are, with $\mathbf{t}_0 = \mathbf{P} \cdot \mathbf{N}$ the traction per unit reference area A_0 ,

$$\oint_{\partial\Omega_0} \mathbf{t}_0 dA_0 = \frac{d}{dt} \int_{\Omega_0} \rho_0 \mathbf{v} d\Omega_0 \quad \Rightarrow \quad \nabla_0 \cdot \mathbf{P} = \rho_0 \dot{\mathbf{v}} \quad \Leftrightarrow \quad \nabla_{0K} P^{iK} = \rho_0 v^i. \quad (21)$$

First Piola–Kirchhoff stress is $\mathbf{P} = J\boldsymbol{\sigma}\mathbf{F}^{-T}$, where $\boldsymbol{\sigma}$ is the Cauchy stress. The balance of angular momentum can then be stated as

$$\oint_{\partial\Omega_0} \mathbf{x} \times \mathbf{t}_0 dA_0 = \frac{d}{dt} \int_{\Omega_0} \mathbf{x} \times \rho_0 \mathbf{v} d\Omega_0 \quad \Rightarrow \quad \mathbf{P}\mathbf{F}^T = \mathbf{F}\mathbf{P}^T \quad \Leftrightarrow \quad P^{iK} F_K^j = F_K^i P^{jK}. \quad (22)$$

Cauchy stress is thus symmetric: $\sigma^{ij} = \sigma^{ji}$.

A microforce system^{28,51} is introduced, here extended to multiple order parameters defined in Section 2.1. Define the internal microforces π_i^η and π_j^ξ and the microscopic stress vectors in the reference configuration $\mathbf{s}_i^\eta$ and $\mathbf{s}_j^\xi$ with corresponding surface forces t_i^η and t_j^ξ :

$$t_i^\eta = \mathbf{s}_i^\eta \cdot \mathbf{N} \quad (i = 1, \dots, k); \quad t_j^\xi = \mathbf{s}_j^\xi \cdot \mathbf{N} \quad (j = 1, \dots, l) \quad [\text{on } \partial\Omega_0]. \quad (23)$$

The following global and local systems are then posited, extending the theory of ME Gurtin⁵¹ to the case with multiple order parameters, but in the absence of microscopic body forces:

$$\begin{aligned} \oint_{\partial\Omega_0} t_i^\eta dA_0 + \int_{\Omega_0} \pi_i^\eta d\Omega_0 &= 0 \quad \Rightarrow \quad \nabla_0 \cdot \mathbf{s}_i^\eta + \pi_i^\eta = 0; \\ \oint_{\partial\Omega_0} t_j^\xi dA_0 + \int_{\Omega_0} \pi_j^\xi d\Omega_0 &= 0 \quad \Rightarrow \quad \nabla_0 \cdot \mathbf{s}_j^\xi + \pi_j^\xi = 0. \end{aligned} \quad (24)$$

2.3.3 Energy

Denote by U and Ψ the internal energy and Helmholtz free energy per unit reference volume, respectively. Let $T > 0$ denote the absolute temperature, and let S denote the entropy per unit reference volume. The usual relationship among these variables

is enforced:

$$U = \Psi + TS. \quad (25)$$

The global balance of energy is stated as follows, accounting for external work due to microscopic surface forces as in other works^{28,51} where here summation is implied over $i = 1, \dots, k$ and $j = 1, \dots, l$:

$$\begin{aligned} \frac{d}{dt} \int_{\Omega_0} U d\Omega_0 + \frac{d}{dt} \int_{\Omega_0} \frac{1}{2} \rho_0 \mathbf{v} \cdot \mathbf{v} d\Omega_0 = \\ \oint_{\partial\Omega_0} \mathbf{t}_0 \cdot \mathbf{v} dA_0 + \oint_{\partial\Omega_0} t_i^\eta \dot{\eta}^i dA_0 + \oint_{\partial\Omega_0} t_i^\xi \dot{\xi}^i dA_0 - \oint_{\partial\Omega_0} \mathbf{Q} \cdot \mathbf{N} dA_0. \end{aligned} \quad (26)$$

The left side is the global rate of internal energy change plus kinetic energy change. The right side accounts for work done by macroscopic and microscopic tractions and heat transfer from $\mathbf{Q}$, the heat flux vector per unit reference area. The local form of Eq. 26 obtained from the divergence theorem and Eqs. 21, 23, and 24 is

$$\dot{U} = \mathbf{P} : \dot{\mathbf{F}} + \mathbf{s}_i^\eta \cdot \nabla_0 \dot{\eta}^i + \mathbf{s}_j^\xi \cdot \nabla_0 \dot{\xi}^j - \pi_i^\eta \dot{\eta}^i - \pi_j^\xi \dot{\xi}^j - \nabla_0 \cdot \mathbf{Q}. \quad (27)$$

Note that ∇_0 and the material time derivative commute. The global and local entropy inequalities are of the usual form^{51,79} in the absence of point heat sources:

$$\frac{d}{dt} \int_{\Omega_0} S d\Omega_0 \geq - \oint_{\partial\Omega_0} \frac{1}{T} \mathbf{Q} \cdot \mathbf{N} dA_0 \quad \Rightarrow \quad T \dot{S} + \nabla_0 \cdot \mathbf{Q} - \frac{1}{T} \mathbf{Q} \cdot \nabla_0 T \geq 0. \quad (28)$$

The local internal dissipation is defined as follows using Eqs. 25 and 26:

$$\mathfrak{D} = T \dot{S} + \nabla_0 \cdot \mathbf{Q} = \mathbf{P} : \dot{\mathbf{F}} + \mathbf{s}_i^\eta \cdot \nabla_0 \dot{\eta}^i + \mathbf{s}_j^\xi \cdot \nabla_0 \dot{\xi}^j - \pi_i^\eta \dot{\eta}^i - \pi_j^\xi \dot{\xi}^j - \dot{\Psi} - \dot{T} S. \quad (29)$$

Assume Fourier conduction in the spatial configuration, where $\mathbf{k}$ is a symmetric and positive-definite conductivity tensor, not necessarily constant, and where $\mathbf{q} = J^{-1} \mathbf{F} \mathbf{Q}$ is the spatial heat flux vector:

$$\mathbf{q} = -\mathbf{k} \nabla T \quad \Rightarrow \quad -\mathbf{Q} \cdot \nabla_0 T = J \nabla T \cdot \mathbf{k} \cdot \nabla T \geq 0. \quad (30)$$

Then the local version of the second law in Eq. 28 reduces to the constraint of non-negative internal dissipation:

$$\mathfrak{D} \geq 0. \quad (31)$$

2.4 Constitutive Theory

Functional forms of constitutive variables are posited, leading to constitutive equations consistent with the balance equations and inequalities of Section 2.3. More specific thermoelastic equations and material coefficients are then derived.

2.4.1 Thermodynamic Potentials and Dissipation

The following functional forms are assumed for free and internal energy densities:

$$\begin{aligned} \Psi &= \Psi(\mathbf{F}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T), \\ U &= U(\mathbf{F}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, S) \quad (i = 1, \dots, k; j = 1, \dots, l). \end{aligned} \quad (32)$$

For brevity, a homogeneous material region in Ω_0 is assumed such that properties do not depend explicitly on $\mathbf{X}$. Dependence on total deformation gradient $\mathbf{F}$, used here to streamline derivations, is replaced by dependence on an objective thermoelastic strain measure later in Section 2.4.2. Macroscopic constitutive variables $\mathbf{P}$ and S depend on the same arguments as free energy, while microscopic forces $\mathbf{s}$ and π are, at least initially, allowed to depend on rates of order parameters:

$$\mathbf{P} = \mathbf{P}(\mathbf{F}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T), \quad S = S(\mathbf{F}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T); \quad (33)$$

$$\begin{aligned} \mathbf{s}_i^\eta &= \mathbf{s}_i^\eta(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T), \quad \mathbf{s}_j^\xi = \mathbf{s}_j^\xi(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T); \\ \pi_i^\eta &= \pi_i^\eta(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T), \quad \pi_j^\xi = \pi_j^\xi(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T). \end{aligned} \quad (34)$$

Expansion of the rate of free energy in Eq. 32 followed by substitution into Eqs. 29 and 31 gives

$$\begin{aligned} \mathfrak{D} &= \left(\mathbf{P} - \frac{\partial \Psi}{\partial \mathbf{F}} \right) : \dot{\mathbf{F}} - \left(S + \frac{\partial \Psi}{\partial T} \right) \dot{T} + \left(\mathbf{s}_i^\eta - \frac{\partial \Psi}{\partial \nabla_0 \eta^i} \right) \cdot \nabla_0 \dot{\eta}^i \\ &\quad + \left(\mathbf{s}_j^\xi - \frac{\partial \Psi}{\partial \nabla_0 \xi^j} \right) \cdot \nabla_0 \dot{\xi}^j - \left(\pi_i^\eta + \frac{\partial \Psi}{\partial \eta^i} \right) \dot{\eta}^i - \left(\pi_j^\xi + \frac{\partial \Psi}{\partial \xi^j} \right) \dot{\xi}^j \geq 0. \end{aligned} \quad (35)$$

The first four products following the equality in Eq. 35 must vanish identically since arguments in parentheses do not depend on rates $\dot{\mathbf{F}}, \dot{T}, \nabla_0 \dot{\eta}^i, \nabla_0 \dot{\xi}^j$:

$$\mathbf{P} = \frac{\partial \Psi}{\partial \mathbf{F}}, \quad S = -\frac{\partial \Psi}{\partial T}; \quad \mathbf{s}_i^\eta = \frac{\partial \Psi}{\partial \nabla_0 \eta^i}, \quad \mathbf{s}_j^\xi = \frac{\partial \Psi}{\partial \nabla_0 \xi^j}. \quad (36)$$

Define the dissipative forces $\hat{\pi}_i^\eta$ and $\hat{\pi}_j^\xi$ as the negative sum of two terms multiplying the order parameter rates:

$$\begin{aligned} & \hat{\pi}_i^\eta(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) \\ &= -[\pi_i^\eta(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) + \partial \Psi(\mathbf{F}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T)/\partial \eta^i], \\ & \hat{\pi}_j^\xi(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) \\ &= -[\pi_j^\xi(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) + \partial \Psi(\mathbf{F}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T)/\partial \xi^j]. \end{aligned} \quad (37)$$

Then the local dissipation inequality reduces to

$$\begin{aligned} \mathfrak{D} &= \hat{\pi}_i^\eta(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) \dot{\eta}^i \\ &+ \hat{\pi}_j^\xi(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) \dot{\xi}^j \geq 0. \end{aligned} \quad (38)$$

Let $T = T(\mathbf{F}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, S)$. Then making a Legendre transformation^{79,91} with Eq. 25 and using Eq. 36,

$$\begin{aligned} \mathbf{P} &= \frac{\partial U}{\partial \mathbf{F}}, \quad T = \frac{\partial U}{\partial S}; \\ \mathbf{s}_i^\eta &= \frac{\partial U}{\partial \nabla_0 \eta^i}, \quad \mathbf{s}_j^\xi = \frac{\partial U}{\partial \nabla_0 \xi^j}; \quad \hat{\pi}_i^\eta = -\pi_i^\eta - \frac{\partial U}{\partial \eta^i}, \quad \hat{\pi}_j^\xi = -\pi_j^\xi - \frac{\partial U}{\partial \xi^j} \end{aligned} \quad (39)$$

are constitutive equalities in terms of entropy rather than temperature as an independent variable.

2.4.2 Logarithmic Thermoelasticity

Dependence of constitutive variables on $\mathbf{F}$ is now replaced with dependence on logarithmic thermoelastic strain $\mathbf{e}^E$ of Eq. 19. The latter, with components referred to intermediate configuration $\bar{\Omega}$, is objective under rotations of the spatial coordinate system so long as the chosen $\bar{\mathbf{g}}_\alpha$ are invariant. First, note for future reference that

$$\mathbf{e}^E(\mathbf{F}, \eta^i, \xi^j) = \frac{1}{2} \ln \left(\left[\mathbf{F} \bar{\mathbf{F}}^{-1}(\eta^i, \xi^j) \right]^T \left[\mathbf{F} \bar{\mathbf{F}}^{-1}(\eta^i, \xi^j) \right] \right). \quad (40)$$

Thus,

$$\begin{aligned} \frac{\partial \mathbf{e}^E}{\partial \mathbf{F}} &= \frac{\partial \mathbf{e}^E}{\partial \mathbf{C}^E} : \frac{\partial \mathbf{C}^E}{\partial \mathbf{F}^E} : \frac{\partial \mathbf{F}^E}{\partial \mathbf{F}} = \mathbf{M}^E : [(\mathbf{F}^E)^T \otimes \bar{\mathbf{F}}^{-1}] \\ &\leftrightarrow \frac{\partial e_{\alpha\beta}^E}{\partial F_J^i} = \frac{\partial \ln C_{\alpha\beta}^E}{\partial C_{\gamma\delta}^E} [(F^E)_\delta^k g_{ik} (\bar{\mathbf{F}}^{-1})_\gamma^J], \end{aligned} \quad (41)$$

where $(\mathbf{M}^E)_{\alpha\beta}^{\gamma\delta} = \partial \ln C_{\alpha\beta}^E / \partial C_{\gamma\delta}^E$ can be calculated via algorithms discussed elsewhere.^{55,89,90} A change of independent variables between $\mathbf{F}$ and $\mathbf{e}^E$ with definitions Eq. 14 leads to the following general formulae:

$$\left. \frac{\partial(\cdot)}{\partial \eta^i} \right|_{\mathbf{F}} = \left. \frac{\partial(\cdot)}{\partial \eta^i} \right|_{\mathbf{e}^E} + \left. \frac{\partial(\cdot)}{\partial \mathbf{e}^E} \right|_{\eta^i} : \left. \frac{\partial \mathbf{e}^E}{\partial \eta^i} \right|_{\mathbf{F}} = \left. \frac{\partial(\cdot)}{\partial \eta^i} \right|_{\mathbf{e}^E} - \left. \frac{\partial(\cdot)}{\partial \mathbf{e}^E} \right|_{\eta^i} : \mathbf{M}^E : (\mathbf{C}^E A_i^\eta \bar{\mathbf{F}}^{-1}), \quad (42)$$

$$\left. \frac{\partial(\cdot)}{\partial \xi^j} \right|_{\mathbf{F}} = \left. \frac{\partial(\cdot)}{\partial \xi^j} \right|_{\mathbf{e}^E} + \left. \frac{\partial(\cdot)}{\partial \mathbf{e}^E} \right|_{\xi^j} : \left. \frac{\partial \mathbf{e}^E}{\partial \xi^j} \right|_{\mathbf{F}} = \left. \frac{\partial(\cdot)}{\partial \xi^j} \right|_{\mathbf{e}^E} - \left. \frac{\partial(\cdot)}{\partial \mathbf{e}^E} \right|_{\xi^j} : \mathbf{M}^E : (\mathbf{C}^E A_j^\xi \bar{\mathbf{F}}^{-1}). \quad (43)$$

Free and internal energy densities per unit reference volume are now expressed as the following potentials for logarithmic thermoelasticity:

$$\begin{aligned} \Psi &= \hat{\Psi}(\mathbf{e}^E, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T), \\ U &= \hat{U}(\mathbf{e}^E, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, S) \quad (i = 1, \dots, k; j = 1, \dots, l). \end{aligned} \quad (44)$$

Define the symmetric thermodynamic conjugate stress tensor Σ , with components $\Sigma^{\alpha\beta}$ as follows, and note from Eqs. 36 and 39 that the constitutive relations for entropy and temperature still apply:

$$\Sigma = \frac{\partial \hat{\Psi}}{\partial \mathbf{e}^E} = \frac{\partial \hat{U}}{\partial \mathbf{e}^E}, \quad S = -\frac{\partial \hat{\Psi}}{\partial T}, \quad T = \frac{\partial \hat{U}}{\partial S}. \quad (45)$$

The first and second equalities in Eq. 45 are verified subsequently in conjunction with Eqs. 36 and 39. The first Piola–Kirchhoff stress obeys, from Eqs. 36, 44, and 45,

$$\begin{aligned} \mathbf{P} &= \Sigma : \frac{\partial \mathbf{e}^E}{\partial \mathbf{F}} = \Sigma : \mathbf{M}^E : [(\mathbf{F}^E)^T \otimes \bar{\mathbf{F}}^{-1}] = \mathbf{F}^E (\Sigma : \mathbf{M}^E) \bar{\mathbf{F}}^{-T} \\ &\leftrightarrow P^{iJ} = (F^E)_\delta^i [\Sigma^{\alpha\beta} (\mathbf{M}^E)_{\alpha\beta}^{\delta\gamma}] (\bar{\mathbf{F}}^{-1})_\gamma^J. \end{aligned} \quad (46)$$

For Eq. 46 to hold simultaneously with Eqs. 36 and 39, both equalities for stress in

Eq. 45 must be true as well. Cauchy stress is then^{55,72}

$$\boldsymbol{\sigma} = J^{-1} \mathbf{F}^E (\boldsymbol{\Sigma} : \mathbf{M}^E) (\mathbf{F}^E)^T. \quad (47)$$

Dissipative forces in Eq. 37 become, with Eqs. 42 and 43,

$$\begin{aligned} \hat{\pi}_i^\eta &= - \left[\pi_i^\eta + \frac{\partial \hat{\Psi}}{\partial \eta^i} \Big|_{\mathbf{e}^E} - \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E \mathbf{A}_i^\eta \bar{F}^{-1}) \right], \\ \hat{\pi}_j^\xi &= - \left[\pi_j^\xi + \frac{\partial \hat{\Psi}}{\partial \xi^j} \Big|_{\mathbf{e}^E} - \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E \mathbf{A}_j^\xi \bar{F}^{-1}) \right], \end{aligned} \quad (48)$$

where thermoelastic driving forces for structural changes or fractures are the third terms on the right sides of each.

Thermoelastic coefficients are defined as follows. Second-order isothermal and isentropic moduli, not necessarily constants, are, respectively,

$$\mathbf{C}^T = \frac{\partial^2 \hat{\Psi}}{\partial \mathbf{e}^E \partial \mathbf{e}^E}, \quad \mathbf{C}^S = \frac{\partial^2 \hat{U}}{\partial \mathbf{e}^E \partial \mathbf{e}^E}. \quad (49)$$

Denote the second-order tensor of thermal expansion coefficients by $\mathbf{a}^E$, thermal stress coefficients by $\boldsymbol{\alpha}^E$, the Grüneisen tensor by $\boldsymbol{\gamma}^E$, and specific heat per unit reference volume at constant strain by c^E :

$$\mathbf{a}^E = \frac{\partial \mathbf{e}^E}{\partial T}, \quad \boldsymbol{\alpha}^E = - \frac{\partial^2 \hat{\Psi}}{\partial \mathbf{e}^E \partial T} = c^E \boldsymbol{\gamma}^E, \quad c^E = \frac{\partial \hat{U}}{\partial T} = T \frac{\partial S}{\partial T} = -T \frac{\partial^2 \hat{\Psi}}{\partial T^2}. \quad (50)$$

Let c^Σ denote specific heat at constant stress. Relationships among thermoelastic coefficients include

$$\boldsymbol{\alpha}^E = \mathbf{a}^E : \mathbf{C}^T, \quad c^\Sigma = c^E + T \mathbf{a}^E : \boldsymbol{\alpha}^E, \quad \mathbf{C}^S = \mathbf{C}^T + (T/c^E) \boldsymbol{\alpha}^E \otimes \boldsymbol{\alpha}^E. \quad (51)$$

Define the collected set of order parameters and their gradients by $\mathbf{z}$, and the collected set of conjugate forces by $\boldsymbol{\zeta}$:

$$\mathbf{z} = \{\eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j\}, \quad \boldsymbol{\zeta} = - \frac{\partial \hat{\Psi}}{\partial \mathbf{z}}. \quad (52)$$

The product of temperature and entropy rate can then be expressed as follows, not-

ing $S = S(\mathbf{e}^E, T, \mathbf{z}) = -\partial\hat{\Psi}/\partial T$:

$$\begin{aligned} T\dot{S} &= T \frac{\partial S}{\partial \mathbf{e}^E} : \dot{\mathbf{e}}^E + T \frac{\partial S}{\partial \mathbf{z}} : \dot{\mathbf{z}} + T \frac{\partial S}{\partial T} \dot{T} \\ &= -T \frac{\partial^2 \hat{\Psi}}{\partial T \partial \mathbf{e}^E} : \dot{\mathbf{e}}^E - T \frac{\partial^2 \hat{\Psi}}{\partial T \partial \mathbf{z}} : \dot{\mathbf{z}} - T \frac{\partial^2 \hat{\Psi}}{\partial T^2} \dot{T} = T \left(\boldsymbol{\alpha}^E : \dot{\mathbf{e}}^E + \frac{\partial \boldsymbol{\zeta}}{\partial T} : \dot{\mathbf{z}} \right) + c^E \dot{T}. \end{aligned} \quad (53)$$

2.4.3 Strain Energy, Phase Energy, and Gradient Energy Densities

More specific forms of free and internal energy densities are now prescribed for crystalline solids. Denote by W^Ψ and W^U two strain energy potentials per unit reference volume that contain all dependence of free and internal energy, respectively, on thermoelastic strain. Let f_η^Ψ and f_η^U denote collective phase energy potentials for the η^i and their gradients, and let f_ξ^Ψ and f_ξ^U denote collective phase energy potentials for the ξ^j and their gradients. Functional forms are assumed for free energy contributions as

$$\begin{aligned} \hat{\Psi}(\mathbf{e}^E, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) &= W^\Psi(\mathbf{e}^E, \eta^i, \xi^j, T) + f_\eta^\Psi(\eta^i, \xi^j, \nabla_0 \eta^i, T) \\ &\quad + f_\xi^\Psi(\eta^i, \xi^j, \nabla_0 \xi^j, T), \end{aligned} \quad (54)$$

and for internal energy contributions as

$$\begin{aligned} \hat{U}(\mathbf{e}^E, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, S) &= W^U(\mathbf{e}^E, \eta^i, \xi^j, S) + f_\eta^U(\eta^i, \xi^j, \nabla_0 \eta^i, S) \\ &\quad + f_\xi^U(\eta^i, \xi^j, \nabla_0 \xi^j, S). \end{aligned} \quad (55)$$

Coupling is enabled for order parameters but not their spatial gradients among the phase energy functions f_η, f_ξ . More general forms are possible, but the present ones are sufficient for this work. Phase energy functions are further decomposed into bulk- and gradient-dependent contributions. For free energy,

$$f_\eta^\Psi(\eta^i, \xi^j, \nabla_0 \eta^i, T) = f_{\eta 0}^\Psi(\eta^i, \xi^j, T) + f_{\eta \nabla}^\Psi(\eta^i, \xi^j, \nabla_0 \eta^i, T), \quad (56)$$

$$f_\xi^\Psi(\eta^i, \xi^j, \nabla_0 \xi^j, T) = f_{\xi 0}^\Psi(\eta^i, \xi^j, T) + f_{\xi \nabla}^\Psi(\eta^i, \xi^j, \nabla_0 \xi^j, T). \quad (57)$$

For internal energy,

$$f_\eta^U(\eta^i, \xi^j, \nabla_0 \eta^i, S) = f_{\eta 0}^U(\eta^i, \xi^j, S) + f_{\eta \nabla}^U(\eta^i, \xi^j, \nabla_0 \eta^i, S), \quad (58)$$

$$f_{\xi}^U(\eta^i, \xi^j, \nabla_0 \eta^i, S) = f_{\xi_0}^U(\eta^i, \xi^j, S) + f_{\xi \nabla}^U(\eta^i, \xi^j, \nabla_0 \xi^j, S). \quad (59)$$

When η^i are associated with phase transformations or deformation twins, a double-well potential in the η^i is common for the f_{η_0} functions.^{17,20,92} When ξ^j are associated with fracture mechanisms, a quadratic potential in the ξ_j is common for the f_{ξ_0} functions.^{10,11,34,36} Quadratic functions of order parameter gradients ($f_{\eta \nabla}$, $f_{\xi \nabla}$) are typically used for any transformation or fracture mechanisms.^{4,11,17,20,34,36,38,39,92,93}

From Eqs. 55–59, more specific forms of thermodynamic forces can be derived from relations introduced in Sections 2.4.1 and 2.4.2:

$$\Sigma = \frac{\partial W^{\Psi}}{\partial \mathbf{e}^E} = \frac{\partial W^U}{\partial \mathbf{e}^E}; \quad (60)$$

$$\mathbf{s}_i^{\eta} = \frac{\partial f_{\eta \nabla}^{\Psi}}{\partial \nabla_0 \eta^i} = \frac{\partial f_{\eta \nabla}^U}{\partial \nabla_0 \eta^i}, \quad \mathbf{s}_j^{\xi} = \frac{\partial f_{\xi \nabla}^{\Psi}}{\partial \nabla_0 \xi^j} = \frac{\partial f_{\xi \nabla}^U}{\partial \nabla_0 \xi^j}; \quad (61)$$

$$\begin{aligned} \hat{\pi}_i^{\eta} &= - \left[\pi_i^{\eta} + \frac{\partial(W^{\Psi} + f_{\eta}^{\Psi} + f_{\xi}^{\Psi})}{\partial \eta^i} - \Sigma : \mathbf{M}^E : (\mathbf{C}^E A_i^{\eta} \bar{F}^{-1}) \right], \\ \hat{\pi}_j^{\xi} &= - \left[\pi_j^{\xi} + \frac{\partial(W^{\Psi} + f_{\eta}^{\Psi} + f_{\xi}^{\Psi})}{\partial \xi^j} - \Sigma : \mathbf{M}^E : (\mathbf{C}^E A_j^{\xi} \bar{F}^{-1}) \right]. \end{aligned} \quad (62)$$

2.5 Order Parameter Kinetics

2.5.1 TDGL Model

Extending prior theory⁵¹ to the case with multiple order parameters, non-negative dissipation can be ensured in Eq. 38 via prescription of dissipative forces of the following forms:

$$\begin{aligned} \hat{\pi}_i^{\eta}(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) &= \sum_{i,m=1}^k \hat{\beta}_{im}^{\eta}(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) \eta^m, \\ \hat{\pi}_j^{\xi}(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) &= \sum_{j,n=1}^l \hat{\beta}_{jn}^{\xi}(\mathbf{F}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) \xi^n, \end{aligned} \quad (63)$$

where $\hat{\beta}^{\eta}$ and $\hat{\beta}^{\xi}$ are symmetric and positive semi-definite. These quantities are, respectively, $k \times k$ and $l \times l$ matrices of kinetic viscosities that are, in general, functions of their indicated arguments. Then the dissipation inequality of Eq. 38

reduces to the following expression that is now always true, where summation is implied on repeated indices for each family of order parameters:

$$\mathfrak{D} = \hat{\beta}_{im}^{\eta} \dot{\eta}^i \dot{\eta}^m + \hat{\beta}_{jn}^{\xi} \dot{\xi}^j \dot{\xi}^n \geq 0. \quad (64)$$

From Eqs. 48 and 63,

$$\begin{aligned} \pi_i^{\eta} &= - \left[\hat{\beta}_{im}^{\eta} \dot{\eta}^m - \frac{\partial \Psi}{\partial \eta^i} \Big|_{\mathbf{F}} \right] = - \left[\hat{\beta}_{im}^{\eta} \dot{\eta}^m - \frac{\partial \hat{\Psi}}{\partial \eta^i} \Big|_{\mathbf{e}^E} + \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E A_i^{\eta} \bar{F}^{-1}) \right]; \\ \pi_j^{\xi} &= - \left[\hat{\beta}_{jn}^{\xi} \dot{\xi}^n - \frac{\partial \Psi}{\partial \xi^j} \Big|_{\mathbf{F}} \right] = - \left[\hat{\beta}_{jn}^{\xi} \dot{\xi}^n - \frac{\partial \hat{\Psi}}{\partial \xi^j} \Big|_{\mathbf{e}^E} + \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E A_j^{\xi} \bar{F}^{-1}) \right]. \end{aligned} \quad (65)$$

Now substitute Eqs. 61 and 65 into the microscopic force balances of Eq. 24:

$$\begin{aligned} \hat{\beta}_{im}^{\eta} \dot{\eta}^m &= - \frac{\delta \Psi}{\delta \eta^i} = - \left[\frac{\partial \Psi}{\partial \eta^i} \Big|_{\mathbf{F}} - \nabla_0 \cdot \frac{\partial \Psi}{\partial \nabla_0 \eta^i} \right] \\ &= - \left[\frac{\partial \hat{\Psi}}{\partial \eta^i} \Big|_{\mathbf{e}^E} - \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E A_i^{\eta} \bar{F}^{-1}) - \nabla_0 \cdot \frac{\partial f_{\eta}^{\Psi}}{\partial \nabla_0 \eta^i} \right]; \\ \hat{\beta}_{jn}^{\xi} \dot{\xi}^n &= - \frac{\delta \Psi}{\delta \xi^j} = - \left[\frac{\partial \Psi}{\partial \xi^j} \Big|_{\mathbf{F}} - \nabla_0 \cdot \frac{\partial \Psi}{\partial \nabla_0 \xi^j} \right] \\ &= - \left[\frac{\partial \hat{\Psi}}{\partial \xi^j} \Big|_{\mathbf{e}^E} - \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E A_j^{\xi} \bar{F}^{-1}) - \nabla_0 \cdot \frac{\partial f_{\xi}^{\Psi}}{\partial \nabla_0 \xi^j} \right]. \end{aligned} \quad (66)$$

When $\hat{\beta}^{\eta}$ and $\hat{\beta}^{\xi}$ are positive-definite and thus invertible, Eq. 66 can be rearranged to provide kinetic equations for all order parameter rates. The notation for variational derivatives $\delta(\cdot)/\delta \eta^i$ and $\delta(\cdot)/\delta \xi^j$ is standard in representations of the TDGL equations,^{39,51} of which Eq. 66 are examples.

The energy balance can be manipulated into a temperature evolution law. Inserting Eq. 53 into the first of Eq. 29, whereby $T \dot{S} = \mathfrak{D} - \nabla_0 \cdot \mathbf{Q}$, produces

$$c^E \dot{T} = \mathfrak{D} - T \left(\boldsymbol{\alpha}^E : \dot{\mathbf{e}}^E + \frac{\partial \zeta}{\partial T} : \dot{\mathbf{z}} \right) + J \nabla \cdot (\mathbf{k} \nabla T). \quad (67)$$

The internal dissipation $\mathfrak{D}$ is given by Eq. 64 for TDGL-type kinetics. Stress power due to inelastic deformation from order parameter rates is embedded in $\mathfrak{D}$ on the right side of Eq. 67, as can be surmised from the rightmost forms in braces in Eq. 66.

Thermoelastic and thermal-phase coupling are in parentheses, and the rightmost term in Eq. 67 accounts for Fourier heat conduction, where $\nabla_0 \cdot \mathbf{Q} = J \nabla \cdot \mathbf{q}$ from Eq. 10.⁷⁹

2.5.2 Irreversibility and Initiation Threshold

Non-negative dissipation is always ensured if Eq. 63 is used, regardless of the signs of order parameter rates $\dot{\eta}^i$ and $\dot{\xi}^j$. When Eq. 66 is implemented for phase kinetics, order parameter values may locally increase or decrease with increasing time according to the signs of driving forces $\delta\Psi/\delta\eta^i$ and $\delta\Psi/\delta\xi^j$. However, in many cases, it is more physically appropriate to restrict transformations to be one-way, such that order parameter rates are always non-negative. Twinning, dislocation motion, and especially fractures are often irreversible in this sense, depending on how order parameters are physically interpreted in terms of inelastic mechanisms. Furthermore, the standard TDGL kinetic laws, and their quasi-static balance laws in the limit of infinite viscosity $||\hat{\beta}|| \rightarrow \infty$, permit nucleation of transformations or fractures without any independent or intrinsic thresholds, depending upon the choices of energy functionals.

A physically realistic and thermodynamically admissible alternative to TDGL-type kinetics in Eq. 63 is postulated as follows. Consider fracture order parameters ξ^j , whose evolution can be constrained to be irreversible by replacing the second of Eq. 66 with

$$\begin{aligned}\dot{\xi}^n &= \left\langle (\hat{\beta}_{jn}^\xi)^{-1} [\mathcal{F}_j - \mathcal{R}_j] \right\rangle H(\hat{\pi}_n^\xi) \geq 0; \\ \mathcal{F}_j &= \mathcal{F}_j \left(\underset{s \in [0, t]}{\mathbf{F}_j} (\mathbf{e}^E(s), S(s), \mathbf{z}(s), \nabla_0 \mathbf{z}(s)) \right) \geq 0, \\ \mathcal{R}_j &= \mathcal{R}_j \left(\underset{s \in [0, t]}{\mathbf{R}_j} (\mathbf{e}^E(s), S(s), \mathbf{z}(s), \nabla_0 \mathbf{z}(s)) \right).\end{aligned}\tag{68}$$

The Macauley bracket operator parses positive values: $\langle(\cdot)\rangle = \frac{1}{2}[(\cdot) + |(\cdot)|]$, and $\hat{\beta}^\xi$ is still symmetric and but now positive-definite by construction, such that it is always invertible. The functional $\mathcal{F}_j$ is a bounded non-negative driving force that depends on the history of local state function $\mathbf{F}_j$. The functional $\mathcal{R}_j$ is a crack resistance, not necessarily always non-negative, that depends on the history of local state function $\mathbf{R}_j$. The Heaviside function H ensures that $\dot{\xi}^n$ is nonzero only when

its conjugate thermodynamic force $\hat{\pi}_n^\xi$ is non-negative [here $H(x) = 1 \forall x \geq 0$], ensuring non-negative dissipation from fracture. Similar ideas have been implemented for phase field fracture modeling published elsewhere,^{28,35} with a history-dependent driving force, but with fracture resistance depending only on current state. For example, $\mathcal{F}$ can be associated with some maximally attained measure of local strain energy density, which when smaller than $\mathcal{R}$, allows for deformation processes that are essentially “elastic to failure” in brittle solids, as opposed to gradual damage accumulation and strain softening that may arise in more standard formulations.¹¹ These differences are examined explicitly later in example problems of Section 5.

Consistency with the remaining theory of Sections 2.1–2.4 is then achieved as follows. Equations 63–66 do not apply, but from Eq. 24,

$$\hat{\pi}_j^\xi = - \left[\frac{\partial \Psi}{\partial \xi^j} \Big|_F + \pi_j^\xi \right] = - \left[\frac{\partial \Psi}{\partial \xi^j} \Big|_F - \nabla_0 \cdot \frac{\partial \Psi}{\partial \nabla_0 \xi^j} \right]. \quad (69)$$

The contribution to $\mathfrak{D}$ in Eq. 67 from this fracture kinetic model is $\hat{\pi}_j^\xi \dot{\xi}^j \geq 0$. This treatment generalizes the irreversible time-dependent theory of Miehe et al.⁹⁴ to the case of multiple fracture order parameters. Generalized irreversible kinetics for the $\dot{\eta}^i$ can be enforced the same way as in Eq. 68 if physically justified.

2.5.3 Remarks on Localization and Interface Velocities

Depending on boundary and initial conditions, localized deformations are often energetically favorable over homogeneous deformations once a critical magnitude of driving force for structural transformation or fracture is attained. Such localized deformation can be expected regardless of dissipative thermal effects, due to elastic energy release from fracture,^{11,35} or to strain accommodation from twinning⁹⁵ or phase transformations involving eigenstrain. The present model, with irreversible kinetics and corresponding viscosities, further accounts for dissipation in the energy balance, leading to potential local temperature rise under adiabatic conditions pertinent to high-strain rate loading. The model allows for temperature dependence of surface energies as well as viscosities. If surface energy or viscosity decreases with increasing temperature (e.g., the latter is physically realistic for [partial]-dislocation mediated transformations including twinning), then adiabatic heating will accelerate strain localization. However, brittle fracture could simultaneously be impeded if a ductile-brittle transition is incorporated in the treatment of fracture surface energy.

The kinetic models in Sections 2.5.1 and 2.5.2 are of standard gradient-flow type, though the latter further incorporate irreversibility and potential threshold constraints on initiation. These models are not enabled with any novel means of addressing supersonic interface velocities. As noted elsewhere,²² existence of interface velocities that exceed the sound velocity of the softer phase in a structural transformation is possible, in general. However, standard phase field kinetic models are unable to support steady velocities of such supersonic interfaces, and spurious results can be expected when they are used in this context for numerical calculations. The same limitations apply for the present theory, whereby treatment of moving phase boundaries should be restricted to the subsonic domain. In calculations of Section 7, existence of a steady structured shock wave moving at Lagrangian velocity D is assumed a priori. In the rising waveform, order parameter fields vary rapidly, as in a phase boundary. Nucleation and growth (e.g., of micro-cracks, slipped regions, or transformation zones) take place simultaneously within the rising waveform. The nonlinear solution demands that $D < (C_l^t/\rho_0)^{1/2}$ in Eq. 274, i.e., that the waveform (moving interface) always travels subsonically with respect to the tangent longitudinal modulus C_l^t .

Now consider crack tip propagation velocities. Prior numerical studies⁹⁶ invoking standard, non-dissipative phase field fracture models in elastodynamics correctly predict mode I crack speeds lower than the limiting Rayleigh wave speed, albeit often higher than those observed experimentally. Viscous dissipation could be added, as available in the present framework, to reduce speeds to realistic levels. Mode II (shear) cracks can propagate along weak planes at intersonic speeds, i.e., faster than the shear wave speed but slower than the longitudinal wave speed, in both experiments and in simulation results of non-dissipative phase field elastodynamics.⁹⁷ Since local elastic strain energy density drives fracture in all such models, the present theory of Sections 2.5.1 and 2.5.2 should offer crack velocity predictions consistent with prior work^{96,97} so long as local driving forces remain sufficient to overcome any prescribed initiation thresholds in the latter case. Increasing viscosities are expected to slow crack propagation and could inhibit intersonic shear fractures. Even in the case of intersonic fracture, cracks always travel slower than the longitudinal wave speed,⁹⁷ consistent with limitations of standard gradient-flow phase field models for generic moving interfaces discussed earlier.

2.6 Third-Order Elasticity

Representative nonlinear constitutive models are now provided for later use on specific material systems in Section 4 and for comparison with their linearized representations derived in Section 3. The general model framework of Section 2.6.1 is applicable to anisotropic or isotropic solids, in single crystalline or polycrystalline forms. Specialization to isotropy, physically most appropriate for random polycrystalline aggregates, follows in Section 2.6.2.

2.6.1 General Formulation

Voigt notation is now adopted for brevity of representation of symmetric second-, fourth-, and sixth-order tensors. Thereby, subscripts $A, B, C, \dots$ that run from 1 to 6 replace symmetric pairs of Greek indices $(\cdot)_{\alpha\beta} \leftrightarrow (\cdot)_A$, etc. Correspondences are

$$11 \leftrightarrow 1, \quad 22 \leftrightarrow 2, \quad 33 \leftrightarrow 3, \quad 23 = 32 \leftrightarrow 4, \quad 13 = 31 \leftrightarrow 5, \quad 12 = 21 \leftrightarrow 6. \quad (70)$$

Stresses and stiffness components retain the same magnitudes in full and Voigt forms. Shear components of strain or compliance may vary by factors of two or four between notation schemes, e.g., $e_4^E = 2e_{23}^E$. Details can be found in several monographs.^{79,98}

An internal energy formulation is presented for subsequent advantageous use in dynamic problems. A reference state from which internal energy and state variable changes are measured is stress- and elastic strain-free ($\Sigma = \mathbf{e}^E = \mathbf{0}$), and is characterized by a datum temperature $T_0 > 0$ and datum entropy $S_0 = 0$, where the latter is chosen for convenience (in this case, $S < 0$ is admissible). Define an indicator function denoting elastic expansion (+1) versus contraction (0) by $\bar{\omega} = H(\text{tr } \mathbf{e}^E) = H(\ln J^E)$, where the Heaviside step function is $H(\cdot)$. The thermoelastic strain energy function is

$$W^U(\mathbf{e}^E, S, \eta^i, \xi^j) = \frac{1}{2} \mathbf{C}^{AB}(\eta^i, \xi^j, \bar{\omega}) e_A^E e_B^E + \frac{1}{6} \mathbf{C}^{ABC}(\eta^i, \xi^j, \bar{\omega}) e_A^E e_B^E e_C^E - T_0 [\gamma^A(\eta^i, \xi^j, \bar{\omega}) e_A^E S - h(S)]. \quad (71)$$

The purely entropic contribution to internal energy accounting for specific heat $c^E = c_0$, which is assumed constant irrespective of structural changes (phases)

or damage, is^{72,98}

$$T_0 h(S) = T_0 S \left[1 + \frac{1}{2} \frac{S}{c_0} + \frac{1}{6} \left(\frac{S}{c_0} \right)^2 + \dots \right]. \quad (72)$$

Certain classes of materials may require more elaborate potentials depending on the η^i to account for different specific heats of phases that can contribute to thermal driving forces for structural transformations.^{39,40,99}

Second- and third-order elastic coefficients are C^{AB} and C^{ABC} , respectively, and the Grüneisen parameters are γ^A . These are usually represented by constants in a homogeneous single crystalline phase,^{55,72} but here generally depend on order parameters. More specific forms are

$$\begin{aligned} C^{AB}(\eta^i, \xi^j, \bar{\omega}) &= C_0^{AB}(\eta^i) \cdot \chi(\xi^j) \cdot \bar{\omega} + C_R^{AB}(\eta^i) \cdot (1 - \bar{\omega}), \\ C^{ABC}(\eta^i, \xi^j, \bar{\omega}) &= C_0^{ABC}(\eta^i) \cdot \chi(\xi^j) \cdot \bar{\omega} + C_R^{ABC}(\eta^i) \cdot (1 - \bar{\omega}), \\ \gamma^A(\eta^i, \xi^j, \bar{\omega}) &= \gamma_0^A(\eta^i) \cdot \chi(\xi^j) \cdot \bar{\omega} + \gamma_R^A(\eta^i) \cdot (1 - \bar{\omega}). \end{aligned} \quad (73)$$

Functions $C_0^{AB}(\eta^i)$, $C_0^{ABC}(\eta^i)$, and $\gamma_0^A(\eta^i)$ smoothly interpolate for the isentropic elastic stiffness and Grüneisen parameters due to changes of crystal structure (e.g., as in solid phase transformations^{17,38}) or lattice orientation (e.g., as in deformation twinning^{20,86}). When $\eta^i = 1$, these parameters correspond to thermoelastic constants for crystals of pure phase i . The ground state is $\eta^i = 0 \forall i \geq 1 \Leftrightarrow \eta^0 = 1$, wherein these parameters correspond to thermoelastic constants of the parent phase. Representative functions are available elsewhere.^{17,20,38,99} Proposed here for interpolation among domains is^{20,38}

$$\begin{aligned} C_0^{AB}(\eta^i) &= C_{0|0}^{AB} + \sum_{i=1}^k (C_{0|i}^{AB} - C_{0|0}^{AB}) \cdot \eta^i [3\eta^i - 2(\eta^i)^2], \\ C_0^{ABC}(\eta^i) &= C_{0|0}^{ABC} + \sum_{i=1}^k (C_{0|i}^{ABC} - C_{0|0}^{ABC}) \cdot \eta^i [3\eta^i - 2(\eta^i)^2], \\ \gamma_0^A(\eta^i) &= \gamma_{0|0}^A + \sum_{i=1}^k (\gamma_{0|i}^A - \gamma_{0|0}^A) \cdot \eta^i [3\eta^i - 2(\eta^i)^2], \end{aligned} \quad (74)$$

where $C_{0|i}^{AB}$, $C_{0|i}^{ABC}$, and $\gamma_{0|i}^A$ are second-order isentropic elastic constants for phase or domain i , with $i = 0$ the parent phase. In local compression ($\bar{\omega} = 0$), certain elastic parameters may not degrade commensurate with fracture in the same way

as for tension ($\bar{\omega} = 1$). The residual thermoelastic coefficients $C_R^{AB}(\eta^i)$, $C_R^{ABC}(\eta^i)$, and $\gamma_R^A(\eta^i)$, which generally depend on crystal anisotropy,⁴⁸ account for stiffness that is maintained under compression, when $\bar{\omega} = 0$. For example, the bulk modulus is typically preserved under compressive fracture, whereas the shear moduli are not.^{7,11,34,48}

The degradation function $\chi(\xi^j) \in [\zeta_0, 1]$ is postulated as follows^{36,81}:

$$\chi(\xi^j) = \zeta_0 + (1 - \zeta_0) \prod_{j=1}^l (1 - \xi^j)^2. \quad (75)$$

This function presumes that different fracture mechanisms (e.g., cleavage on multiple planes) at the same material location X contribute in a geometric (i.e., multiplicative) way to strength reduction. The specific form of χ used here is augmented by the residual factor $0 < \zeta_0 \ll 1$ that preserves a minimal stiffness to avoid numerical instabilities when tangent stiffness would otherwise vanish entirely.^{34,36,44,81} The same function χ is used to modulate all second- and third-order elastic coefficients as well as all Grüneisen parameters. The latter choice is consistent with Eqs. 50 and 51 if thermal expansion coefficients and specific heat are unaffected by the ξ^j .

Now consider inelastic deformation $\bar{\mathbf{F}}$, where Eq. 12 is assumed to hold. Let the reference state with order parameter values $(\cdot)_0$ correspond to a homogeneous single-phase body, such that $\eta_0^i = 0 \forall i = 1, \dots, k$. Furthermore, assume that no fractures, voids, pores or other damage entities exist in the reference state, such that $\xi_0^j = 0 \forall j = 1, \dots, l$. Then

$$\mathbf{F}^\xi(\xi_0^j) = \mathbf{1}, \quad \mathbf{F}^\eta(\eta_0^i) = \mathbf{1} \quad \Rightarrow \quad \bar{\mathbf{F}}_0 = \mathbf{1}, \quad (i, j \geq 1), \quad (76)$$

where $\bar{\mathbf{F}}_0$ is the now null residual deformation of the reference state. Residual deformation from fracture and damage mechanisms embodied in $\mathbf{F}^\xi$ may generally be anisotropic and may include both shearing and normal separation on cleavage planes, for example.^{47,55,72,100,101} However, volume change from ξ is usually expansive, so long as no pore crushing takes place. Denote by $\bar{\varphi}$ the dilatation from damage (e.g., the inelastic free volume change induced from crack opening or cav-

itation). Measured per unit volume in configuration $\bar{\Omega}$,⁶¹

$$\bar{\varphi}(\xi^j) = 1 - \frac{1}{J^\xi(\xi^j)} = 1 - \frac{\sqrt{G}}{\sqrt{g} \det[\mathbf{F}^\xi(\xi^j)]} \Leftrightarrow \bar{J}(\xi^j) = \frac{1}{1 - \bar{\varphi}(\xi^j)}. \quad (77)$$

Residual deformation from structural changes embodied in $\mathbf{F}^\eta$ varies depending on the mechanisms quantified by the order parameters η^i . When these represent activity of deformation twinning systems,^{20,43} or of other simple shearing, slip, or shear localization modes on crystallographic planes,^{58,70} then $\mathbf{F}^\eta$ is isochoric with $J^\eta = 1$, but $\mathbf{F}^\eta$ is generally not symmetric, i.e., it includes non-negligible rotation. For other kinds of phase transformations, $\mathbf{F}^\eta$ is usually not isochoric, but it is often treated as symmetric, with all rotations embedded in $\mathbf{F}^E$.^{38,39,99}

Assume that damage ensues by cleavage fractures on l different low-energy crystallographic planes,⁸⁰ each characterized by a unit normal vector $\mathbf{M}^j$ in the reference configuration. Then the functions in Eq. 59 are prescribed as generalizations of those proposed in other works^{36,81}:

$$f_\xi^U(\eta^i, \xi^j, S) = \sum_{j=1}^l \frac{\Upsilon^j(\eta^i, T^e(S))}{l_\xi} (\xi^j)^2 + \sum_{j=1}^l \Upsilon^j(\eta^i, T^e(S)) \cdot l_\xi \cdot \boldsymbol{\omega}^j : (\nabla_0 \xi^j \otimes \nabla_0 \xi^j). \quad (78)$$

The first sum on the right is $f_{\xi 0}^U$, the second $f_{\xi \nabla}^U$. The regularization length l_ξ , which could be related to atomic-scale displacements in the vicinity of cleavage surfaces,^{102,103} is assumed identical among all crack systems j . The fracture surface energy per unit reference area is Υ^j , which generally depends on the family of cleavage plane (via j), the crystallographic phase (via η^i), and the effective temperature T^e , for example, accounting for a ductile-to-brittle transition. Since S , rather than T , is the independent thermal variable in the internal energy-based formulation, fracture surface energy is more conveniently parameterized by the temperature attained under stress-free conditions from Eq. 72:

$$T^e(S) = T_0 \frac{dh(S)}{dS} = T_0 \left[1 + \frac{S}{c_0} + \frac{1}{2} \left(\frac{S}{c_0} \right)^2 + \dots \right]. \quad (79)$$

The anisotropy tensor ω^j is defined as^{36,48,81}

$$\omega^j = \mathbf{1} + \hat{\alpha}^j \cdot (\mathbf{1} - \mathbf{M}^j \otimes \mathbf{M}^j), \quad (80)$$

where each $\hat{\alpha}^j \geq 0$ is a parameter, that when nonzero, penalizes fractures not occurring on planes $\mathbf{M}^j$. When $\hat{\alpha}^j = 0 \forall j$, then fracture energies are isotropic. Generalization of $f_{\xi \nabla}^U$ has been undertaken to account for other prescriptions of anisotropy in terms of structure tensors pertinent to the symmetry group of the material.¹⁰⁴ When the fracture energy is anisotropic, the effective width of the fracture zone varies from l_ξ according to the relative orientation of $\mathbf{M}^j$ to that of the fractured material region wherein $\xi^j > 0$.¹⁰⁴

Implicitly assumed in Eq. 78 is that energies associated with each cleavage plane j are decoupled and combine simply in an additive way. There is no energetic penalty, and conversely no energetic bonus, when multiple damage systems are operative at the same material point $\mathbf{X}$. A kinetic equation for fracture evolution (TDGL type) consistent with these assumptions is that of Eq. 66, where here decoupling manifests from $\hat{\beta}_{jn}^\xi \rightarrow \hat{\beta}_j^\xi \delta_{jn}$ (no sum on j):

$$\hat{\beta}_j^\xi \dot{\xi}^j = -\frac{\delta \Psi}{\delta \xi^j} = -\left[\frac{\partial \hat{\Psi}}{\partial \xi^j} \Big|_{e^E} - \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E \mathbf{A}_j^\xi \bar{\mathbf{F}}^{-1}) - \nabla_0 \cdot \frac{\partial f_{\xi \nabla}^U}{\partial \nabla_0 \xi^j} \right]. \quad (\text{no sum}) \quad (81)$$

In other words, the original matrix $\hat{\beta}_{jn}^\xi$ is now diagonal. The viscosity-type functions $\hat{\beta}_j^\xi$ (dimensions of stress·time) most generally can depend on all state variables as well as order parameter rates as in Eq. 63. In the current formulation, to allow for rate-, temperature-, and pressure-dependence of fractures that may vary with phase,

$$\hat{\beta}_j^\xi = \hat{\beta}_j^\xi(\dot{\xi}^j, T, p, \eta^i). \quad (82)$$

When $\hat{\beta}_j^\xi = 0 \forall j = 1, \dots, l$, then a rate-independent and non-dissipative formulation for fracture is recovered, whereby Eq. 81 produces the standard equilibrium equation for phase field fracture.^{34,45,49}

Finally consider the phase and gradient energy contributions from other structural transformations (solid-solid phase changes, deformation twinning, partial dislocation slip, etc.) that are embodied by order parameters η^i . The functions in Eq. 58

are posited as

$$f_{\eta^0}^U(\eta^i, \xi^j, S) = \hat{\chi}(\xi^j) \cdot \bar{f}_{\eta^0}^U(\eta^i, S), \quad (83)$$

$$f_{\eta^\nabla}^U(\nabla_0 \eta^i, S) = \hat{\chi}(\xi^j) \cdot \bar{f}_{\eta^\nabla}^U(\nabla_0 \eta^i, T^e(S)), \quad (84)$$

where degradation of phase and surface energy from damage is effected by setting $\hat{\chi} = \chi$ of Eq. 75.⁴⁴ Degradation of these energies is alternatively omitted when $\hat{\chi} = 1$ is prescribed. The phase energy $\bar{f}_{\eta^0}^U$ includes the energy barriers for homogeneous as well as stress-free (i.e., temperature- or entropy-driven) transformations. As noted already, assumed is that the unstressed reference state at $T = T_0$ and $S = 0$ is homogeneous of phase 0, i.e., $\eta^0 = 1$ and $\eta^i = 0 \forall i > 0$, and undamaged, $\xi^j = 0 \forall j$. If total internal energy $U = W^U + f_\eta^U + f_\xi^U$ is assumed to have a null reference value (i.e., $U_0 = 0$), then $\bar{f}_{\eta^0}^U(\eta^0 = 1, S = 0) = 0$, meaning a well exists at $\eta^0 = 1$. If η^i represent twin systems, then zero-energy wells also exist for any $\eta^i = 1$. A candidate energy function for twinning is²⁰

$$\begin{aligned} \bar{f}_{\eta^0}^U(\eta^i, T^e(S)) = & \sum_{i=1}^k 12 \frac{\Gamma^i(T^e(S))}{l_\eta} (\eta^i)^2 (1 - \eta^i)^2 \\ & + \sum_{i=1}^{k-1} \sum_{j=i+1}^k \frac{\Xi^{ij}(T^e(S))}{l_\eta} (\eta^i \eta^j)^2 (1 - \eta^i - \eta^j). \end{aligned} \quad (85)$$

The phase or twin boundary surface energy per unit reference area for isolated system i , relative to phase 0, is Γ^i , and is generally temperature dependent. Existence of more than two phases (e.g., at a triple point) is penalized by the function Ξ^{ij} . Similar constructions for martensitic transformations, including thermal barriers not contained in Eq. 85, are reported elsewhere.^{16,38,99} The regularization length l_η , which can be related to atomic perturbations near an interface,^{20,103} is assumed the same for all η^i for simplicity.

Assume that gradient interfacial energy $f_{\eta^\nabla}^U$ is isotropic, and that interface surface stresses do not exist. Then the following function is presumed:

$$\bar{f}_{\eta^\nabla}^U(\nabla_0 \eta^i, T^e(S)) = \sum_{i=1}^l \sum_{j=1}^l \frac{3}{4} \Gamma^{ij}(T^e(S)) \cdot l_\eta \cdot |\nabla_0 \eta^i| |\nabla_0 \eta^j|. \quad (86)$$

Matrix Γ^{ij} accounts for temperature-dependent surface energy associated with gradients of η^i and η^j . Generally, coupling is permissible between gradients of different order parameters $i \neq j$.⁴⁰ When energies are decoupled, as assumed for

twinning in,²⁰ but not necessarily equal among variants, then $\Gamma^{ij} = \Gamma^i \delta^{ij}$ (no sum). When energies are equal among variants, then $\Gamma^{ij} = \Gamma \delta^{ij}$. Generalization to include anisotropy and surface stresses is presented in the references.^{39,40,99}

A TDGL-type kinetic equation for phase evolution consistent with f_η^U is that inferred from Eq. 66, where coupling is admitted from nonzero off-diagonal entries of $\hat{\beta}_{im}^\eta$:

$$\hat{\beta}_{im}^\eta \dot{\eta}^m = -\frac{\delta \Psi}{\delta \eta^i} = -\left[\frac{\partial \hat{\Psi}}{\partial \eta^i} \Big|_{\mathbf{e}^E} - \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E \mathbf{A}_i^\eta \bar{\mathbf{F}}^{-1}) - \nabla_0 \cdot \frac{\partial f_{\eta \nabla}^U}{\partial \nabla_0 \eta^i} \right]. \quad (87)$$

$(i \geq 1; \text{ summation on } m = 1, \dots, k)$

Decoupled kinetics are attained if matrix $\hat{\beta}_{im}^\eta$ is prescribed diagonal. The viscosity-type functions $\hat{\beta}_{im}^\eta$ (dimensions of stress·time) most generally can depend on all state variables as well as order parameter rates as in Eq. 63. In the current formulation, analogous to Eq. 82, to allow for rate-, temperature-, and pressure-dependence of phase transformation kinetics or twinning modes that may vary with phase or domain,

$$\hat{\beta}_i^\eta = \hat{\beta}_i^\eta(\dot{\eta}^i, \eta^i, T, p). \quad (88)$$

When $\hat{\beta}_i^\eta = 0 \forall i = 1, \dots, k$, then a rate-independent and non-dissipative formulation for structural transformations is recovered. In that case, setting the right side of Eq. 87 equal to zero produces the standard equilibrium equation for twinning or solid phase changes.^{20,105}

2.6.2 Isotropy

The framework of Section 2.6.1 is now specialized to isotropic (e.g., certain polycrystalline) materials. Structural changes are characterized by a single order parameter $\eta = \eta^i = \eta^1$, and $i = k = 1$ in Eq. 1, such that $\eta^0 = 1 - \eta$ quantifies the parent phase. Fracture is likewise characterized by a single order parameter $\xi = \xi^j = \xi^1$, and $j = l = 1$ in Eq. 3. The reference state is a homogeneous medium Ω_0 with $\eta = 0$ and $\xi = 0$.

With regard to inelastic deformation $\bar{\mathbf{F}}$, Eq. 12 is again assumed to hold. Equations 76 and 77 also apply. Deformation incurred from damage is assumed purely

dilatational^{53,106}:

$$\mathbf{F}^\xi(\xi) = [J^\xi(\xi)]^{1/3} \mathbf{1} = [1 - \bar{\varphi}(\xi)]^{-1/3} \mathbf{1}; \quad \bar{\varphi}(\xi) = \phi(\xi) \bar{\varphi}_0 = (3\xi^2 - 2\xi^3) \bar{\varphi}_0. \quad (89)$$

Here, $\bar{\varphi}(\mathbf{X}, t)$ is the local free volume or residual porosity induced from damage (e.g., crack opening or cavitation), and $\bar{\varphi}_0 \in [0, 1)$ is the maximum local free volume attained at $(\mathbf{X}, t)$ when $\xi(\mathbf{X}, t) = 1$, assumed to be a material constant. A frequently used^{15,20,38} polynomial interpolation function with vanishing endpoint derivatives is ϕ . Note that $\bar{\varphi}$ persists when the material is elastically unloaded. Recoverable deformation from damage entities is contained in $\mathbf{F}^E$.

Residual deformation from other structural changes, $\mathbf{F}^\eta(\eta)$, is not necessarily spherical. However, in an isotropic solid, the material response should be independent of any (inelastic) rotations of the microstructure. This can be ensured by restricting $\mathbf{F}^\eta(\eta)$ to be a stretch, i.e., a symmetric tensor, similarly to the usual practice of omitting plastic spin in isotropic finite plasticity theory.^{107,108} Similarly to prior works,^{16,38,99}

$$\begin{aligned} \mathbf{F}^\eta(\eta) &= \mathbf{1} + \mathbf{e}^\eta(\eta) = \mathbf{1} + \phi(\eta) \mathbf{e}_0^\eta = \mathbf{1} + (3\eta^2 - 2\eta^3) \mathbf{e}_0^\eta; \\ (e^\eta)_{IJ} &= (e^\eta)_{JI}; \quad [(F^\eta)_K^\alpha = g_K^\alpha + g_I^\alpha G^{IJ} (e^\eta)_{JK}] . \end{aligned} \quad (90)$$

An example is the collective inelastic strain manifested from numerous twinning systems in a non-textured polycrystalline aggregate. The full transformation strain at $\eta = 1$ is the symmetric matrix of material constants $\mathbf{e}_0^\eta$. The shifter between reference and intermediate coordinate frames (Clayton,⁸² p. 98) is $g_K^\alpha = \bar{\mathbf{g}}^\alpha \cdot \mathbf{G}_K$.

Substitution of Eq. 89 and Eq. 90 into Eq. 14 gives

$$\begin{aligned} \mathbf{A}^\xi(\xi, \eta) &= \frac{2\xi(1 - \xi) \bar{\varphi}_0}{[1 - (3\xi^2 - 2\xi^3) \bar{\varphi}_0]^{4/3}} [\mathbf{1} + (3\eta^2 - 2\eta^3) \mathbf{e}_0^\eta], \\ \mathbf{A}^\eta(\xi, \eta) &= \frac{6\eta(1 - \eta)}{[1 - (3\xi^2 - 2\xi^3) \bar{\varphi}_0]^{1/3}} \mathbf{e}_0^\eta. \end{aligned} \quad (91)$$

Furthermore,

$$\bar{\mathbf{F}}^{-1}(\xi, \eta) = [1 - (3\xi^2 - 2\xi^3) \bar{\varphi}_0]^{1/3} [\mathbf{1} + (3\eta^2 - 2\eta^3) \mathbf{e}_0^\eta]^{-1}. \quad (92)$$

Thermoelastic strain energy accounts for isotropic elasticity, isotropic thermal ex-

pansion, and specific heat. A nonlinear pressure-volume response is administered, but higher-order shear elastic coefficients are not included. An isotropic solid has three independent third-order elastic constants^{56,79,98}; here, only a single nonlinear elastic coefficient is included via the ambient pressure derivative of the bulk modulus. The rationale is that a brittle material (e.g., ceramic or mineral) can sustain large compressive pressures, for example, under shock loading conditions, but that deviatoric stresses are limited due to fractures that degrade the shear modulus before higher-order shear elastic coefficients, difficult to measure and thus unknown for most polycrystalline solids, are necessary.^{58,72} The corresponding thermoelastic strain energy function is

$$W^U(\mathbf{e}^E, S, \eta, \xi) = \frac{1}{2}B(\eta, \xi, \bar{\omega}) \cdot (\text{tr} \mathbf{e}^E)^2 \left[1 - \frac{1}{3}\{B'_0(\eta) - 2\} \cdot (\text{tr} \mathbf{e}^E) \right] \\ + G(\eta, \xi) \cdot (\mathbf{e}'^E : \mathbf{e}'^E) - T_0 [\gamma(\eta, \xi, \bar{\omega}) \cdot (\text{tr} \mathbf{e}^E) \cdot S - h(S)]. \quad (93)$$

The deviatoric thermoelastic strain is $\mathbf{e}'^E = \mathbf{e}^E - \frac{1}{3}(\text{tr} \mathbf{e}^E)\mathbf{1}$; this does not contribute to J^E . The purely entropic contribution $h(S)$ is identical to that of Eq. 72, where c_0 is specific heat. The phase- and fracture-dependent bulk modulus, shear modulus, and Grüneisen parameter are B , G , and γ . Dimensionless third-order elastic parameter B'_0 accounts for a change in tangent bulk stiffness with pressure or volume changes. Simpler forms of Eqs. 73 and 74 now apply:

$$B(\eta, \xi, \bar{\omega}) = B_0(\eta) \cdot [\chi(\xi) \cdot \bar{\omega} + (1 - \bar{\omega})], \quad G(\eta, \xi) = G_0(\eta) \cdot \chi(\xi), \quad (94) \\ \gamma(\eta, \xi, \bar{\omega}) = \gamma_0(\eta) \cdot [\chi(\xi) \cdot \bar{\omega} + (1 - \bar{\omega})];$$

$$B_0(\eta) = B_{0|0} + (B_{0|1} - B_{0|0}) \cdot \phi(\eta), \quad B'_0(\eta) = B'_{0|0} + (B'_{0|1} - B'_{0|0}) \cdot \phi(\eta), \\ G_0(\eta) = G_{0|0} + (G_{0|1} - G_{0|0}) \cdot \phi(\eta), \quad \gamma_0(\eta) = \gamma_{0|0} + (\gamma_{0|1} - \gamma_{0|0}) \cdot \phi(\eta), \quad (95)$$

recalling $\phi(x) = 3x^2 - 2x^3$. According to Eq. 94, the bulk modulus and Grüneisen parameter degrade with fracture in tension ($\bar{\omega} = 1$) but not compression ($\bar{\omega} = 0$), as in prior works.^{7,34,48} The shear modulus degrades irrespective of $\bar{\omega}$. Note that in a homogeneous phase i , $\gamma_{0|i} = A_{0|i}^E B_{0|i} / c_{0|i}^\Sigma$, where $A_{0|i}^E = \text{tr}(\mathbf{a}_{0|i}^E)$ is the volumetric thermal expansion coefficient and $c_{0|i}^\Sigma$ is specific heat at constant stress/pressure,^{79,98} so the assumption of equivalent degradation of B and γ with ξ and stress state is

justified. The degradation function $\chi(\xi) \in [\zeta_0, 1]$ is, from Eq. 75 with $j = l = 1$,

$$\chi(\xi) = \zeta_0 + (1 - \zeta_0)(1 - \xi)^2. \quad (96)$$

The same function χ is used in prior nonlinear phase field theories for fracture.^{34,44} Such quadratic degradation is standard in isotropic phase field models.^{10,11}

For isotropic damage measured by a single order parameter $\xi = \xi^1$, the functions in Eq. 97 are the following reductions of those in Eq. 78:

$$f_\xi^U(\eta, \xi, S) = \Upsilon(\eta, T^e(S)) \left[\frac{1}{l_\xi} \xi^2 + l_\xi |\nabla_0 \xi|^2 \right]. \quad (97)$$

The effective fracture surface energy per unit reference area is Υ , which can depend on phase and temperature, the latter via T^e of Eq. 79. If the polycrystal is a composite, then effects of thermal residual stresses on fracture toughness¹⁰⁹ can be incorporated via dependence of Υ on T^e . When $\Upsilon = \text{constant}$, the standard gradient energy functional for geometrically nonlinear phase field fracture^{34,35} is recovered. The TDGL-type kinetic equation for fracture of Eq. 66 and viscosity of Eq. 82 are, in the present case,

$$\begin{aligned} \hat{\beta}^\xi \dot{\xi} &= -\frac{\delta \Psi}{\delta \xi} = - \left[\frac{\partial \hat{\Psi}}{\partial \xi} \Big|_{\mathbf{e}^E} - \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E \mathbf{A}^\xi \bar{\mathbf{F}}^{-1}) - 2l_\xi \nabla_0 \cdot (\Upsilon \nabla_0 \xi) \right]; \\ \hat{\beta}^\xi &= \hat{\beta}^\xi(\dot{\xi}, \eta, T, p) \geq 0. \end{aligned} \quad (98)$$

If fracture is irreversible with possible initiation threshold, then Eq. 98 can be replaced with the following specific version of Eq. 68:

$$\begin{aligned} \dot{\xi} &= \left\langle \frac{1}{\hat{\beta}^\xi} [\mathcal{F} - \mathcal{R}] \right\rangle \mathbf{H}(\hat{\pi}^\xi) \geq 0; \quad \hat{\pi}^\xi = - \frac{\partial \Psi}{\partial \xi} \Big|_{\mathbf{F}} + 2l_\xi \nabla_0 \cdot (\Upsilon \nabla_0 \xi); \\ \hat{\beta}^\xi &= \hat{\beta}^\xi(\dot{\xi}, \eta, T, p) > 0. \end{aligned} \quad (99)$$

Consider phase and gradient energies from the single order parameter η . Functions in Eq. 58 are posited as

$$f_{\eta 0}^U(\eta, \xi, S) = \hat{\chi}(\xi) \cdot \bar{f}_{\eta 0}^U(\eta, S), \quad f_{\eta \nabla}^U(\nabla_0 \eta, S) = \hat{\chi}(\xi) \cdot \bar{f}_{\eta \nabla}^U(\nabla_0 \eta, T^e(S)), \quad (100)$$

where $\hat{\chi} = \chi$ for degradation or $\hat{\chi} = 1$ otherwise. The phase energy $\bar{f}_{\eta 0}^U$ includes

the energy barriers for homogeneous as well as stress-free (i.e., temperature- or entropy-driven) transformations. If total internal energy U is assumed to have a null reference value (i.e., $U_0 = 0$), then $\bar{f}_{\eta 0}^U(\eta = 0, S = 0) = 0$, meaning at least one well exists at $\eta = 0$. As in Eq. 86, assume that gradient interfacial energy $f_{\eta \nabla}^U$ is isotropic and that interface surface stresses do not exist. Then

$$\bar{f}_{\eta \nabla}^U(\nabla_0 \eta, T^e(S)) = \frac{3}{4} \Gamma(T^e(S)) \cdot l_\eta \cdot |\nabla_0 \eta|^2. \quad (101)$$

The temperature-dependent surface energy density is Γ . Generalization for surface stresses is presented by VI Levitas.^{39,40} The TDGL-type or Allen–Cahn^{51,92} kinetic equation for phase evolution consistent with f_η^U is, with $\hat{\beta}^\eta$ a non-negative viscosity function:

$$\begin{aligned} \hat{\beta}^\eta \dot{\eta} &= -\frac{\delta \Psi}{\delta \eta} = - \left[\frac{\partial \hat{\Psi}}{\partial \eta} \Big|_{\mathbf{e}^E} - \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E \mathbf{A}^\eta \bar{\mathbf{F}}^{-1}) - \frac{3}{2} l_\eta \nabla_0 \cdot (\Gamma \nabla_0 \eta) \right]; \\ \hat{\beta}^\eta &= \hat{\beta}^\eta(\dot{\eta}^i, \eta^i, T, p) \geq 0. \end{aligned} \quad (102)$$

Lastly, for subsequent comparison with stresses derived in the linearized model of Section 3, the thermodynamic stress $\boldsymbol{\Sigma}$ is computed via differentiation of Eq. 93:

$$\boldsymbol{\Sigma} = \frac{\partial \hat{U}}{\partial \mathbf{e}^E} = \frac{\partial W^U}{\partial \mathbf{e}^E} = \mathbf{B} \left[1 - \frac{1}{2} \{ \mathbf{B}'_0 - 2 \} (\text{tr} \mathbf{e}^E) \right] (\text{tr} \mathbf{e}^E) \mathbf{1} + 2\mathbf{G} \mathbf{e}'^E - T_0 \gamma S \mathbf{1}. \quad (103)$$

Cauchy stress $\boldsymbol{\sigma}$ then follows from Eq. 47. For hydrostatic thermoelastic loading [$\mathbf{F}^E = (J^E)^{1/3} \mathbf{1}$ and $\boldsymbol{\sigma} = -p \mathbf{1}$, with p the pressure], the result reduces to the logarithmic pressure-volume-entropy equation of state (EOS)^{57,72,110}:

$$p = -\frac{\ln J^E}{J} \mathbf{B} \left[1 - \frac{1}{2} \{ \mathbf{B}'_0 - 2 \} (\ln J^E) \right] + \frac{T_0 \gamma S}{J}. \quad (104)$$

2.6.3 Initial Stress

Constituents of many polycrystalline materials support residual stresses, meaning a convenient choice of reference = initial state is not stress-free. For example, unequal thermal expansion coefficients among phases contributes to residual stresses in many ceramics when cooled from a higher processing temperature to the reference (e.g., ambient or room) temperature.^{70,109,111} The theory of Sections 2.6.1 and

2.6.2 can be augmented to allow for an initial thermodynamic stress tensor $\tilde{\Sigma}$, following DC Wallace.¹¹² In this case, all strains vanish at the reference state at $S = 0$ and $T = T_0$, but stresses do not.

For the anisotropic model, Eq. 71 is augmented as

$$\begin{aligned} W^U(\mathbf{e}^E, S, \eta^i, \xi^j) = & \tilde{\Sigma}^A(\eta^i, \xi^j, \bar{\omega}) e_A^E + \frac{1}{2} \mathbf{C}^{AB}(\eta^i, \xi^j, \bar{\omega}) e_A^E e_B^E \\ & + \frac{1}{6} \mathbf{C}^{ABC}(\eta^i, \xi^j, \bar{\omega}) e_A^E e_B^E e_C^E - T_0 [\gamma^A(\eta^i, \xi^j, \bar{\omega}) e_A^E S - h(S)], \end{aligned} \quad (105)$$

leading to, with $\mathbf{C}^{(2)}$ and $\mathbf{C}^{(3)}$ the second- and third-order elastic coefficients in tensor notation,

$$\Sigma = \frac{\partial W^U}{\partial \mathbf{e}^E} = \tilde{\Sigma} + \mathbf{C}^{(2)} : \mathbf{e}^E + \frac{1}{2} (\mathbf{C}^{(3)} : \mathbf{e}^E) : \mathbf{e}^E - T_0 \gamma S. \quad (106)$$

The initial stress, which is symmetric with components $\tilde{\Sigma}^{\alpha\beta}$ referred to the intermediate configuration (tensor notation) and $\tilde{\Sigma}^A$ (Voigt notation), potentially depends on order parameters and elastic volume change in a general way, similarly to the elastic coefficients in Eqs. 73 and 74:

$$\begin{aligned} \tilde{\Sigma}^A(\eta^i, \xi^j, \bar{\omega}) = & \tilde{\Sigma}_0^A(\eta^i) \cdot \chi(\xi^j) \cdot \bar{\omega} + \tilde{\Sigma}_R^A(\eta^i) \cdot (1 - \bar{\omega}), \\ \tilde{\Sigma}_0^A(\eta^i) = & \tilde{\Sigma}_{0|0}^A + \sum_{i=1}^k (\tilde{\Sigma}_{0|i}^A - \tilde{\Sigma}_{0|0}^A) \cdot \eta^i [3\eta^i - 2(\eta^i)^2]. \end{aligned} \quad (107)$$

For isotropic solids, $\tilde{\Sigma}$ is a spherical tensor, i.e., $\tilde{\Sigma} = \tilde{\Sigma} \mathbf{1}$, with $\tilde{\Sigma}$ a scalar denoting an initial tensile pressure when positive in sign. Strain energy, total thermodynamic stress, and order parameter dependencies in the context of the isotropic theory of Section 2.6.2 become

$$\begin{aligned} W^U(\mathbf{e}^E, S, \eta, \xi) = & \tilde{\Sigma}(\eta, \xi, \bar{\omega}) \cdot (\text{tr} \mathbf{e}^E) \\ & + \frac{1}{2} \mathbf{B}(\eta, \xi, \bar{\omega}) \cdot (\text{tr} \mathbf{e}^E)^2 \left[1 - \frac{1}{3} \{ \mathbf{B}'_0(\eta) - 2 \} \cdot (\text{tr} \mathbf{e}^E) \right] \\ & + \mathbf{G}(\eta, \xi) \cdot (\mathbf{e}'^E : \mathbf{e}'^E) - T_0 [\gamma(\eta, \xi, \bar{\omega}) \cdot (\text{tr} \mathbf{e}^E) \cdot S - h(S)], \end{aligned} \quad (108)$$

$$\boldsymbol{\Sigma} = \frac{\partial W^U}{\partial \mathbf{e}^E} = \tilde{\Sigma} \mathbf{1} + \mathbf{B} \left[1 - \frac{1}{2} \{ \mathbf{B}'_0 - 2 \} (\text{tr} \mathbf{e}^E) \right] (\text{tr} \mathbf{e}^E) \mathbf{1} + 2\mathbf{G} \mathbf{e}'^E - T_0 \gamma S \mathbf{1}, \quad (109)$$

$$\tilde{\Sigma}(\eta, \xi, \bar{\omega}) = \tilde{\Sigma}_0(\eta) \cdot [\chi(\xi) \cdot \bar{\omega} + (1 - \bar{\omega})], \quad \tilde{\Sigma}_0(\eta) = \tilde{\Sigma}_{0|0} + (\tilde{\Sigma}_{0|1} - \tilde{\Sigma}_{0|0}) \cdot \phi(\eta). \quad (110)$$

Initial stress affects driving forces for fracture and other microstructure kinetics in Eqs. 81, 87, 98, and 102.

3. Linearized Theory

The nonlinear phase field theory of Section 2 is recast in the context of geometric linearity. Reference position of a material element is $\mathbf{X}$, and t is time. The solid body in its undeformed state is again labeled Ω_0 , with unit outward normal $\mathbf{N}(\mathbf{X})$ on boundary $\partial\Omega_0$. Definitions and properties of order parameters η^i and ξ^j are unchanged from those given in Section 2.1. The linearized theory is intended for study of problems where volume changes may be finite but shears and rigid body rotations remain small. The geometrically nonlinear theory of Section 2 is advocated for problems involving finite shear strains and/or finite rotations.

3.1 Kinematics

Basis vectors are $\mathbf{G}_K(\mathbf{X}) = \partial_K \mathbf{X}$, and the metric has components $G_{IJ} = \mathbf{G}_I \cdot \mathbf{G}_J$. The gradient operator for covariant differentiation is $\nabla_0(\cdot) = \partial_K(\cdot) \otimes \mathbf{G}^K$. The displacement vector $\mathbf{u}$ and its gradient $\mathbf{h}$ are

$$\mathbf{u}(\mathbf{X}, t) = \mathbf{x}(\mathbf{X}, t) - \mathbf{X}, \quad \mathbf{h}(\mathbf{X}, t) = \nabla_0 \mathbf{u}(\mathbf{X}, t). \quad (111)$$

Derivations generally admit curvilinear coordinates X^K over Ω_0 embedded in Euclidean 3-space. Recalling $\nabla_0 J G_{KL} = 0$,^{79,82} the total strain tensor is

$$\boldsymbol{\epsilon} = \frac{1}{2} (\mathbf{h} + \mathbf{h}^T) \quad \leftrightarrow \quad \epsilon_{IJ} = \frac{1}{2} (\nabla_0 I u^K G_{KJ} + \nabla_0 J u^K G_{IK}). \quad (112)$$

In the linear theory, volume change is measured by

$$d\Omega/d\Omega_0 = 1 + \nabla_0 \cdot \mathbf{u} = 1 + \text{tr} \mathbf{h} = 1 + \text{tr} \boldsymbol{\epsilon}. \quad (113)$$

Particle velocity and acceleration are

$$\mathbf{v}(\mathbf{X}, t) = \dot{\mathbf{u}}(\mathbf{X}, t), \quad \dot{\mathbf{v}}(\mathbf{X}, t) = \ddot{\mathbf{u}}(\mathbf{X}, t). \quad (114)$$

Compatibility conditions for $\mathbf{h}$ that ensure existence of $\mathbf{u}$ on a simply connected domain Ω_0 are

$$\nabla_0 \times \mathbf{h} = \mathbf{0} \quad \leftrightarrow \quad \epsilon^{IJK} \nabla_{0J} h_K^L = \epsilon^{IJK} \nabla_{0J} \nabla_{0K} u^L = 0. \quad (115)$$

An additive decomposition of displacement gradient into thermoelastic ($\mathbf{h}^E$) and residual parts applies ($\bar{\mathbf{h}}$), leading to an additive decomposition of strain:

$$\begin{aligned} \mathbf{h}(\mathbf{X}, t) &= \mathbf{h}^E(\mathbf{X}, t) + \bar{\mathbf{h}}(\eta^i(\mathbf{X}, t), \xi^j(\mathbf{X}, t)), \\ \boldsymbol{\epsilon}(\mathbf{X}, t) &= \boldsymbol{\epsilon}^E(\mathbf{X}, t) + \bar{\boldsymbol{\epsilon}}(\eta^i(\mathbf{X}, t), \xi^j(\mathbf{X}, t)). \end{aligned} \quad (116)$$

Analogously to Eq. 12, an additive split of residual distortion and strain is often useful:

$$\begin{aligned} \bar{\mathbf{h}}(\eta^i(\mathbf{X}, t), \xi^j(\mathbf{X}, t)) &= \mathbf{h}^\xi(\xi^j(\mathbf{X}, t)) + \mathbf{h}^\eta(\eta^i(\mathbf{X}, t)), \\ \bar{\boldsymbol{\epsilon}}(\eta^i(\mathbf{X}, t), \xi^j(\mathbf{X}, t)) &= \boldsymbol{\epsilon}^\xi(\xi^j(\mathbf{X}, t)) + \boldsymbol{\epsilon}^\eta(\eta^i(\mathbf{X}, t)). \end{aligned} \quad (117)$$

The strain rate obeys an additive decomposition, and thermoelastic and residual volume changes are measured by the isotropic parts of corresponding strain tensors:

$$\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{\epsilon}}^E + \dot{\bar{\boldsymbol{\epsilon}}}; \quad d\bar{\Omega} = (1 + \text{tr } \boldsymbol{\epsilon}^E)^{-1} d\Omega = (1 + \text{tr } \bar{\boldsymbol{\epsilon}}) d\Omega_0. \quad (118)$$

Define the following structure tensors that replace Eq. 14 in the linearized theory:

$$\mathbf{A}_j^\xi = \partial \bar{\mathbf{h}} / \partial \xi^j, \quad \mathbf{A}_i^\eta = \partial \bar{\mathbf{h}} / \partial \eta^i. \quad (119)$$

From Eqs. 115 and 119,

$$-\epsilon^{PQR} \nabla_{0Q} (h^E)_R^L = \epsilon^{PQR} \nabla_{0Q} \bar{h}_R^L = \epsilon^{PQR} \left[(A_j^\xi)_R^L \nabla_{0Q} \xi^j + (A_i^\eta)_R^L \nabla_{0Q} \eta^i \right]. \quad (120)$$

When $\bar{h}$ manifests from plastic slip, then such non-vanishing curl terms are often physically linked to geometrically necessary dislocations.^{83,84,113}

3.2 Balance Laws and Thermodynamics

As in Section 2, mass transport, body forces, and point heat sources are omitted for brevity; the latter two can be added without difficulty. In what follows in Section 3.2, global laws, from which local versions are obtained using the same procedures followed in Section 2.3, are also omitted. The symmetric stress tensor field is denoted by $\mathbf{P}(\mathbf{X}, t)$ and traction is $\mathbf{t}_0 = \mathbf{P} \cdot \mathbf{N}$. Mass conservation of Eq. 20 still applies, with $J \rightarrow 1 + \nabla_0 \cdot \mathbf{u}$ and $\nabla \cdot \mathbf{v} \rightarrow \nabla_0 \cdot \dot{\mathbf{u}}$ in the linearized theory (∇ and ∇_0 are indistinguishable). Local balance laws of linear and angular momentum are

$$\nabla_0 \cdot \mathbf{P} = \rho_0 \dot{\mathbf{v}}, \quad \mathbf{P} = \mathbf{P}^T. \quad (121)$$

Local micro-force balances are identical to those of Eq. 24:

$$\nabla_0 \cdot \mathbf{s}_i^\eta + \pi_i^\eta = 0, \quad \nabla_0 \cdot \mathbf{s}_j^\xi + \pi_j^\xi = 0. \quad (122)$$

Notation for internal energy, free energy, entropy, and temperature (U, Ψ, S, T) introduced in Section 2.3 still holds, as does Eq. 25. Heat flux is $\mathbf{Q}$. The local energy balance of Eq. 27 is replaced with

$$\dot{U} = \mathbf{P} : \dot{\mathbf{h}} + \mathbf{s}_i^\eta \cdot \nabla_0 \dot{\eta}^i + \mathbf{s}_j^\xi \cdot \nabla_0 \dot{\xi}^j - \pi_i^\eta \dot{\eta}^i - \pi_j^\xi \dot{\xi}^j - \nabla_0 \cdot \mathbf{Q}. \quad (123)$$

From symmetry of $\mathbf{P}$, the distortion rate $\dot{\mathbf{h}}$ in Eq. 123 can be replaced with $\dot{\epsilon}$, but the former proves advantageous for later derivations. The local entropy inequality from Eq. 28 is unchanged, and the internal dissipation becomes, noting $\mathbf{Q} = -\mathbf{k} \nabla_0 T$ for conduction of the type in Eq. 30,

$$\mathfrak{D} = T \dot{S} + \nabla_0 \cdot \mathbf{Q} = \mathbf{P} : \dot{\mathbf{h}} + \mathbf{s}_i^\eta \cdot \nabla_0 \dot{\eta}^i + \mathbf{s}_j^\xi \cdot \nabla_0 \dot{\xi}^j - \pi_i^\eta \dot{\eta}^i - \pi_j^\xi \dot{\xi}^j - \dot{\Psi} - \dot{T} S \geq 0. \quad (124)$$

3.3 Constitutive Theory

3.3.1 Thermodynamic Potentials and Dissipation

Equations of Section 2.4.1 apply, but with $\mathbf{F}$ replaced by $\mathbf{h}$:

$$\begin{aligned} \Psi &= \Psi(\mathbf{h}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T), \\ U &= U(\mathbf{h}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, S) \quad (i = 1, \dots, k; j = 1, \dots, l); \end{aligned} \quad (125)$$

$$\mathbf{P} = \mathbf{P}(\mathbf{h}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T), \quad S = S(\mathbf{h}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T); \quad (126)$$

$$\begin{aligned} \mathbf{s}_i^\eta &= \mathbf{s}_i^\eta(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T), \quad \mathbf{s}_j^\xi = \mathbf{s}_j^\xi(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T); \\ \pi_i^\eta &= \pi_i^\eta(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T), \quad \pi_j^\xi = \pi_j^\xi(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T); \end{aligned} \quad (127)$$

$$\mathbf{P} = \frac{\partial \Psi}{\partial \mathbf{h}} = \frac{\partial \Psi}{\partial \boldsymbol{\epsilon}}, \quad S = -\frac{\partial \Psi}{\partial T}; \quad \mathbf{s}_i^\eta = \frac{\partial \Psi}{\partial \nabla_0 \eta^i}, \quad \mathbf{s}_j^\xi = \frac{\partial \Psi}{\partial \nabla_0 \xi^j}; \quad (128)$$

$$\begin{aligned} \hat{\pi}_i^\eta(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) &= -[\pi_i^\eta(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) \\ &\quad + \partial \Psi(\mathbf{h}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) / \partial \eta^i], \\ \hat{\pi}_j^\xi(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) &= -[\pi_j^\xi(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) \\ &\quad + \partial \Psi(\mathbf{h}, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) / \partial \xi^j]; \end{aligned} \quad (129)$$

$$\begin{aligned} \mathfrak{D} &= \hat{\pi}_i^\eta(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) \dot{\eta}^i \\ &\quad + \hat{\pi}_j^\xi(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) \dot{\xi}^j \geq 0; \end{aligned} \quad (130)$$

$$\begin{aligned} \mathbf{P} &= \frac{\partial U}{\partial \mathbf{h}} = \frac{\partial U}{\partial \boldsymbol{\epsilon}}, \quad T = \frac{\partial U}{\partial S}; \quad \mathbf{s}_i^\eta = \frac{\partial U}{\partial \nabla_0 \eta^i}, \quad \mathbf{s}_j^\xi = \frac{\partial U}{\partial \nabla_0 \xi^j}; \\ \hat{\pi}_i^\eta &= -\pi_i^\eta - \frac{\partial U}{\partial \eta^i}, \quad \hat{\pi}_j^\xi = -\pi_j^\xi - \frac{\partial U}{\partial \xi^j}. \end{aligned} \quad (131)$$

Consistency with the balance of angular momentum and invariance of energy under rotations $\frac{1}{2}(\mathbf{h} - \mathbf{h}^T)$ requires that dependence of constitutive variables upon $\mathbf{h}$ is only through $\boldsymbol{\epsilon}(\mathbf{h})$.

3.3.2 Small-Strain Thermoelasticity

Dependence of constitutive variables on $\mathbf{h}$ is now replaced with dependence on thermoelastic strain $\boldsymbol{\epsilon}^E$ of Eq. 116. Note

$$\boldsymbol{\epsilon}^E(\mathbf{h}, \eta^i, \xi^j) = \frac{1}{2} (\mathbf{h} + \mathbf{h}^T) - \bar{\boldsymbol{\epsilon}}(\eta^i, \xi^j). \quad (132)$$

Thus,

$$\frac{\partial \epsilon_{IJ}^E}{\partial h_{KL}} = \frac{1}{2} (\delta_I^K \delta_J^L + \delta_J^K \delta_I^L). \quad (133)$$

A change of independent variables between $\mathbf{h}$ and $\boldsymbol{\epsilon}^E$ with definitions Eq. 119 leads to the following general formulae:

$$\left. \frac{\partial(\cdot)}{\partial \eta^i} \right|_{\mathbf{h}} = \left. \frac{\partial(\cdot)}{\partial \eta^i} \right|_{\boldsymbol{\epsilon}^E} + \left. \frac{\partial(\cdot)}{\partial \boldsymbol{\epsilon}^E} \right|_{\eta^i} : \left. \frac{\partial \boldsymbol{\epsilon}^E}{\partial \eta^i} \right|_{\mathbf{h}} = \left. \frac{\partial(\cdot)}{\partial \eta^i} \right|_{\boldsymbol{\epsilon}^E} - \frac{1}{2} \left. \frac{\partial(\cdot)}{\partial \boldsymbol{\epsilon}^E} \right|_{\eta^i} : [\mathbf{A}_i^\eta + (\mathbf{A}_i^\eta)^T], \quad (134)$$

$$\left. \frac{\partial(\cdot)}{\partial \xi^j} \right|_{\mathbf{h}} = \left. \frac{\partial(\cdot)}{\partial \xi^j} \right|_{\boldsymbol{\epsilon}^E} + \left. \frac{\partial(\cdot)}{\partial \boldsymbol{\epsilon}^E} \right|_{\xi^j} : \left. \frac{\partial \boldsymbol{\epsilon}^E}{\partial \xi^j} \right|_{\mathbf{h}} = \left. \frac{\partial(\cdot)}{\partial \xi^j} \right|_{\boldsymbol{\epsilon}^E} - \frac{1}{2} \left. \frac{\partial(\cdot)}{\partial \boldsymbol{\epsilon}^E} \right|_{\xi^j} : [\mathbf{A}_j^\xi + (\mathbf{A}_j^\xi)^T]. \quad (135)$$

Free and internal energy densities per unit reference volume are now expressed as the following potentials for geometrically linear thermoelasticity:

$$\begin{aligned} \Psi &= \hat{\Psi}(\boldsymbol{\epsilon}^E, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T), \\ U &= \hat{U}(\boldsymbol{\epsilon}^E, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, S) \quad (i = 1, \dots, k; j = 1, \dots, l). \end{aligned} \quad (136)$$

Define the symmetric thermodynamic conjugate stress tensor $\boldsymbol{\Sigma}$, with components Σ^{IJ} as follows, and note from Eqs. 128 and 131 that the constitutive relations for entropy and temperature still apply:

$$\boldsymbol{\Sigma} = \frac{\partial \hat{\Psi}}{\partial \boldsymbol{\epsilon}^E} = \frac{\partial \hat{U}}{\partial \boldsymbol{\epsilon}^E}, \quad S = -\frac{\partial \hat{\Psi}}{\partial T}, \quad T = \frac{\partial \hat{U}}{\partial S}. \quad (137)$$

The stress $\mathbf{P}$ then obeys, from Eqs. 128, 133, 136, and 137,

$$P^{IJ} = \Sigma^{KL} \frac{\partial \epsilon_{KL}^E}{\partial h_{IJ}} = \frac{1}{2} \Sigma^{KL} (\delta_I^K \delta_J^L + \delta_J^K \delta_I^L) = \Sigma^{IJ} \Rightarrow \boldsymbol{\Sigma} = \mathbf{P}. \quad (138)$$

Dissipative forces in Eq. 129 become, with Eqs. 134 and 135 and the symmetry of $\mathbf{P}$,

$$\hat{\pi}_i^\eta = - \left[\pi_i^\eta + \left. \frac{\partial \hat{\Psi}}{\partial \eta^i} \right|_{\boldsymbol{\epsilon}^E} - \mathbf{P} : \mathbf{A}_i^\eta \right], \quad \hat{\pi}_j^\xi = - \left[\pi_j^\xi + \left. \frac{\partial \hat{\Psi}}{\partial \xi^j} \right|_{\boldsymbol{\epsilon}^E} - \mathbf{P} : \mathbf{A}_j^\xi \right], \quad (139)$$

where thermoelastic driving forces for structural changes or fractures are the third terms in braces on right sides.

Thermoelastic coefficients and their relations are as follows, where the same notation from Section 2.4.2 is used, but with $\boldsymbol{\epsilon}^E$ replacing $\mathbf{e}^E$ as the independent strain variable:

$$\mathbf{C}^T = \frac{\partial^2 \hat{\Psi}}{\partial \boldsymbol{\epsilon}^E \partial \boldsymbol{\epsilon}^E}, \quad \mathbf{C}^S = \frac{\partial^2 \hat{U}}{\partial \boldsymbol{\epsilon}^E \partial \boldsymbol{\epsilon}^E}; \quad (140)$$

$$\mathbf{a}^E = \frac{\partial \boldsymbol{\epsilon}^E}{\partial T}, \quad \boldsymbol{\alpha}^E = -\frac{\partial^2 \hat{\Psi}}{\partial \boldsymbol{\epsilon}^E \partial T} = c^E \boldsymbol{\gamma}^E, \quad c^E = \frac{\partial \hat{U}}{\partial T} = T \frac{\partial S}{\partial T} = -T \frac{\partial^2 \hat{\Psi}}{\partial T^2}; \quad (141)$$

$$\boldsymbol{\alpha}^E = \mathbf{a}^E : \mathbf{C}^T, \quad c^\Sigma = c^E + T \mathbf{a}^E : \boldsymbol{\alpha}^E, \quad \mathbf{C}^S = \mathbf{C}^T + (T/c^E) \boldsymbol{\alpha}^E \otimes \boldsymbol{\alpha}^E; \quad (142)$$

Define the collected set of order parameters and their gradients by $\mathbf{z}$, and the collected set of conjugate forces by $\boldsymbol{\zeta}$ as in Eq. 52. Then the product of temperature and entropy rate can be expressed as

$$\begin{aligned} T\dot{S} &= T \frac{\partial S}{\partial \boldsymbol{\epsilon}^E} : \dot{\boldsymbol{\epsilon}}^E + T \frac{\partial S}{\partial \mathbf{z}} : \dot{\mathbf{z}} + T \frac{\partial S}{\partial T} \dot{T} \\ &= -T \frac{\partial^2 \hat{\Psi}}{\partial T \partial \boldsymbol{\epsilon}^E} : \dot{\boldsymbol{\epsilon}}^E - T \frac{\partial^2 \hat{\Psi}}{\partial T \partial \mathbf{z}} : \dot{\mathbf{z}} - T \frac{\partial^2 \hat{\Psi}}{\partial T^2} \dot{T} = T \left(\boldsymbol{\alpha}^E : \dot{\boldsymbol{\epsilon}}^E + \frac{\partial \boldsymbol{\zeta}}{\partial T} : \dot{\mathbf{z}} \right) + c^E \dot{T}. \end{aligned} \quad (143)$$

3.3.3 Strain Energy, Phase Energy, and Gradient Energy Densities

Notation parallels that of Section 2.4.3, where W^Ψ and W^U are strain energy potentials that contain all dependence of free and internal energy, respectively, on $\boldsymbol{\epsilon}^E$. Let f_η^Ψ and f_η^U denote collective phase energy potentials for the η^i and their gradients, and let f_ξ^Ψ and f_ξ^U denote collective phase energy potentials for the ξ^j and their gradients:

$$\begin{aligned} \hat{\Psi}(\boldsymbol{\epsilon}^E, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) &= W^\Psi(\boldsymbol{\epsilon}^E, \eta^i, \xi^j, T) \\ &\quad + f_\eta^\Psi(\eta^i, \xi^j, \nabla_0 \eta^i, T) + f_\xi^\Psi(\eta^i, \xi^j, \nabla_0 \xi^j, T); \end{aligned} \quad (144)$$

$$\begin{aligned} \hat{U}(\boldsymbol{\epsilon}^E, \eta^i, \xi^j, \nabla_0 \eta^i, \nabla_0 \xi^j, S) &= W^U(\boldsymbol{\epsilon}^E, \eta^i, \xi^j, S) \\ &\quad + f_\eta^U(\eta^i, \xi^j, \nabla_0 \eta^i, S) + f_\xi^U(\eta^i, \xi^j, \nabla_0 \xi^j, S); \end{aligned} \quad (145)$$

$$f_\eta^\Psi(\eta^i, \xi^j, \nabla_0 \eta^i, T) = f_{\eta 0}^\Psi(\eta^i, \xi^j, T) + f_{\eta \nabla}^\Psi(\eta^i, \xi^j, \nabla_0 \eta^i, T); \quad (146)$$

$$f_\xi^\Psi(\eta^i, \xi^j, \nabla_0 \xi^j, T) = f_{\xi 0}^\Psi(\eta^i, \xi^j, T) + f_{\xi \nabla}^\Psi(\eta^i, \xi^j, \nabla_0 \xi^j, T); \quad (147)$$

$$f_\eta^U(\eta^i, \xi^j, \nabla_0 \eta^i, S) = f_{\eta 0}^U(\eta^i, \xi^j, S) + f_{\eta \nabla}^U(\eta^i, \xi^j, \nabla_0 \eta^i, S); \quad (148)$$

$$f_\xi^U(\eta^i, \xi^j, \nabla_0 \xi^j, S) = f_{\xi 0}^U(\eta^i, \xi^j, S) + f_{\xi \nabla}^U(\eta^i, \xi^j, \nabla_0 \xi^j, S). \quad (149)$$

From Eqs. 144–149,

$$\mathbf{P} = \frac{\partial W^\Psi}{\partial \boldsymbol{\epsilon}^E} = \frac{\partial W^U}{\partial \boldsymbol{\epsilon}^E}; \quad \mathbf{s}_i^\eta = \frac{\partial f_{\eta \nabla}^\Psi}{\partial \nabla_0 \eta^i} = \frac{\partial f_{\eta \nabla}^U}{\partial \nabla_0 \eta^i}, \quad \mathbf{s}_j^\xi = \frac{\partial f_{\xi \nabla}^\Psi}{\partial \nabla_0 \xi^j} = \frac{\partial f_{\xi \nabla}^U}{\partial \nabla_0 \xi^j}; \quad (150)$$

$$\begin{aligned} \hat{\pi}_i^\eta &= - \left[\pi_i^\eta + \frac{\partial(W^\Psi + f_\eta^\Psi + f_\xi^\Psi)}{\partial \eta^i} - \mathbf{P} : \mathbf{A}_i^\eta \right], \\ \hat{\pi}_j^\xi &= - \left[\pi_j^\xi + \frac{\partial(W^\Psi + f_\eta^\Psi + f_\xi^\Psi)}{\partial \xi^j} - \mathbf{P} : \mathbf{A}_j^\xi \right]. \end{aligned} \quad (151)$$

3.4 Order Parameter Kinetics

Derivations of Section 2.5 become the following for geometric linearity:

$$\begin{aligned} \hat{\pi}_i^\eta(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) &= \sum_{i,m=1}^k \hat{\beta}_{im}^\eta(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) \eta^m, \\ \hat{\pi}_j^\xi(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) &= \sum_{j,n=1}^l \hat{\beta}_{jn}^\xi(\mathbf{h}, \eta^i, \xi^j, \dot{\eta}^i, \dot{\xi}^j, \nabla_0 \eta^i, \nabla_0 \xi^j, T) \xi^n; \end{aligned} \quad (152)$$

$$\mathfrak{D} = \hat{\beta}_{im}^\eta \dot{\eta}^i \dot{\eta}^m + \hat{\beta}_{jn}^\xi \dot{\xi}^j \dot{\xi}^n \geq 0; \quad (153)$$

$$\begin{aligned} \pi_i^\eta &= - \left[\hat{\beta}_{im}^\eta \dot{\eta}^m - \frac{\partial \Psi}{\partial \eta^i} \Big|_{\mathbf{h}} \right] = - \left[\hat{\beta}_{im}^\eta \dot{\eta}^m - \frac{\partial \hat{\Psi}}{\partial \eta^i} \Big|_{\boldsymbol{\epsilon}^E} + \mathbf{P} : \mathbf{A}_i^\eta \right], \\ \pi_j^\xi &= - \left[\hat{\beta}_{jn}^\xi \dot{\xi}^n - \frac{\partial \Psi}{\partial \xi^j} \Big|_{\mathbf{h}} \right] = - \left[\hat{\beta}_{jn}^\xi \dot{\xi}^n - \frac{\partial \hat{\Psi}}{\partial \xi^j} \Big|_{\boldsymbol{\epsilon}^E} + \mathbf{P} : \mathbf{A}_j^\xi \right]; \end{aligned} \quad (154)$$

$$\begin{aligned} \hat{\beta}_{im}^\eta \dot{\eta}^m &= - \frac{\delta \Psi}{\delta \eta^i} = - \left[\frac{\partial \Psi}{\partial \eta^i} \Big|_{\mathbf{h}} - \nabla_0 \cdot \frac{\partial \Psi}{\partial \nabla_0 \eta^i} \right] \\ &= - \left[\frac{\partial \hat{\Psi}}{\partial \eta^i} \Big|_{\boldsymbol{\epsilon}^E} - \mathbf{P} : \mathbf{A}_i^\eta - \nabla_0 \cdot \frac{\partial f_{\eta \nabla}^\Psi}{\partial \nabla_0 \eta^i} \right], \\ \hat{\beta}_{jn}^\xi \dot{\xi}^n &= - \frac{\delta \Psi}{\delta \xi^j} = - \left[\frac{\partial \Psi}{\partial \xi^j} \Big|_{\mathbf{h}} - \nabla_0 \cdot \frac{\partial \Psi}{\partial \nabla_0 \xi^j} \right] \\ &= - \left[\frac{\partial \hat{\Psi}}{\partial \xi^j} \Big|_{\boldsymbol{\epsilon}^E} - \mathbf{P} : \mathbf{A}_j^\xi - \nabla_0 \cdot \frac{\partial f_{\xi \nabla}^\Psi}{\partial \nabla_0 \xi^j} \right]; \end{aligned} \quad (155)$$

$$c^E \dot{T} = \hat{\beta}_{im}^\eta \dot{\eta}^i \dot{\eta}^m + \hat{\beta}_{jn}^\xi \dot{\xi}^j \dot{\xi}^n - T \left(\boldsymbol{\alpha}^E : \dot{\boldsymbol{\epsilon}}^E + \frac{\partial \zeta}{\partial T} : \dot{\mathbf{z}} \right) + \nabla_0 \cdot (\mathbf{k} \nabla_0 T). \quad (156)$$

Irreversibility and initiation constraints such as those contained in Eq. 68 can be used in place of Eq. 155 if appropriate.

3.5 Geometrically Linear Elasticity

A general anisotropic framework suitable for small strains is described in Section 3.5.1. Specialization to isotropy, with extension to high-pressure regimes, is given in Section 3.5.2.

3.5.1 Linear Anisotropic Formulation

Voigt notation of Eq. 70 is followed, where indices $A, B, \dots$ run from 1 to 6. As in Section 2.6, an internal energy-based formulation is proposed for dynamic problems. The thermoelastic strain energy function is, with the tension versus compression indicator function $\bar{\omega} = H(\text{tr } \epsilon^E)$ and $H(\cdot)$ the unit step (Heaviside) function,

$$W^U(\epsilon^E, S, \eta^i, \xi^j) = \frac{1}{2} C^{AB}(\eta^i, \xi^j, \bar{\omega}) \epsilon_A^E \epsilon_B^E - T_0 [\gamma^A(\eta^i, \xi^j, \bar{\omega}) \epsilon_A^E S - h(S)]. \quad (157)$$

Elastic constants of orders three and higher are omitted in the context of linear thermoelasticity. Entropy function $h(S)$ accounting for specific heat is identical to Eq. 72 with effective temperature $T^e(S)$, while second-order elastic coefficients and Grüneisen parameters are defined according to the same scheme as used in the nonlinear theory:

$$\begin{aligned} T_0 h(S) &= T_0 S \left[1 + \frac{1}{2} \frac{S}{c_0} + \frac{1}{6} \left(\frac{S}{c_0} \right)^2 + \dots \right], \\ T^e(S) &= T_0 \frac{dh(S)}{dS} = T_0 \left[1 + \frac{S}{c_0} + \frac{1}{2} \left(\frac{S}{c_0} \right)^2 + \dots \right]; \end{aligned} \quad (158)$$

$$\begin{aligned} C^{AB}(\eta^i, \xi^j, \bar{\omega}) &= C_0^{AB}(\eta^i) \cdot \chi(\xi^j) \cdot \bar{\omega} + C_R^{AB}(\eta^i) \cdot (1 - \bar{\omega}), \\ \gamma^A(\eta^i, \xi^j, \bar{\omega}) &= \gamma_0^A(\eta^i) \cdot \chi(\xi^j) \cdot \bar{\omega} + \gamma_R^A(\eta^i) \cdot (1 - \bar{\omega}); \end{aligned} \quad (159)$$

$$\begin{aligned} C_0^{AB}(\eta^i) &= C_{0|0}^{AB} + \sum_{i=1}^k (C_{0|i}^{AB} - C_{0|0}^{AB}) \cdot \eta^i [3\eta^i - 2(\eta^i)^2], \\ \gamma_0^A(\eta^i) &= \gamma_{0|0}^A + \sum_{i=1}^k (\gamma_{0|i}^A - \gamma_{0|0}^A) \cdot \eta^i [3\eta^i - 2(\eta^i)^2]; \end{aligned} \quad (160)$$

$$\chi(\xi^j) = \zeta_0 + (1 - \zeta_0) \prod_{j=1}^l (1 - \xi^j)^2. \quad (161)$$

Inelastic kinematic relations with reference state conditions are given in terms of components of distortion $\bar{\mathbf{h}} = \mathbf{h}^\xi + \mathbf{h}^\eta$ in Eq. 117, where $\bar{\varphi}$ is free volume fraction ($\approx$ most accurate for $\bar{\varphi} \ll 1$):

$$\mathbf{h}^\xi(\xi_0^j) = \mathbf{0}, \quad \mathbf{h}^\eta(\eta_0^i) = \mathbf{0} \quad \Rightarrow \quad \bar{\mathbf{h}}_0 = \mathbf{0}, \quad (i, j \geq 1), \quad (162)$$

$$\bar{\varphi}(\xi^j) = \frac{\text{tr} \mathbf{h}^\xi}{1 + \text{tr} \mathbf{h}^\xi} \approx \text{tr} \mathbf{h}^\xi \quad \Leftrightarrow \quad \text{tr} \mathbf{h}^\xi = \frac{\bar{\varphi}(\xi^j)}{1 - \bar{\varphi}(\xi^j)} \approx \bar{\varphi}(\xi^j). \quad (163)$$

Damage ensues by cleavage fractures on l different low-energy crystallographic planes, each characterized by a unit normal vector $\mathbf{M}^j$. Then, as in Section 2.6.1, energy functions are

$$\begin{aligned} f_\xi^U(\eta^i, \xi^j, S) &= f_{\xi_0}^U(\eta^i, \xi^j, S) + f_{\xi \nabla}^U(\eta^i, \nabla_0 \xi^j, S) \\ &= \sum_{j=1}^l \frac{\Upsilon^j(\eta^i, T^e(S))}{l_\xi} (\xi^j)^2 + \sum_{j=1}^l \Upsilon^j(\eta^i, T^e(S)) \cdot l_\xi \cdot \boldsymbol{\omega}^j : (\nabla_0 \xi^j \otimes \nabla_0 \xi^j); \end{aligned} \quad (164)$$

$$\boldsymbol{\omega}^j = \mathbf{1} + \hat{\alpha}^j \cdot (\mathbf{1} - \mathbf{M}^j \otimes \mathbf{M}^j); \quad (165)$$

while TDGL-type kinetic equations are

$$\begin{aligned} \hat{\beta}_j^\xi \dot{\xi}^j &= -\frac{\delta \Psi}{\delta \xi^j} = -\left[\frac{\partial \hat{\Psi}}{\partial \xi^j} \Big|_{\epsilon^E} - \mathbf{P} : \mathbf{A}_j^\xi - \nabla_0 \cdot \frac{\partial f_{\xi \nabla}^U}{\partial \nabla_0 \xi^j} \right], \\ \hat{\beta}_j^\xi &= \hat{\beta}_j^\xi(\dot{\xi}^j, \eta^i, T, p). \quad (\text{no sum}) \end{aligned} \quad (166)$$

Other structural transformations are measured by η^i . Energy functions carried over from Section 2.6.1 are

$$f_{\eta_0}^U(\eta^i, \xi^j, S) = \hat{\chi}(\xi^j) \cdot \bar{f}_{\eta_0}^U(\eta^i, S), \quad f_{\eta \nabla}^U(\nabla_0 \eta^i, S) = \hat{\chi}(\xi^j) \cdot \bar{f}_{\eta \nabla}^U(\nabla_0 \eta^i, T^e(S)); \quad (167)$$

and a candidate energy function for twinning is²⁰

$$\begin{aligned} \bar{f}_{\eta 0}^U(\eta^i, T^e(S)) &= \sum_{i=1}^k 12 \frac{\Gamma^i(T^e(S))}{l_\eta} (\eta^i)^2 (1 - \eta^i)^2 \\ &+ \sum_{i=1}^{k-1} \sum_{j=i+1}^k \frac{\Xi^{ij}(T^e(S))}{l_\eta} (\eta^i \eta^j)^2 (1 - \eta^i - \eta^j). \end{aligned} \quad (168)$$

For isotropic $f_{\eta \nabla}^U$, in the absence of surface stresses,

$$\bar{f}_{\eta \nabla}^U(\nabla_0 \eta^i, T^e(S)) = \sum_{i=1}^l \sum_{j=1}^l \frac{3}{4} \Gamma^{ij}(T^e(S)) \cdot l_\eta \cdot |\nabla_0 \eta^i| |\nabla_0 \eta^j|. \quad (169)$$

The TDGL-type kinetic equations are

$$\begin{aligned} \hat{\beta}_{im}^\eta \dot{\eta}^m &= -\frac{\delta \Psi}{\delta \eta^i} = -\left[\frac{\partial \hat{\Psi}}{\partial \eta^i} \Big|_{\mathbf{e}^E} - \mathbf{P} : \mathbf{A}_i^\eta - \nabla_0 \cdot \frac{\partial f_{\eta \nabla}^U}{\partial \nabla_0 \eta^i} \right], \\ \hat{\beta}_i^\eta &= \hat{\beta}_i^\eta(\dot{\eta}^i, \eta^i, T, p), \quad (i \geq 1; \text{ sum on } m = 1, \dots, k). \end{aligned} \quad (170)$$

3.5.2 Isotropy

The model framework of Section 3.5.1 is specialized to isotropic materials. As in Section 2.6.2, structural changes are characterized by a single order parameter $\eta = \eta^i = \eta^1$, and $i = k = 1$ in Eq. 1, such that $\eta^0 = 1 - \eta$ quantifies the parent phase. Fracture is characterized by a $\xi = \xi^j = \xi^1$, and $j = l = 1$ in Eq. 3. The reference state is homogeneous: $\xi(\mathbf{X}) = \eta(\mathbf{X}) = 0 \forall \mathbf{X} \in \Omega_0$. With regard to inelastic deformation $\bar{\mathbf{h}}$, Eq. 117 is again assumed to hold, and Eqs. 162 and 163 apply. Deformation from damage is dilatational:

$$\mathbf{h}^\xi(\xi) = \frac{1}{3} \text{tr}\{\mathbf{h}^\xi(\xi)\} \mathbf{1} = \frac{\bar{\varphi}(\xi)}{3 - 3\bar{\varphi}(\xi)} \mathbf{1}; \quad \bar{\varphi}(\xi) = \phi(\xi) \bar{\varphi}_0 = (3\xi^2 - 2\xi^3) \bar{\varphi}_0. \quad (171)$$

Residual deformation from other structural changes, $\mathbf{h}^\eta(\eta)$, is not necessarily spherical, but it is chosen symmetric for isotropic solids:

$$\begin{aligned} \mathbf{h}^\eta(\eta) &= \mathbf{e}^\eta(\eta) = \phi(\eta) \mathbf{e}_0^\eta = (3\eta^2 - 2\eta^3) \mathbf{e}_0^\eta; \\ (e^\eta)_{IJ} &= (e^\eta)_{JI}; \quad [(\mathbf{h}^\eta)_K^J = (e^\eta)_{IK} G^{IJ}]. \end{aligned} \quad (172)$$

Substitution of Eqs. 171 and 172 into Eq. 119 gives

$$\mathbf{A}^\xi(\xi) = \frac{\bar{\varphi}'(\xi)}{3 - 3\bar{\varphi}(\xi)} \mathbf{1} = \frac{2\xi(1 - \xi)\bar{\varphi}_0}{1 - (3\xi^2 - 2\xi^3)\bar{\varphi}_0} \mathbf{1}, \quad \mathbf{A}^\eta(\eta) = \phi'(\eta)\mathbf{e}_0^\eta = 6\eta(1 - \eta)\mathbf{e}_0^\eta. \quad (173)$$

Thermoelastic strain energy accounts for isotropic elasticity, isotropic thermal expansion, and specific heat. As in Section 2.6.2, a nonlinear pressure-volume response is administered, here via a coefficient β'_0 . Thus, material nonlinearity in the pressure-volume response is captured, but geometric nonlinearity is not (a fundamental limitation inherent in the theory of Section 3). The thermoelastic strain energy nearly matches Eq. 93, with $\mathbf{e}^E$ replaced with its linear approximation $\boldsymbol{\epsilon}^E$:

$$\begin{aligned} W^U(\boldsymbol{\epsilon}^E, S, \eta, \xi) = & \frac{1}{2} \mathbf{B}(\eta, \xi, \bar{\omega}) \cdot (\text{tr} \boldsymbol{\epsilon}^E)^2 \left[1 - \frac{1}{3} \beta'_0(\eta) \cdot (\text{tr} \boldsymbol{\epsilon}^E) \right] \\ & + \mathbf{G}(\eta, \xi) \cdot (\boldsymbol{\epsilon}'^E : \boldsymbol{\epsilon}'^E) - T_0 [\gamma(\eta, \xi, \bar{\omega}) \cdot (\text{tr} \boldsymbol{\epsilon}^E) \cdot S - h(S)]. \end{aligned} \quad (174)$$

The linear deviatoric thermoelastic strain is $\boldsymbol{\epsilon}'^E = \boldsymbol{\epsilon}^E - \frac{1}{3}(\text{tr} \boldsymbol{\epsilon}^E) \mathbf{1}$; this does not contribute to volume change. Analogs of Eqs. 94–102 are as follows:

$$\begin{aligned} \mathbf{B}(\eta, \xi, \bar{\omega}) &= \mathbf{B}_0(\eta) \cdot [\chi(\xi) \cdot \bar{\omega} + (1 - \bar{\omega})], \quad \mathbf{G}(\eta, \xi) = \mathbf{G}_0(\eta) \cdot \chi(\xi), \\ \gamma(\eta, \xi, \bar{\omega}) &= \gamma_0(\eta) \cdot [\chi(\xi) \cdot \bar{\omega} + (1 - \bar{\omega})]; \end{aligned} \quad (175)$$

$$\begin{aligned} \mathbf{B}_0(\eta) &= \mathbf{B}_{0|0} + (\mathbf{B}_{0|1} - \mathbf{B}_{0|0}) \cdot \phi(\eta), \quad \beta'_0(\eta) = \beta'_{0|0} + (\beta'_{0|1} - \beta'_{0|0}) \cdot \phi(\eta), \\ \mathbf{G}_0(\eta) &= \mathbf{G}_{0|0} + (\mathbf{G}_{0|1} - \mathbf{G}_{0|0}) \cdot \phi(\eta), \quad \gamma_0(\eta) = \gamma_{0|0} + (\gamma_{0|1} - \gamma_{0|0}) \cdot \phi(\eta); \end{aligned} \quad (176)$$

$$\chi(\xi) = \zeta_0 + (1 - \zeta_0)(1 - \xi)^2; \quad (177)$$

$$f_\xi^U(\eta, \xi, S) = \Upsilon(\eta, T^e(S)) \left[\frac{1}{l_\xi} \xi^2 + l_\xi |\nabla_0 \xi|^2 \right]; \quad (178)$$

$$\hat{\beta}^\xi \dot{\xi} = -\frac{\delta \Psi}{\delta \xi} = - \left[\frac{\partial \hat{\Psi}}{\partial \xi} \Big|_{\boldsymbol{\epsilon}^E} - \mathbf{P} : \mathbf{A}^\xi - 2l_\xi \nabla_0 \cdot (\Upsilon \nabla_0 \xi) \right]; \quad \hat{\beta}^\xi = \hat{\beta}^\xi(\dot{\xi}, \eta, T) \geq 0; \quad (179)$$

$$f_{\eta 0}^U(\eta, \xi, S) = \hat{\chi}(\xi) \cdot \bar{f}_{\eta 0}^U(\eta, S), \quad f_{\eta \nabla}^U(\nabla_0 \eta, S) = \hat{\chi}(\xi) \cdot \bar{f}_{\eta \nabla}^U(\nabla_0 \eta, T^e(S)); \quad (180)$$

$$\bar{f}_{\eta \nabla}^U(\nabla_0 \eta, T^e(S)) = \frac{3}{4} \Gamma(T^e(S)) \cdot l_\eta \cdot |\nabla_0 \eta|^2, \quad (181)$$

$$\hat{\beta}^\eta \dot{\eta} = -\frac{\delta \Psi}{\delta \eta} = -\left[\frac{\partial \hat{\Psi}}{\partial \eta} \Big|_{\epsilon^E} - \mathbf{P} : \mathbf{A}^\eta - \frac{3}{2} l_\eta \nabla_0 \cdot (\Gamma \nabla_0 \eta) \right]; \quad \hat{\beta}^\eta = \hat{\beta}^\eta(\dot{\eta}, \eta, T) \geq 0. \quad (182)$$

Irreversibility and threshold constraints such as Eq. 99 for fracture can be likewise applied, replacing Eq. 179.

For comparison with stress Eq. 103 derived in the nonlinear thermoelastic model of Section 2, the thermodynamic stress $\Sigma = \mathbf{P}$ is computed from Eq. 174:

$$\mathbf{P} = \Sigma = \frac{\partial \hat{U}}{\partial \epsilon^E} = \frac{\partial W^U}{\partial \epsilon^E} = \mathbf{B} \left[1 - \frac{1}{2} \beta'_0 (\text{tr} \epsilon^E) \right] (\text{tr} \epsilon^E) \mathbf{1} + 2\mathbf{G} \epsilon'^E - T_0 \gamma S \mathbf{1}. \quad (183)$$

Classical linear isotropic thermoelasticity is recovered when $\beta'_0 = 0$. For hydrostatic thermoelastic loading $[\mathbf{h}^E = \frac{1}{3} \{\text{tr}(\epsilon^E)\} \mathbf{1}]$ and $\mathbf{P} = -p \mathbf{1}$, with p the pressure], following equation of state arises that can be compared with Eq. 104:

$$p = -(\text{tr} \epsilon^E) \mathbf{B} \left[1 - \frac{1}{2} \beta'_0 \cdot (\text{tr} \epsilon^E) \right] + T_0 \gamma S. \quad (184)$$

Compared now are outcomes of the thermoelastic parts of isotropic models for the nonlinear theory (Section 2.6.2) and the present geometrically linear theory augmented with β'_0 to address the high-pressure response. Homogeneous uniaxial strain compression is considered since high pressures are achieved, and since similar loading conditions are studied in Sections 6 and 7. In Cartesian coordinates with compression along the X_1 -axis, deformation is of the form $x_1 = (1 - \epsilon)X_1$, with $x_2 = X_2$ and $x_3 = X_3$. Compressive strain is ϵ . The deformation gradient is $\mathbf{F} = \mathbf{1} - \epsilon \mathbf{G}_1 \otimes \mathbf{G}_1$. The distortion is $\mathbf{h} = -\epsilon \mathbf{G}_1 \otimes \mathbf{G}_1$. Exact volume change is $J - 1 = F_{11} - 1 = -\epsilon$. Linearized volume change is $\text{tr}(\mathbf{h}) = -\epsilon$ and is exact in this case.

Isentropic conditions with purely elastic loading are considered, and all material coefficients are constants ($\mathbf{B} = \mathbf{B}_0$, $\mathbf{G} = \mathbf{G}_0$, etc.). For the nonlinear theory of Section 2.6.2,

$$e_{11}^E = \ln(1 - \epsilon); \quad e_{11}^{E'} = \frac{2}{3} \ln(1 - \epsilon), \quad e_{22}^{E'} = e_{33}^{E'} = -\frac{1}{3} \ln(1 - \epsilon); \quad (185)$$

$$\begin{aligned}\Sigma_{11} &= B \left[1 - \frac{1}{2} \{B'_0 - 2\} \ln(1 - \epsilon) \right] \ln(1 - \epsilon) + \frac{4}{3} G \ln(1 - \epsilon), \\ \Sigma_{22} = \Sigma_{33} &= B \left[1 - \frac{1}{2} \{B'_0 - 2\} \ln(1 - \epsilon) \right] \ln(1 - \epsilon) - \frac{2}{3} G \ln(1 - \epsilon);\end{aligned}\quad (186)$$

$$\begin{aligned}\sigma &= \frac{\Sigma}{J}, \quad P = -\sigma_{11} = -\frac{\Sigma_{11}}{J}, \\ p &= -\frac{1}{3} \text{tr} \sigma = \frac{B}{J} \left[1 - \frac{1}{2} \{B'_0 - 2\} \ln(1 - \epsilon) \right] \ln(1 - \epsilon).\end{aligned}\quad (187)$$

Here, $P = -\sigma_{11}$ is the axial compressive (Cauchy) stress and p the pressure. For the linear theory of Section 3.5.2,

$$\epsilon_{11}^E = -\epsilon; \quad \epsilon_{11}^{E'} = -\frac{2}{3}\epsilon, \quad \epsilon_{22}^{E'} = \epsilon_{33}^{E'} = \frac{1}{3}\epsilon; \quad (188)$$

$$\begin{aligned}P_{11} = \Sigma_{11} &= -B \left[1 + \frac{1}{2} \beta'_0 \epsilon \right] \epsilon - \frac{4}{3} G \epsilon, \\ P_{22} = \Sigma_{22} = \Sigma_{33} = P_{33} &= -B \left[1 + \frac{1}{2} \beta'_0 \epsilon \right] \epsilon + \frac{2}{3} G \epsilon;\end{aligned}\quad (189)$$

$$P = -P_{11} = B \left[1 + \frac{1}{2} \beta'_0 \epsilon \right] \epsilon + \frac{4}{3} G \epsilon, \quad p = -\frac{1}{3} \text{tr} \mathbf{P} = B \left[1 + \frac{1}{2} \beta'_0 \epsilon \right] \epsilon. \quad (190)$$

In the nonlinear theory, B'_0 is equal to the derivative of the isentropic tangent bulk modulus with respect to pressure at the reference state in a homogeneous elastic solid.^{55,57,72} In the geometrically linear theory, β'_0 is not precisely defined physically, but instead is treated as a corrective parameter to bring the predicted pressure from Eq. 190 into agreement with that obtained from Eq. 187.

Crystalline solids tend to have values of $2 \lesssim B'_0 \lesssim 6$, though outliers exist.^{72,114} The correspondence $\beta'_0 = 2B'_0 - 1$ is satisfactory to match pressures obtained from geometrically linear and nonlinear models for $\Xi = B'_0 = \frac{1}{2}(\beta'_0 + 1) \in [3, 5]$, a range appropriate for the specific ceramic materials investigated later in this work. Results for p (pressure) and P (axial stress) are compared in Fig. 2a and Fig. 2b, respectively, for $\epsilon \in [0, 0.2]$. Values are normalized by B . Pressure does not depend on shear modulus for the present conditions, but axial stress does. Shear modulus is chosen representatively as $G = \frac{3}{5}B$, corresponding to Poisson's ratio $\nu = (3B - 2G)/(6B + 2G) = \frac{1}{4}$. Agreement for pressure between geometrically linear and nonlinear models is clear from Fig. 2a. Axial stress P is under-predicted by the geometrically linear model at larger compression due to differences between linear and logarithmic deviatoric strain measures. However, in many real crystalline

solids, relaxation of deviatoric stress due to inelasticity mechanisms (e.g., slip, twinning, fracture, shear localization) would ensue for $\epsilon \lesssim 0.1$, before severe discrepancies with the nonlinear theory would be attained.

3.5.3 Initial Stress

Initial stress of Section 2.6.3 can be included in the same way for the geometrically linear theory. Denote the initial (e.g., residual) stress by the symmetric tensor $\tilde{\mathbf{P}}$, with components $\tilde{P}^A$ in Voigt notation. For anisotropic linear thermoelasticity, Eq. 157 and corresponding stress are augmented as

$$W^U(\boldsymbol{\epsilon}^E, S, \eta^i, \xi^j) = \tilde{P}^A(\eta^i, \xi^j, \bar{\omega}) \epsilon_A^E + \frac{1}{2} \mathbf{C}^{AB}(\eta^i, \xi^j, \bar{\omega}) \epsilon_A^E \epsilon_B^E - T_0 [\gamma^A(\eta^i, \xi^j, \bar{\omega}) \epsilon_A^E S - h(S)], \quad (191)$$

$$\mathbf{P} = \frac{\partial W^U}{\partial \boldsymbol{\epsilon}^E} = \tilde{\mathbf{P}} + \mathbf{C}^{(2)} : \boldsymbol{\epsilon}^E - T_0 \gamma S. \quad (192)$$

Analogously to interpolations in Eq. 107,

$$\begin{aligned} \tilde{P}^A(\eta^i, \xi^j, \bar{\omega}) &= \tilde{P}_0^A(\eta^i) \cdot \chi(\xi^j) \cdot \bar{\omega} + \tilde{P}_R^A(\eta^i) \cdot (1 - \bar{\omega}), \\ \tilde{P}_0^A(\eta^i) &= \tilde{P}_{0|0}^A + \sum_{i=1}^k (\tilde{P}_{0|i}^A - \tilde{P}_{0|0}^A) \cdot \eta^i [3\eta^i - 2(\eta^i)^2]. \end{aligned} \quad (193)$$

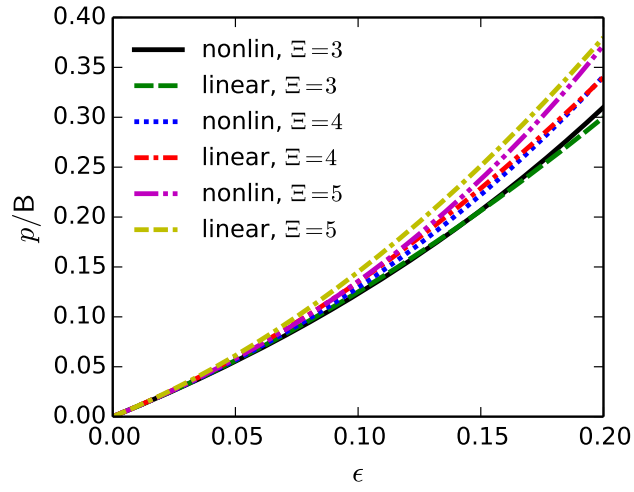
For isotropic solids, $\tilde{\mathbf{P}}$ is a spherical tensor: $\tilde{\mathbf{P}} = \tilde{P} \mathbf{1}$, with $\tilde{P}$ a scalar tensile pressure when positive. Strain energy, total stress, and order parameter dependencies in the context of the isotropic theory of Section 3.5.2 become

$$\begin{aligned} W^U(\boldsymbol{\epsilon}^E, S, \eta, \xi) &= \tilde{P}(\eta, \xi, \bar{\omega}) \cdot (\text{tr} \boldsymbol{\epsilon}^E) + \frac{1}{2} \mathbf{B}(\eta, \xi, \bar{\omega}) \cdot (\text{tr} \boldsymbol{\epsilon}^E)^2 \left[1 - \frac{1}{3} \beta'_0(\eta) \cdot (\text{tr} \boldsymbol{\epsilon}^E) \right] \\ &\quad + \mathbf{G}(\eta, \xi) \cdot (\boldsymbol{\epsilon}'^E : \boldsymbol{\epsilon}'^E) - T_0 [\gamma(\eta, \xi, \bar{\omega}) \cdot (\text{tr} \boldsymbol{\epsilon}^E) \cdot S - h(S)], \end{aligned} \quad (194)$$

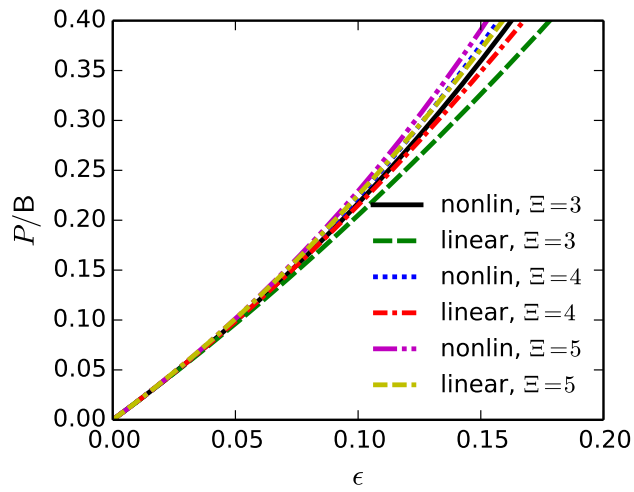
$$\mathbf{P} = \frac{\partial W^U}{\partial \boldsymbol{\epsilon}^E} = \tilde{P} \mathbf{1} + \mathbf{B} \left[1 - \frac{1}{2} \beta'_0(\text{tr} \boldsymbol{\epsilon}^E) \right] (\text{tr} \boldsymbol{\epsilon}^E) \mathbf{1} + 2\mathbf{G} \boldsymbol{\epsilon}'^E - T_0 \gamma S \mathbf{1}, \quad (195)$$

$$\tilde{P}(\eta, \xi, \bar{\omega}) = \tilde{P}_0(\eta) \cdot [\chi(\xi) \cdot \bar{\omega} + (1 - \bar{\omega})], \quad \tilde{P}_0(\eta) = \tilde{P}_{0|0} + (\tilde{P}_{0|1} - \tilde{P}_{0|0}) \cdot \phi(\eta). \quad (196)$$

Thermoelastic driving forces in kinetic laws of Eqs. 166, 170, 179, and 182 are



(a) pressure



(b) axial stress

Fig. 2 Comparison of geometrically linear and nonlinear thermoelasticity models for isentropic uniaxial strain compression: (a) pressure p versus compressive strain ϵ (b) axial compressive stress P versus compressive strain ϵ

notably affected by initial stress $\tilde{P}$.

4. Material Models and Symmetry Conditions

Specialization of the frameworks of Sections 2 and 3 to describe behaviors of three polycrystalline ceramic materials— B_4C , TiB_2 , and a composite blend of both B_4C and TiB_2 —follows next. Pertinent constitutive relations and corresponding parameters are described in each case. Most parameters are obtained from fundamental measurements (e.g., standard thermoelastic properties) or logical physical assumptions, without calibration in numerical studies. Of approximately 25 parameters for each material, only four are calibrated to match response curves in Sections 5, 6, or 7.

4.1 Boron Carbide

The isotropic frameworks of Section 2.6.2 and Section 3.5.2 are used for polycrystals with random grain orientations. The order parameter representing fracture is ξ , and the structural change order parameter η represents the crystal-to-glass solid state phase transformation, i.e., amorphization, driven by high pressure and shear.^{62,115–118} Dislocation motion is not observed in B_4C at temperatures up to 1500 K,¹¹⁹ a domain within which all calculations herein belong.

4.1.1 Thermoelasticity

Thermoelastic potentials are Eq. 93 for the geometrically and materially nonlinear theory and Eq. 174 for the geometrically linear theory with high-pressure correction (Section 3.5.2). Thermoelastic properties, with supporting references, are listed in Table 1. Previous work¹¹⁷ suggests that elastic constants, though not fully characterized for the glassy phase, should vary little among phases. For this reason and for simplicity, thermoelastic coefficients are assumed independent of η , such that $W^U = W^U(\mathbf{e}^E, S, \xi)$ in the nonlinear model and $W^U = W^U(\boldsymbol{\epsilon}^E, S, \xi)$ in the linear model.

4.1.2 Phase Field Energy

The internal energy contribution from ξ consists of the sum of quadratic terms in ξ and $|\nabla_0 \xi|$ in Eq. 97 and Eq. 178, where the two corresponding material parameters are surface energy Υ and regularization length l_ξ . Dependence of fracture surface energy Υ on temperature is omitted, since strength and fracture toughness are ef-

fectively constant from room temperature to 1500 K.¹¹⁹ Dependence of f_ξ^U on η is omitted since any differences in fracture properties of the amorphous phase versus the crystal phase are unknown. Surface energy is related to plane strain fracture toughness K_{IC} , which is readily measured experimentally, via¹²⁰

$$K_{IC}^2 = 2\psi_R E_0 \Upsilon / (1 - \nu^2), \quad 1 \leq \psi_R \lesssim 4. \quad (197)$$

Young's modulus and Poisson's ratio are E_0 and ν . The value of roughness factor $\psi_R = 2$ is used herein, which has been used elsewhere for polycrystalline diamond,¹²⁰ another very hard ceramic that fractures intragranularly similar to B_4C . No standard means of measuring the regularization length l_ξ is known for polycrystals.^{28,35} Therefore, following prior work,^{28,35} l_ξ is prescribed such that the peak load supported by a material element in tension as predicted by the phase field model matches the tensile strength P_T of the material, which is measurable (e.g., via a direct tensile test, or a multi-point bend-flexure test often used for ceramics). The analytical homogeneous solution given by the phase model is, for linear elastic response,^{11,35,95}

$$P_T = \frac{3}{16} \sqrt{6E_0 \Upsilon / l_\xi}. \quad (198)$$

Combining Eqs. 197 and 198, given the two measurable properties K_{IC} and P_T , the fracture energy is found from Eq. 197, and the regularization length is

$$l_\xi = \frac{27}{256} \frac{K_{IC}^2 (1 - \nu^2)}{\psi_R P_T^2}. \quad (199)$$

This approach alleviates a potentially unrealistic $l_\xi^{-1/2}$ dependence of peak strength on regularization length^{35,48} when the fracture energy and regularization length are prescribed as independent parameters.

Equations 197–199 are derived under assumptions of quasi-static fracture using linear isotropic elasticity and the standard phase field model,^{11,94} whereby Υ has a known interpretation as fracture energy in the Griffith sense. When a non-traditional model for fracture kinetics is invoked—incorporating elastic nonlinearity, thermal effects, and dissipative viscous effects, as well as possible coupling with other structural transformations—the total energy consumed by fracture processes will differ from that of the standard linear model. Nonetheless, the present kinetic theory of Eq. 201 or Eq. 204, in the absence of thermoelastic driving force ($\tilde{\mathcal{F}} = 0$) and in the

quasi-static limit, reduces to the phase equilibrium equation $\tilde{\mathcal{R}} = 2\xi - 2l_\xi^2 \nabla_0^2 \xi = 0$ with system energy $\int f_\xi^U d\Omega_0 = (\Upsilon/l_\xi) \int (\xi^2 + l_\xi^2 |\nabla_0 \xi|^2) d\Omega_0$. This equilibrium condition and system energy are identical to those of standard models,^{11,35} for which Υ and l_ξ have known physical interpretations related to toughness and crack width that are likewise adopted in the present work. In other words, Υ and l_ξ are assigned based on static property data such that the present theory reproduces the standard classical result in the absence of phase field dynamics (e.g., a regularized stationary crack).

Now consider transformation parameter η . Energy contributions are introduced in Eqs. 100 and 180, where for the present application, $\chi = 1$ for simplicity since the effect of fracture on phase energy density is not known. Bulk energy $f_{\eta 0}^U$ depends only on η . It consists of a double-well transformation barrier^{53,58,105} characterizing resistance to amorphization that may be preceded by twinning¹²¹ and a cubic potential accounting for the difference in energies of the glass and crystal phases.^{105,106,122} Specifically,

$$f_{\eta 0}^U(\eta) = \bar{f}_{\eta 0}^U(\eta) = A\eta^2(1-\eta)^2 + \Xi\eta^2(3-2\eta); \quad df_{\eta 0}^U(0)/d\eta = df_{\eta 0}^U(1)/d\eta = 0. \quad (200)$$

Vanishing endpoint derivatives at $\eta = 0, 1$ result in null corresponding thermodynamic driving forces for homogeneous end states. Gradient contributions $f_{\eta \nabla}^U = \bar{f}_{\eta \nabla}^U$ are quadratic forms given by Eq. 101 and Eq. 181. Surface energy of phase boundaries $\Gamma = \frac{1}{12}Al_\eta$ is constant, where l_η is the regularization length.

The value of Ξ is obtained from density functional theory (DFT)¹²² as the difference in ground state energies between the two phases. The value of A is calibrated to observations on the high-pressure response⁶² later in Section 6.2. In a single crystal, l_η could be prescribed a value on the order of 1 nm,^{47,58,105,106} commensurate with widths of observed amorphous bands.^{62,123} In a polycrystal, l_η is interpreted as a phenomenological parameter separating transformed and parent domains, where the regularization length l_η is assumed to resolve shear localization processes^{58,77} at the same scale as fracture, so is nominally assumed $l_\eta = l_\xi$. Parameter studies with other l_η/l_ξ are undertaken in Section 7, and have been reported in other work on different ceramics.¹²⁴ When A and Ξ are prescribed independently from l_η , the latter does not affect the solution of problems wherein order parameter η is spatially homogeneous.

4.1.3 Phase Field Kinetics

Addressed first is the kinetic law for evolution of the fracture order parameter ξ . Two kinetic equations are studied later in this work. The first is the classical TDGL-type equation whereby ξ evolves in time to minimize free energy of the material. From Eqs. 39, 55, 62, and 97, the TDGL fracture equation for an isotropic solid can be written as follows in non-dimensional form upon dividing both sides of Eq. 98 by Υ/l_ξ :

$$\tilde{\beta}\dot{\xi} = -\frac{l_\xi}{\Upsilon} \frac{\delta\Psi}{\delta\xi} = \tilde{\mathcal{F}} - \tilde{\mathcal{R}}, \quad \tilde{\beta} = \hat{\beta}^\xi \frac{l_\xi}{\Upsilon}. \quad (201)$$

The dimensionless thermoelastic driving force and geometric resistance³⁵ are, respectively,

$$\tilde{\mathcal{F}} = -\frac{l_\xi}{\Upsilon} \left[\frac{\partial W^U}{\partial \xi} - \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E \mathbf{A}^\xi \bar{\mathbf{F}}^{-1}) \right], \quad (202)$$

$$\tilde{\mathcal{R}} = 2(\xi - l_\xi^2 \nabla_0^2 \xi). \quad (203)$$

The second kinetic law is a version of Eq. 99 ensuring irreversible damage growth and a threshold for brittle-elastic behavior that depends on local stress state. In dimensionless form,

$$\tilde{\beta}\dot{\xi} = \langle \tilde{\mathcal{F}} - \tilde{\mathcal{R}} \rangle, \quad (204)$$

where $\tilde{\beta}$ and $\tilde{\mathcal{R}}$ are defined identically to versions in Eqs. 201 and 203. The thermoelastic driving force accounts for effects of triaxiality on fracture behavior, noting that most ceramic and brittle polycrystalline materials demonstrate pressure-dependent strength, whereby fractures (e.g., crack opening and extension) are inhibited with increasing confinement.^{28,125,126} Specifically, motivated by similar generalized forms³⁵ for brittle elastic materials,

$$\tilde{\mathcal{F}} = -\frac{d\chi(\xi)}{d\xi} \left\langle \frac{W^E + \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E \mathbf{A}^\xi \bar{\mathbf{F}}^{-1}) - \tilde{W}(\tilde{\sigma})}{\tilde{W}(\tilde{\sigma})} \right\rangle, \quad (205)$$

$$W^E(\mathbf{e}^E, S) = W^U(\mathbf{e}^E, S; \xi = 0) - T_0 h(S).$$

The thermoelastic energy density of the non-degraded solid, W^E , drives evolution of ξ , as does the conjugate mechanical force $\boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E \mathbf{A}^\xi \bar{\mathbf{F}}^{-1})$.

The threshold for onset of fracture depends on the triaxiality ratio $\tilde{\sigma}$, i.e., the ratio of mean stress to von Mises effective stress. The threshold energy is linearly interpolated among three measurable values for triaxiality ratios corresponding to

uniaxial stress tension ($\tilde{W}_T$), uniaxial stress compression ($\tilde{W}_C$), and uniaxial strain compression ($\tilde{W}_H$):

$$\tilde{W} = \begin{cases} \tilde{W}_T & (\tilde{\sigma} \geq \tilde{\sigma}_T) \\ \tilde{W}_T + (\tilde{W}_C - \tilde{W}_T) \cdot (\tilde{\sigma} - \tilde{\sigma}_T) / (\tilde{\sigma}_C - \tilde{\sigma}_T) & (\tilde{\sigma}_C \leq \tilde{\sigma} \leq \tilde{\sigma}_T) \\ \tilde{W}_C + (\tilde{W}_H - \tilde{W}_C) \cdot (\tilde{\sigma} - \tilde{\sigma}_C) / (\tilde{\sigma}_H - \tilde{\sigma}_C) & (\tilde{\sigma}_H \leq \tilde{\sigma} \leq \tilde{\sigma}_C) \\ \tilde{W}_H & (\tilde{\sigma} \leq \tilde{\sigma}_H). \end{cases} \quad (206)$$

Triaxiality ratios at discrete stress states are the following, where the linear elastic approximation is used for state $(\cdot)_H$:

$$\tilde{\sigma} = \frac{\text{tr} \boldsymbol{\sigma}}{\sigma_V} = -\frac{3p}{(\frac{3}{2} \boldsymbol{\sigma}' : \boldsymbol{\sigma}')^{1/2}}; \quad \tilde{\sigma}_T = 1, \quad \tilde{\sigma}_C = -1, \quad \tilde{\sigma}_H = -\frac{1+\nu}{1-2\nu}. \quad (207)$$

Recalling that P_T denotes static unconfined tensile strength, and denoting by P_C the measurable unconfined compressive strength of the material and P_H the Hugoniot elastic limit⁷² of the material, corresponding elastic strain energy densities are defined as follows, assuming linear response up to fracture initiation:

$$\tilde{W}_T = \frac{1}{2} \frac{P_T^2}{E_0}, \quad \tilde{W}_C = \frac{1}{2} \frac{P_C^2}{E_0}, \quad \tilde{W}_H = \frac{1}{2} \frac{P_H^2}{B_0 + \frac{4}{3} G_0}. \quad (208)$$

Values of P_C and P_H measured experimentally are given in Table 1 with source references. Viscosity coefficient $\tilde{\beta}$ listed in Table 1 is assigned following comparisons of predictions with experimental data in Sections 5.2, 6.2, and 7.2.

Geometrically linearized versions of Eqs. 201–208 are identical with the following two exceptions. First, strain energy density depends on linear elastic strain $\boldsymbol{\epsilon}^E$ rather than logarithmic elastic strain $\boldsymbol{e}^E$, so W^U and W^E are modified accordingly in Eq. 205. Secondly, the conjugate mechanical force is of a simpler form in the linear model, such total forces $\tilde{\mathcal{F}}$ in Eqs. 202 and 205 become, respectively,

$$\tilde{\mathcal{F}} = \begin{cases} -\frac{l_\xi}{\Upsilon} \left[\frac{\partial W^U}{\partial \xi} - \boldsymbol{P} : \boldsymbol{A}^\xi \right] & \text{(TDGL-type kinetics)} \\ -\frac{d\chi(\xi)}{d\xi} \left\langle \frac{W^E + \boldsymbol{P} : \boldsymbol{A}^\xi - \tilde{W}(\tilde{\sigma})}{\tilde{W}(\tilde{\sigma})} \right\rangle & \text{(irreversible with threshold).} \end{cases} \quad (209)$$

Notably, the alternative irreversible kinetic theory in Eqs. 204–209 departs from the usual variational format of the standard phase field theory wherein the driving force

for kinetics is the δ -derivative of free energy with respect to ξ . Various other models have been posited to address fractures for general stress states that are not always realistically captured by the standard model. Nucleation and propagation criteria based on strain or strain energy partitioning into tensile and compressive parts have been used,^{11,48,94} as have principal stress-based criteria.³⁵ A recent alternative¹²⁷ augments the Euler–Lagrange equation in a popular variational model^{4,10} with an external driving force. This driving force incorporates a strength surface, essentially accounting for stress-state dependent nucleation. The model proposed here in Eqs. 204–209 accounts for stress-state dependent nucleation via the triaxiality rather than via a Drucker–Prager type strength surface.¹²⁷ The presently proposed model precisely accounts for differing strengths in uniaxial stress tension, uniaxial stress compression, and uniaxial strain compression; its accuracy, when extrapolated to general 2D and 3D stress states, remains to be tested in future numerical implementations.

Now consider the structural order parameter η . Transformation kinetics considered in this work for amorphization are limited to energy minimizing, TDGL-type evolution. Using Eqs. 39, 55, 62, and 200, and noting that $\partial\hat{\Psi}/\partial\eta = \partial\hat{U}/\partial\eta = \mathrm{d}f_{\eta 0}^U/\mathrm{d}\eta$ since W^U does not depend on η , a dimensionless form of TDGL equation in Eq. 102 is obtained by dividing both sides by Ξ :

$$\bar{\beta}_A \dot{\eta} = -\frac{1}{\Xi} \frac{\delta\Psi}{\delta\eta} = \bar{\mathcal{F}} - \bar{\mathcal{R}}, \quad \bar{\beta}_A = \hat{\beta}^\eta/\Xi = \bar{\beta} \cdot \left[1 - \frac{T - T_0}{T - T_M}\right]. \quad (210)$$

Apparent viscosity $\bar{\beta}_A$ decreases linearly with temperature from the ambient (constant) value $\bar{\beta}$, increasing the transformation rate as melting is approached.^{62,63} The dimensionless thermoelastic driving force and geometric resistance are, respectively,

$$\begin{aligned} \bar{\mathcal{F}} &= \frac{1}{\Xi} \boldsymbol{\Sigma} : \mathbf{M}^E : (\mathbf{C}^E \mathbf{A}^\eta \bar{\mathbf{F}}^{-1}), \\ \bar{\mathcal{R}} &= \frac{1}{\Xi} \frac{\mathrm{d}f_{\eta 0}^U}{\mathrm{d}\eta} = 6\eta(1 - \eta) + \frac{A}{\Xi} \left[2\eta(1 - \eta)(1 - 2\eta) - \frac{1}{8} l_\eta^2 \nabla_0^2 \eta \right]. \end{aligned} \quad (211)$$

Identical equations hold for the geometrically linear case, where more general relation Eq. 182 becomes Eq. 210, with the exception that $\bar{\mathcal{F}} = \mathbf{P} : \mathbf{A}^\eta/\Xi$ in the linear analog of Eq. 211. The value of viscosity coefficient $\bar{\beta}$ listed in Table 1 is chosen based on comparison of model results with experimental observations in Sections

6.2 and 7.2.

4.1.4 Inelastic Kinematics

The total inelastic deformation $\bar{\mathbf{F}} = \mathbf{F}^\xi \mathbf{F}^\eta$ is presumed to obey Eq. 12. In the linearized theory, Eq. 117 applies, $\bar{\mathbf{h}} = \mathbf{h}^\xi + \mathbf{h}^\eta$, with $\bar{\epsilon} = \epsilon^\xi + \epsilon^\eta$ for inelastic strains.

The contribution from fracture, as described by order parameter ξ , in the isotropic case is given by the spherical deformations of Eq. 89 in the nonlinear theory and Eq. 171 in the geometrically linear theory. The lone material parameter is $\bar{\varphi}_0$, representing the maximum free volume increase due to cavitation or crack opening locally where $\xi = 1$. Values up to several percent have been explored in other works^{105,124} for compressive loading; these are of the same order of magnitude as values inferred from experiments on rocks and other ceramic materials.^{128,129} Specific values of $\bar{\varphi}_0$ are unknown for polycrystalline B_4C , so parameter studies with $\bar{\varphi}_0 = 0$ and $\bar{\varphi}_0 = 0.01$ are undertaken later in this work, to enable a general understanding of effects of bulking on predictions of the model. The latter choice is shown to enable agreement of predicted stress with shock Hugoniot data.^{60,75}

Inelastic deformation from structural changes associated with η , here amorphization, is described by Eq. 90 in the nonlinear theory and Eq. 172 in the linear case. Volume change is respectively measured by $J^\eta = \det \mathbf{F}^\eta \sqrt{\bar{g}/\bar{G}}$ in the nonlinear framework, and by $\text{tr} \epsilon^\eta \approx J^\eta - 1$ in the linear framework. Six components of the symmetric strain tensor $\mathbf{e}_0^\eta$ must be provided for arbitrary deformation histories, for both nonlinear and linear representations. However, for isotropic response and symmetric loading conditions, discussed in Section 4.4, $\mathbf{e}_0^\eta = \mathbf{e}_0^\eta(J_1^\eta, \epsilon^\eta)$, where ϵ^η is the effective deviatoric inelastic strain. The quantity ϵ^η is the scalar work conjugate to the von Mises effective stress σ_V . For simple shear by an amount γ^η , for example, $\sqrt{3}\epsilon^\eta = \gamma^\eta$ and $\sigma_V = \sqrt{3}\tau$, where τ is the shear component of Cauchy stress. High resolution transmission electron microscopy on recovered samples of B_4C containing amorphous bands⁶² produces the value of ϵ^η in Table 1, which is similar to the total inelastic strain used in theoretical studies⁵⁸ based on atomic simulation results.¹²¹ The known densification upon amorphization of 4%^{121,130,131} provides $J_1^\eta = J^\eta|_{\eta=1}$ quoted in Table 1.

4.2 Titanium Diboride

Isotropic frameworks of Sections 2.6.2 and 3.5.2 are used. Fracture is represented by ξ . The structural change order parameter η represents limited slip of partial and full dislocations on the basal plane, with corresponding stacking fault formation for the former.^{53,70,132} Slip generally is precluded except in cases where high confining pressures (e.g., shock compression or indentation) limit fracture that otherwise accommodates load relaxation,^{56,64,133} or at very high temperatures ($T \gtrsim 2000$ K) where dislocation mobility increases.¹³⁴

4.2.1 Thermoelasticity

Thermoelastic potentials are Eqs. 93 and 174 for respective nonlinear and linear theory with high-pressure correction (Section 3.5.2). Thermoelastic properties are listed in Table 2 with source references. Elastic coefficients vary among materials produced by different manufacturers; hence, several values of certain constants are listed for subsequent calculations in which model predictions are compared with data for particular materials. Specifically, those properties measured on material subjected to high-pressure experiments, sourced from Cercom (now under CoorsTek), are listed in parentheses.^{65,76,135} The bulk modulus and Poisson's ratio are notably lower in this material than those reported for other polycrystalline TiB_2 materials tabulated in the literature.^{65,136} As is usually assumed in crystalline plasticity models,⁷⁹ dislocations leave thermoelastic coefficients unchanged, such that W^U does not depend on η .

4.2.2 Phase Field Energy

The internal energy contribution from ξ is given by Eqs. 97 and 178. Dependence of fracture energy and tensile strength for regimes studied in the present work, with $T \lesssim 800\text{K}$, is omitted since flexure strength is relatively temperature-independent in this range.¹³⁶ Equations 197–199 are used to obtain surface energy and regularization length from measured toughness and tensile strength.

Relations 100 and 180 apply for phase energy from η , where $\chi = 1$ again for simplicity since the effect of fracture on dislocation energy is not known. The bulk internal energy contribution from η is given by Eq. 200, though coefficients A and Ξ now have different physical meanings. The present phase field representation of dislocation energy generalizes the single slip model for TiB_2 single crystals of prior research.^{53,70,132} The double-well potential with coefficient A accounts for intrinsic

sis dislocation glide resistance as well as nucleation barriers, and is calibrated to polycrystalline high-pressure-shear response data^{56,65,76} in Section 6.3. The cubic potential with coefficient Ξ accounts for the stored elastic energy of dislocation lines. Denote by b and b_0 the magnitudes of the partial slip vector and full Burgers vector for basal slip, and denote by ρ_D and ρ_S the scalar transient dislocation density and saturation dislocation density, both measured as line length per unit reference volume in Ω_0 . Stored elastic energy per unit volume from dislocation lines is approximated as $\frac{1}{2}G_0b^2\rho_D$.⁷⁹ Then the following relationships apply among the order parameter, Burgers vector, dislocation density, and energy coefficient:

$$\Xi = \frac{1}{2}G_0b_0^2\rho_S, \quad (\rho_D/\rho_S)(b/b_0)^2 = \phi(\eta) = \eta^2(3 - 2\eta). \quad (212)$$

Gradient contributions $f_{\eta\nabla}^U = \bar{f}_{\eta\nabla}^U$ are quadratic forms in respective Eqs. 101 and 181, and surface energy is $\Gamma = \frac{1}{12}Al_\eta$, where l_η is viewed as a phenomenological regularization parameter at the polycrystal scale. For homogeneous order parameter fields, l_η does not affect model predictions when A and Ξ are prescribed independently. For heterogeneous fields, $l_\eta/l_\xi = 1$ is assumed nominally, with other values explored parametrically in Section 7.3.

4.2.3 Phase Field Kinetics

Identical forms of fracture kinetic equations to those in Section 4.1.3 are used for polycrystalline TiB₂, specifically Eqs. 201–208. Corresponding strength parameters P_C and P_H measured experimentally are given in Table 2 with references. Viscosity coefficient $\tilde{\beta}$ is calibrated following analysis in Sections 5.3 and 6.3. Identical kinetic laws for η to those of Section 4.1.3 are also invoked for TiB₂, where now dislocation nucleation and glide are described rather than solid state amorphization. Viscosity coefficient $\bar{\beta}$ in Table 2 is obtained via comparison of model results with experimental observations in Sections 6.3 and 7.3.

4.2.4 Inelastic Kinematics

The general treatment discussed in Section 4.1.4 applies for TiB₂. The possible contribution to inelastic strain from fracture is given by Eqs. 89 and 171, where $\bar{\varphi}_0$ is likewise not known precisely so is varied from 0 to 0.01 in forthcoming calculations. Inelastic deformation from restricted dislocation slip associated with η is described by Eq. 90 in the nonlinear theory and Eq. 172 in the linear model. For isotropic polycrystalline material and symmetric loading conditions of the sort described in

Section 4.4 and implemented in Sections 5, 6, and 7, it follows that $\mathbf{e}_0^\eta = \mathbf{e}_0^\eta(J_1^\eta, \epsilon^\eta)$. Effective deviatoric plastic strain^{53,70,132} and residual volume change from dislocations at state $\eta = 1$ are, respectively,^{71,72}

$$\epsilon^\eta = \frac{1}{2}\gamma^\eta = \frac{1}{2}\rho_S b_0 \bar{x}, \quad J_1^\eta = 1 + \frac{\Xi}{G_0} \left(G'_0 - \frac{G_0}{B_0} \right). \quad (213)$$

From published findings,^{53,64,133} the mean slipped distance of dislocations in shock-loaded TiB₂ is $\bar{x} = 50$ nm, the saturation density is $\rho_D = 10^{15} \text{m}^{-2}$, and $b_0 = 0.303$ nm for basal slip,⁷⁰ furnishing the value of ϵ^η in Table 2. Volume change J_1^η can be obtained from various analytical derivations,^{137–140} where G'_0 is the ambient pressure derivative of the shear modulus. For this material, volume change from dislocation lines is positive (i.e., expansive), but very small.

4.3 Ceramic Composite

The ceramic composite, discussed in recent papers,^{70,78} consists of 77% by volume B₄C and 23% by volume TiB₂. It is referred to as B₄C-TiB₂, with a mass density just under 3.0 g/cc. Some comparisons with data on another B₄C-TiB₂ composite with 35% by volume TiB₂^{67–69} (density of 3.2 g/cc) are also made later in this work, since fully comprehensive data and properties do not exist for materials of either composition. Isotropic frameworks of Sections 2.6.2 and 3.5.2 are used. Fracture is represented by ξ , which occurs in both phases of the composite and along grain and phase boundaries.^{70,78} Order parameter η represents limited slip of partial and full dislocations in the TiB₂ phase, since such dislocations and stacking faults have been observed after hardness testing on the composite.^{70,78} Amorphization has not been observed in B₄C grains within the composite, though it may be possible under extreme loading conditions. However, to maintain simplicity of the model (only two order parameters in the isotropic case), amorphization is not addressed for the composite in the present work.

4.3.1 Thermoelasticity

Thermoelastic potentials are Eqs. 93 and 174. Thermoelastic properties, with supporting references, are listed in Table 3. Second-order elastic constants have been measured directly, as indicated by supporting references. Other properties that have not been measured are calculated using a mixture rule (e.g., Voigt-type averages) of properties of constituent phases from Tables 1 and 2, assuming 23% by volume of the TiB₂ phase. As in Section 4.2.1, strain energy density is assumed unaffected

by η since dislocations are not expected to substantially affect thermoelastic coefficients.

4.3.2 Phase Field Energy

As was the case for the other two ceramics, the internal energy contribution from ξ is included in Eqs. 97 and 178. The fracture contribution to internal energy density is addressed in the same manner as in Sections 4.1.2 and 4.2.2, though different material properties apply as is evident from Table 3. The order parameter η represents effects of partial and full dislocations and stacking faults, but only in the TiB_2 grains of the composite. The same equations referenced in Section 4.2.2 apply (e.g., Eqs. 100 and 180 with $\chi = 1$), as does Eq. 200 for the bulk energy contribution. However, parameters A and Ξ are modified since dislocations are present only in the TiB_2 , and not the B_4C , grains. Let v_1 denote the volume fraction of TiB_2 in the composite. Then the saturation density $\rho_S \rightarrow v_1 \rho_S$ such that $\Xi \rightarrow v_1 \Xi$ for the composite relative to pure TiB_2 . Similarly, energy per unit total composite volume associated with slip and nucleation resistance $A \rightarrow v_1 A$. Thus, in a material saturated with dislocations where $\eta = 1$, internal energy per total volume of the composite is v_1 that of the pure TiB_2 grains within.

4.3.3 Phase Field Kinetics

Forms of fracture kinetic equations nearly identical to those in Section 4.1.3 are used for the B_4C - TiB_2 composite, specifically Eqs. 201–208. The only difference from the framework of Sections 4.1.3 and 4.2.3 is augmentation of the crack growth resistance due to the effect of temperature change on residual stresses. This phenomenon arises from the mismatch in thermal expansion coefficients of B_4C and TiB_2 grains in the composite.^{70,141,142} These residual stresses are thought to contribute to increased toughness of the composite relative to monolithic polycrystalline B_4C and TiB_2 .^{70,78} When temperature T increases above room temperature T_0 , residual stresses are relaxed and the toughening decreases. The analytical solution from a self-consistent theory¹⁰⁹ is used to estimate the effect of temperature change on fracture toughness entering the crack resistance, leading to a reduction that manifests from relaxation of thermal residual stresses with heating. Thermoelastic properties from Tables 1 and 2 are used, along with thermal expansion coefficients for each phase.^{136,143} The result is $K_{IC}(T) = K_{IC}(T_0) \cdot [1 - c_K(T - T_0)]$, where $c_K = -(dK/dT)/K_{IC}(T_0)$ computed using the theory¹⁰⁹ is given in Table 3. The corresponding dimensionless kinetic resistance entering Eqs. 201 and 204 be-

comes the following for the composite since $\Upsilon \propto K_{IC}^2$ via Eq. 197:

$$\tilde{\mathcal{R}} = 2(\xi - l_\xi^2 \nabla_0^2 \xi)[1 - c_K(T - T_0)]^2. \quad (214)$$

Static tensile and compressive strength parameters P_C and P_H measured experimentally are listed in Table 3 with references. Viscosity coefficient $\tilde{\beta}$ is calibrated following analysis in Sections 5.4 and 6.4. The same kinetic laws for η to those of Section 4.1.3 are also invoked for the composite, where as in Section 4.2.3, dislocation nucleation and limited glide are described rather than amorphization. Viscosity coefficient $\tilde{\beta}$ listed in Table 3 is assumed to match that used for the pure TiB_2 material since mobile dislocations are assumed only to nucleate within crystals of this phase of the composite.

4.3.4 Inelastic Kinematics

The treatment of inelastic deformation is identical to that described in Section 4.2.4. Dilatation from fracture or cavitation is addressed by material property $\bar{\varphi}_0$, where values of 0 and 0.01 are again explored parametrically. Inelastic deformation from dislocation glide in the TiB_2 phase is characterized, for isotropic symmetric response, by the two parameters ϵ^η and J_1^η . Since dislocations are assumed only to exist in the TiB_2 grains of the composite, with volume fraction of TiB_2 denoted by v_1 , it follows that $\rho_S \rightarrow v_1 \rho_S$ and, as mentioned already in Section 4.3.2, $\Xi \rightarrow v_1 \Xi$ from pure TiB_2 to the composite. The end result is a fractional reduction of parameters defined in Eq. 213 according to $v_1 = 0.23$ for the present material composition, with values shown in Table 3.

Table 1 Boron carbide: physical properties or parameters for polycrystalline B₄C at $T_0 = 295$ K (except T_M)

Parameter (units)	Definition	Value	Reference or source
B_0 (GPa)	bulk modulus	205	Vogler, ⁶⁰ Swab ⁷³
G_0 (GPa)	shear modulus	187	[same as above]
E_0 (GPa)	Young's modulus	430	
ν (-)	Poisson's ratio	0.15	
B'_0 (-)	pressure derivative of bulk modulus	4.7	Dodd ¹⁴⁴
β'_0 (-)	nonlinear correction	8.4	$\beta'_0 \approx 2B'_0 - 1$; see Section 3.5.2
G'_0 (-)	pressure derivative of shear modulus	0.8	Dodd ¹⁴⁴
C'_0 (-)	fourth-order elastic constant	20	calibrated to Vogler ⁶⁰ ; see Section 6.2
ρ_0 (g/cm ³)	mass density	2.51	Dandekar, ¹⁴⁵ Vogler ⁶⁰
γ_0 (-)	Grüneisen parameter	1.28	Dandekar, ¹⁴⁵ Clayton ⁶¹
c_0 (MPa/K)	specific heat at constant volume	2.41	Dandekar, ¹⁴⁵ Dodd ¹⁴⁴
T_M (K)	melt temperature (at $p \gtrsim 50$ GPa)	2500 (≈ 2000)	Zhao ⁶²
K_{IC} (MPa·m ^{1/2})	fracture toughness	2.5	Paliwal ⁷⁴
P_T (GPa)	static tensile strength	0.45	Swab ⁷³
l_ξ (μ m)	fracture regularization length	1.6	Eq. 199
l_η/l_ξ (-)	amorphization regularization length	1	assumed
Ξ (GPa)	energy difference between glass and crystal phases	0.188	Fanchini, ¹²² Clayton ⁵³
A (GPa)	energy barrier for transformation, nonlinear (linear) theory	20 (29)	calibrated to Zhao ⁶² ; see Section 6.2
φ_0 (-)	bulking coefficient from fracture under pressure-shear loading	0 or 0.01	assumed
ϵ^η (-)	max inelastic shear accommodation by amorphous phase	0.5	An, ¹²¹ Zhao ⁶²
J_1^η (-)	density ratio of crystalline to amorphous phase	0.96	Yan, ¹³⁰ An ¹²¹
P_C (GPa)	static unconfined compressive strength	6.1	Swab ⁷³
P_H (GPa)	Hugoniot elastic limit (HEL)	18.0	Vogler ⁶⁰
$\tilde{\beta}$ (s)	viscosity for crack kinetics	$1 \cdot 10^{-7}$	calibrated to Vogler ⁶⁰ in Section 7.2
β (s)	viscosity for transformation kinetics	$1 \cdot 10^{-9}$	calibrated to Zhao ⁶² in Section 6.2

Table 2 Titanium diboride: physical properties or parameters for TiB₂ at $T_0 = 295$ K (except T_M)

Parameter (units)	Definition	Value	Reference or source
B_0 (GPa)	bulk modulus	240 (193)	Munro ¹³⁶ (Dandekar ⁶⁵)
G_0 (GPa)	shear modulus	255 (249)	[same as above]
E_0 (GPa)	Young's modulus	565 (522)	
ν (-)	Poisson's ratio	0.11 (0.05)	
B'_0 (-)	pressure derivative of bulk modulus	3.91 (2.02)	Dodd ¹⁴⁶ (Dandekar ^{65,147})
β'_0 (-)	nonlinear correction	6.82	$\beta'_0 \approx 2B'_0 - 1$; see Section 3.5.2
G'_0 (-)	pressure derivative of shear modulus	2.53	Dodd ¹⁴⁶
ρ_0 (g/cm ³)	mass density	4.51	Dodd, ¹⁴⁶ Dandekar ⁶⁵
γ_0 (-)	Grüneisen parameter	1.31	
c_0 (MPa/K)	specific heat at constant volume	2.78	Munro ¹³⁶
T_M (K)	melt temperature	3500	Munro ¹³⁶
K_{IC} (MPa·m ^{1/2})	fracture toughness	6.2	Munro ¹³⁶
P_T (GPa)	static tensile strength	0.40	Munro ¹³⁶
l_ξ (μm)	fracture regularization length	12.6	Munro ¹³⁶
l_η/l_ξ (-)	slip regularization length	1	Eq. 199
Ξ (GPa)	stored energy coefficient for dislocation lines	0.012	assumed
A (GPa)	energy barrier for slip	0.2	Clayton ^{53,70}
φ_0 (-)	bulking coefficient from fracture under pressure-shear loading	0 or 0.01	calibrated to Dandekar, ⁶⁵ Grady ⁷⁶ in Section 6.3
ϵ'' (-)	saturation inelastic shear accommodation from slip	$7.6 \cdot 10^{-3}$	assumed
$J_1^n - 1$ (-)	expansion from dislocations at saturation	$6.7 \cdot 10^{-5}$	Eq. 213
P_C (GPa)	static unconfined compressive strength	6.0	Eq. 213
P_H (GPa)	Hugoniot elastic limit (first plastic wave)	7.0	Blumenthal ¹⁴⁸
p_L (GPa)	locking pressure for crack arrest	4	Dandekar, ⁶⁵ Grady ⁷⁶
$\tilde{\beta}$ (s)	viscosity for crack kinetics	$1 \cdot 10^{-7}$	calibrated to Dandekar ⁶⁵ in Section 6.3
β (s)	viscosity for transformation kinetics	$5 \cdot 10^{-7}$	calibrated in Sections 5.3 and 6.3 calibrated to Grady ⁷⁶ in Section 7.3

Table 3 Ceramic composite: properties or parameters for B₄C-23 vol. % TiB₂, $v_1 = 0.23$, at $T_0 = 295$ K

Parameter (units)	Definition	Value	Reference or source
B_0 (GPa)	bulk modulus	211	Clayton, ⁷⁰ Brennan ¹⁴⁹
G_0 (GPa)	shear modulus	200	[same as above]
E_0 (GPa)	Young's modulus	456	
ν (-)	Poisson's ratio	0.14	
B'_0 (-)	pressure derivative of bulk modulus	4.52	mixture rule
β'_0 (-)	nonlinear correction	8.04	$\beta'_0 \approx 2B'_0 - 1$; see Section 3.5.2
ρ_0 (g/cm ³)	mass density	2.98	Rubink, ⁷⁸ Clayton ⁷⁰
γ_0 (-)	Grüneisen parameter	1.29	mixture rule
c_0 (MPa/K)	specific heat at constant volume	2.50	mixture rule
K_{IC} (MPa·m ^{1/2})	fracture toughness	6.9	Rubink ⁷⁸
P_T (GPa)	static tensile strength	0.52	Rubink ⁷⁸
l_ξ (μ m)	fracture regularization length	9.1	Eq. 199
l_η/l_ξ (-)	slip regularization length	1	assumed
Ξ (GPa)	stored energy coefficient for dislocation lines	0.003	$v_1 \times$ value in Table 2
A (GPa)	energy barrier for slip	0.046	[same as above]
ϵ^η (-)	saturation inelastic shear accommodation from slip	$1.7 \cdot 10^{-3}$	Eq. 213
$J_1^\eta - 1$ (-)	expansion from dislocations at saturation	$1.6 \cdot 10^{-5}$	Eq. 213
P_C (GPa)	static unconfined compressive strength	5.3	Gao ⁶⁷
P_H (GPa)	Hugoniot elastic limit	16.0	Gao ⁶⁸
β (s)	viscosity for crack kinetics	$3 \cdot 10^{-4}$	calibrated to Gao, ⁶⁷ Rubink ⁷⁸ in Section 5.4
$\bar{\beta}$ (s)	viscosity for transformation kinetics	$5 \cdot 10^{-7}$	same as in Table 2
c_K (1/K)	thermal residual stress effect on toughness	$1.2 \cdot 10^{-4}$	Taya ¹⁰⁹

4.4 Symmetry Reductions for Axisymmetric Uniaxial Loading

Calculations invoke specific forms of geometry, kinematics, and governing equations in cylindrical curvilinear coordinates. The nonlinear description follows in Sections 4.4.1 and 4.4.2, with geometric linearization discussed in Section 4.4.3.

4.4.1 Geometry and Kinematics

Referential and spatial cylindrical coordinates are denoted, respectively, by the triplets (R, Θ, Z) and (r, θ, z) . A right circular cylindrical domain of material is modeled for calculations of Sections 5, 6, and 7. In Sections 5 and 6, $Z \in [0, L_0]$, while an infinite length $Z \in (-\infty, \infty)$ is examined in wave propagation studies of Section 7. In all cases, $R \in [0, R_0]$ and $\Theta \in (-\pi, \pi]$.

Motions and order parameter fields studied herein are of the following axisymmetric forms, or are subsets of these forms:

$$r = r(R, t), \quad \theta = \Theta, \quad z = z(Z, t); \quad \xi = \xi(R, Z, t), \quad \eta = \eta(R, Z, t). \quad (215)$$

Natural basis vectors in configurations Ω_0 and Ω are, respectively, $(\mathbf{G}_R, \mathbf{G}_\Theta, \mathbf{G}_Z)$ and $(\mathbf{g}_r, \mathbf{g}_\theta, \mathbf{g}_z)$. In physical components,⁸² dimensionless basis vectors are $(\mathbf{G}_R, \mathbf{E}_\Theta, \mathbf{G}_Z)$ and $(\mathbf{g}_r, \mathbf{e}_\theta, \mathbf{g}_z)$, where $\mathbf{E}_\Theta = \mathbf{G}_\Theta/R$ and $\mathbf{e}_\theta = \mathbf{g}_\theta/r$. Metric tensors are $\mathbf{G} = \text{diag}(1, R^2, 1)$ and $\mathbf{g} = \text{diag}(1, r^2, 1)$. The deformation gradient and Jacobian determinant are

$$\begin{aligned} \mathbf{F} &= \partial_R r \mathbf{g}_r \otimes \mathbf{G}^R + \mathbf{g}_\theta \otimes \mathbf{G}^\Theta + \partial_Z z \mathbf{g}_z \otimes \mathbf{G}^Z \\ &= \partial_R r \mathbf{g}_r \otimes \mathbf{G}^R + \frac{r}{R} \mathbf{e}_\theta \otimes \mathbf{E}^\Theta + \partial_Z z \mathbf{g}_z \otimes \mathbf{G}^Z, \\ J &= (\partial_R r) \frac{r}{R} (\partial_Z z). \end{aligned} \quad (216)$$

As first proposed* in a monograph,⁷⁹ first analyzed in a paper,⁸⁸ and first implemented for solutions of geometrically nonlinear inelasticity problems in other papers,^{47,59} coincident (i.e., shifted) basis vectors from Ω_0 are used in intermediate configuration $\bar{\Omega}$:

$$\bar{\mathbf{g}}_\alpha = \delta_\alpha^K \mathbf{G}_K, \quad \bar{\mathbf{g}}^\alpha = \delta_A^\alpha \mathbf{G}^K; \quad \bar{g}_{\alpha\beta} = \delta_\alpha^J G_{JK} \delta_\beta^K, \quad \bar{g} = G. \quad (217)$$

*An equivalent metric $\bar{g}_{\alpha\beta}(\mathbf{X}) = \delta_\alpha^J G_{JK}(\mathbf{X}) \delta_\beta^K$ was posited by JC Simo,¹⁵⁰ but corresponding basis vectors and Christoffel symbols on $\bar{\Omega}$ were not.

Torsion and Riemann–Christoffel curvature tensors constructed from $\bar{g}_{\alpha\beta}$ using geometric definitions do not generally vanish in configuration $\bar{\Omega}$ as proven in analysis elsewhere.^{82,88} These features are inconsequential herein, where covariant differentiation is performed in Ω_0 as opposed to anholonomic space $\bar{\Omega}$ as considered in other work,⁶¹ for example. The almost universally applied assumption in the finite plasticity literature, $\bar{g}_{\alpha\beta} = \delta_{\alpha\beta}$,^{87,151} is inefficient and unwieldy for analysis of cylindrical geometries, as well as other problems best described in general curvilinear coordinate systems.

Elastic and inelastic deformation gradients are diagonal. The former, in natural coordinates, is as follows, with determinant $J^E = (g/\bar{g})^{1/2} \det \mathbf{F}^E$:

$$\begin{aligned}\mathbf{F}^E &= (F^E)_R^r \mathbf{g}_r \otimes \mathbf{G}^R + (F^E)_\Theta^\theta \mathbf{g}_\theta \otimes \mathbf{G}^\Theta + (F^E)_Z^z \mathbf{g}_z \otimes \mathbf{G}^Z, \\ J^E &= (F^E)_R^r (F^E)_\Theta^\theta (F^E)_Z^z \frac{r}{R}.\end{aligned}\quad (218)$$

The logarithmic thermoelastic strain of Eq. 19 consists of three diagonal mixed-variant components:

$$\begin{aligned}(e^E)_R^R &= \ln[(F^E)_R^r], & (e^E)_\Theta^\Theta &= \ln \left[\frac{r}{R} (F^E)_\Theta^\theta \right], & (e^E)_Z^Z &= \ln[(F^E)_Z^z]; \\ \text{tr} \mathbf{e}^E &= \ln \left[(F^E)_R^r (F^E)_\Theta^\theta (F^E)_Z^z \frac{r}{R} \right].\end{aligned}\quad (219)$$

Total inelastic deformation $\bar{\mathbf{F}} = \mathbf{F}^\xi \mathbf{F}^\eta$ is diagonal, where $\mathbf{F}^\xi$ is spherical according to Eq. 89:

$$(F^\xi)_R^R = (F^\xi)_\Theta^\Theta = (F^\xi)_Z^Z = [1 - \bar{\varphi}_0(3\xi^2 - 2\xi^3)]^{-1/3}. \quad (220)$$

Deformation associated with η is diagonal, where from Eq. 90,

$$\mathbf{F}^\eta = \mathbf{G}_K \otimes \mathbf{G}^K + (3\eta^2 - 2\eta^3) \left[(e_0^\eta)_R^R \mathbf{G}_R \otimes \mathbf{G}^R + (e_0^\eta)_\Theta^\Theta \mathbf{G}_\Theta \otimes \mathbf{G}^\Theta + (e_0^\eta)_Z^Z \mathbf{G}_Z \otimes \mathbf{G}^Z \right]. \quad (221)$$

Components of $\mathbf{e}_0^\eta(\epsilon^\eta, J_1^\eta)$ are of the following form for cylindrical axisymmetric problems in an isotropic body, in terms of deviatoric inelastic strain parameter ϵ^η

and volumetric inelastic strain parameter J_1^η introduced in Section 4.1.4:

$$(e_0^\eta)_R^R = (e_0^\eta)_\Theta^\Theta = (J_1^\eta)^{1/3} \exp\left(\pm \frac{1}{2} \epsilon^\eta\right) - 1, \quad (e_0^\eta)_Z^Z = (J_1^\eta)^{1/3} \exp(\mp \epsilon^\eta) - 1. \quad (222)$$

For compressive straining in the Z -direction, $\epsilon^\eta > 0$, and vice versa for extension along Z .

From Eq. 215, and using Christoffel symbols of the Levi–Civita connection from G_{AB} ⁸² $\Gamma_{\Theta R}^\Theta = \Gamma_{R\Theta}^\Theta = 1/R$ and $\Gamma_{\Theta\Theta}^R = -R$, the material gradient and Laplacian of order parameter fields are

$$\begin{aligned} \nabla_0 \xi &= \partial_R \xi \mathbf{G}^R + \partial_Z \xi \mathbf{G}^Z, & \nabla_0^2 \xi &= \frac{1}{R} \partial_R (R \partial_R \xi) + \partial_{ZZ}^2 \xi; \\ \nabla_0 \eta &= \partial_R \eta \mathbf{G}^R + \partial_Z \eta \mathbf{G}^Z, & \nabla_0^2 \eta &= \frac{1}{R} \partial_R (R \partial_R \eta) + \partial_{ZZ}^2 \eta. \end{aligned} \quad (223)$$

Finally, the density of geometrically necessary dislocations^{79,83,84} is constructed for analysis of cases in which the deviatoric part of $\mathbf{F}^\eta$ accounts for plastic slip. Define the deviatoric inelastic deformation gradient as

$$\bar{\mathbf{F}}^\eta(\eta) = \mathbf{1} + \bar{\mathbf{e}}_0^\eta \phi(\eta), \quad \bar{\mathbf{e}}_0^\eta(\epsilon^\eta) = \mathbf{e}_0^\eta(\epsilon^\eta; J_1^\eta = 1). \quad (224)$$

The geometrically necessary dislocation density (GND) tensor considered herein is the two-point tensor

$$\rho_G = -\nabla_0 \times \bar{\mathbf{F}}^\eta \quad \leftrightarrow \quad \rho_G^{\alpha J} = \epsilon^{JKL} \partial_L (\bar{\mathbf{F}}^\eta)_K^\alpha = \frac{1}{\sqrt{G}} e^{JKL} \partial_L (\bar{\mathbf{F}}^\eta)_K^\alpha. \quad (225)$$

Use of Eq. 225 is restricted in this work to plane-wave problems of Section 7, whereby $\bar{\mathbf{F}}^\eta = \bar{\mathbf{F}}^\eta(Z, t)$ and $\eta = \eta(Z, t)$. In this class of problems, the GND tensor has two components, equal in magnitude and opposite in sign.^{72,108} From plastic incompressibility and material symmetry, $(\bar{\mathbf{F}}^\eta)_R^R = (\bar{\mathbf{F}}^\eta)_\Theta^\Theta = [(\bar{\mathbf{F}}^\eta)_Z^Z]^{-1/2}$, the GND tensor can be derived as

$$\begin{aligned} \rho_G &= \frac{1}{2R} [(\bar{\mathbf{F}}^\eta)_Z^Z]^{-3/2} \partial_Z (\bar{\mathbf{F}}^\eta)_Z^Z (\mathbf{G}_R \otimes \mathbf{G}_\Theta - \mathbf{G}_\Theta \otimes \mathbf{G}_R) \\ &= \frac{1}{2R} [(\bar{\mathbf{F}}^\eta)_Z^Z]^{-3/2} (\bar{\mathbf{e}}_0^\eta)_Z^Z \frac{d\phi}{d\eta} \partial_Z \eta (\mathbf{G}_R \otimes \mathbf{G}_\Theta - \mathbf{G}_\Theta \otimes \mathbf{G}_R). \end{aligned} \quad (226)$$

The scalar magnitude of geometrically necessary dislocations, measured as line

length per unit volume, is then, with b_0 the Burgers vector magnitude,

$$\rho_G = \frac{1}{b_0} |\boldsymbol{\rho}_G : \boldsymbol{\rho}_G|^{1/2} = \frac{\sqrt{2}}{b_0} [(\bar{F}^\eta)_Z^Z]^{-3/2} |6(\bar{e}_0^\eta)_Z^Z \eta(1 - \eta) \partial_Z \eta|. \quad (227)$$

4.4.2 Stresses and Balance Laws

For an isotropic solid under the symmetric deformation modes of Section 4.4.1, stress tensors are diagonal. From constitutive equality Eq. 45 and thermoelastic potential Eq. 93, the conjugate stress $\boldsymbol{\Sigma} = \partial \hat{U} / \partial \mathbf{e}^E$ consists of three nonzero components:

$$\begin{aligned} \Sigma_R^R &= B \left[1 - \frac{1}{2} \{B'_0 - 2\} \cdot (\text{tr} \mathbf{e}^E) \right] (\text{tr} \mathbf{e}^E) + 2G(e'^E)_R^R - T_0 \gamma S, \\ \Sigma_\Theta^\Theta &= B \left[1 - \frac{1}{2} \{B'_0 - 2\} \cdot (\text{tr} \mathbf{e}^E) \right] (\text{tr} \mathbf{e}^E) + 2G(e'^E)_\Theta^\Theta - T_0 \gamma S, \\ \Sigma_Z^Z &= B \left[1 - \frac{1}{2} \{B'_0 - 2\} \cdot (\text{tr} \mathbf{e}^E) \right] (\text{tr} \mathbf{e}^E) + 2G(e'^E)_Z^Z - T_0 \gamma S. \end{aligned} \quad (228)$$

First Piola–Kirchhoff and Cauchy stress components are found simply from Eqs. 46 and 47 as

$$P_r^R = J \sigma_r^r / F_R^r = \Sigma_r^r / \partial_R r, \quad P_\theta^\Theta = J \sigma_\theta^\theta / F_\Theta^\theta = \Sigma_\Theta^\Theta, \quad P_z^Z = J \sigma_z^z / F_Z^z = \Sigma_Z^Z / \partial_Z z. \quad (229)$$

Mass conservation Eq. 20 is as follows in Lagrangian rate form, noting that the velocity vector is $\mathbf{v} = \dot{r} \mathbf{g}_r + \dot{z} \mathbf{g}_z$:

$$-\dot{\rho} / \rho = \dot{J} / J = \frac{1}{r} \partial_r (r \dot{r}) + \partial_z \dot{z}. \quad (230)$$

Linear momentum conservation law Eq. 21 reduces to two non-trivial equations, where the total covariant derivative operation^{79,82} is applied towards the divergence of two-point tensor field $\mathbf{P}(R, Z, t)$:

$$\partial_R P_r^R + \frac{1}{R} \left(P_r^R - \frac{R}{r} P_\theta^\Theta \right) = \rho_0 \ddot{r}, \quad \partial_Z P_z^Z = \rho_0 \ddot{z}. \quad (231)$$

From Eqs. 45, 97, and 101, conjugate forces to order parameter gradients are

$$\mathbf{s}^\xi = 2\Upsilon l_\xi \nabla_0 \xi, \quad \mathbf{s}^\eta = \frac{3}{2} \Gamma l_\eta \nabla_0 \eta. \quad (232)$$

Microforce balances in Eq. 24 become, with Eq. 223,

$$\pi^\xi = -2\Upsilon l_\xi \left[\frac{1}{R} \partial_R (R \partial_R \xi) + \partial_{ZZ}^2 \xi \right], \quad \pi^\eta = -\frac{3}{2} \Gamma l_\eta \left[\frac{1}{R} \partial_R (R \partial_R \eta) + \partial_{ZZ}^2 \eta \right]. \quad (233)$$

The energy balance in Eq. 29 is $T\dot{S} = \mathfrak{D} - \nabla_0 \cdot \mathbf{Q}$. For adiabatic problems, heat flux vanishes. Internal dissipation is given in general form by Eq. 38. For the kinetic equations outlined in Sections 4.1, 4.2, and 4.3, entropy production in the adiabatic case becomes

$$T\dot{S} = \mathfrak{D} = \hat{\pi}^\xi \dot{\xi} + \hat{\pi}^\eta \dot{\eta} = \hat{\pi}^\xi \dot{\xi} + \bar{\beta}_A^\eta \Xi \dot{\eta}^2. \quad (234)$$

When the TDGL kinetic law for $\dot{\xi}$ from Eq. 201, is invoked, then $\hat{\pi}^\xi \dot{\xi} = \tilde{\beta} \Upsilon \dot{\xi}^2 / l_\xi$ is the contribution from fracture to dissipation. Otherwise, when Eq. 204 applies, Eq. 69 is used to obtain $\hat{\pi}^\xi$.

From Eqs. 45 and 93 and truncating $h(S)$ in Eq. 72 to second order in S , temperature is

$$T = T_0 \cdot (1 + S/c_0 - \gamma \text{tr} \mathbf{e}^E). \quad (235)$$

For isothermal problems, $T = T_0 = \text{constant}$, such that $S = c_0 \gamma \text{tr}(\mathbf{e}^E)$. Heat transport compensates for internal dissipation $\mathfrak{D} \geq 0$ such that $\dot{T} = 0$. Values of elastic constants in Tables 1, 2, and 3 correspond to isentropic moduli. The reference shear modulus, G_0 , of isotropic solids is identical under isentropic or isothermal conditions. The ratio of isentropic to isothermal bulk moduli is equal to the ratio of specific heat at constant pressure to specific heat at constant volume^{79,112}: $B_0^S/B_0^T = c_0^\Sigma/c_0^E = 1 + \gamma_0 T_0 \text{tr}(\mathbf{a}_0^E)$. For thermoelastic properties of B_4C and TiB_2 , $\gamma_0 T_0 \text{tr}(\mathbf{a}_0^E) \lesssim 0.008$, such that the difference in bulk moduli is less than 1% at room temperature, which is on the order of accuracy of experimental measurements. Hence, the distinction between isothermal and isentropic elastic constants is safely ignored when isothermal problems are studied later.

4.4.3 Alternative Intermediate Basis Vectors

An equivalent and equally efficient description of the nonlinear problem is afforded by use of coincident basis vectors between Ω and $\bar{\Omega}$. In this description,

first proposed in the monograph⁷⁹ and analyzed geometrically by the author in later works,^{82,88} Eq. 217 is replaced with

$$\bar{\mathbf{g}}_\alpha = \delta_\alpha^k \mathbf{g}_k, \quad \bar{\mathbf{g}}^\alpha = \delta_k^\alpha \mathbf{g}^k; \quad \bar{g}_{\alpha\beta} = \delta_\alpha^j g_{jk} \delta_\beta^k, \quad \bar{g} = g. \quad (236)$$

The shifter tensor between reference and spatial basis vectors, with components $g_J^i = \mathbf{g}^i \cdot \mathbf{G}_J$, has the following non-vanishing components and determinant for cylindrical coordinate systems when $\theta = \Theta$ ⁸²:

$$g_R^r = g_Z^z = 1, \quad g_\Theta^\theta = 1/g_\theta^\Theta = R/r; \quad \det(g_J^i) = \sqrt{G/g} = R/r. \quad (237)$$

The elastic deformation gradient is written as follows in terms of the basis Eq. 236:

$$\mathbf{F}^E = (F^E)_r^r \mathbf{g}_r \otimes \mathbf{g}^r + (F^E)_\theta^\theta \mathbf{g}_\theta \otimes \mathbf{g}^\theta + (F^E)_z^z \mathbf{g}_z \otimes \mathbf{g}^z, \quad J^E = (F^E)_r^r (F^E)_\theta^\theta (F^E)_z^z. \quad (238)$$

The logarithmic thermoelastic strain consists of three diagonal mixed-variant components:

$$(e^E)_r^r = \ln[(F^E)_r^r], \quad (e^E)_\theta^\theta = \ln[(F^E)_\theta^\theta], \quad (e^E)_z^z = \ln[(F^E)_z^z]; \quad (239)$$

$$\text{tre}^E = \ln[(F^E)_r^r (F^E)_\theta^\theta (F^E)_z^z].$$

Total inelastic deformation $\bar{\mathbf{F}} = \mathbf{F}^\xi \mathbf{F}^\eta$ remains diagonal, but now $\mathbf{F}^\xi$ contains coordinate factors associated with the shifter tensor:

$$(F^\xi)_K^\alpha = (J^\xi)^{1/3} g_K^i \delta_i^\alpha; \quad (F^\xi)_R^r = \frac{R}{r} (F^\xi)_\Theta^\theta = (F^\xi)_Z^z = [1 - \bar{\varphi}_0(3\xi^2 - 2\xi^3)]^{-1/3}. \quad (240)$$

Deformation tensor $\mathbf{F}^\eta = (F^\eta)_J^I \mathbf{G}_I \otimes \mathbf{G}^J$ is unchanged from its representation in Section 4.4.1, but total inelastic deformation becomes $\bar{F}_K^\alpha = \delta_i^\alpha g_J^i \bar{F}_K^J$. Note also that in the present case, $(F^E)_r^r = (F^E)_{r_R}^r$, $(F^E)_z^z = (F^E)_{z_Z}^z$, and $(F^E)_\theta^\theta = (F^E)_{\Theta}^\theta g_\theta^\Theta = (F^E)_\Theta^\theta (r/R)$. If $F_\Theta^\theta = \partial_\Theta \theta = 1$ and $\bar{F}_\Theta^\theta$ are imposed, then

$$(F^E)_\theta^\theta = F_\Theta^\theta (\bar{F}^{-1})_\theta^\Theta = \partial_\Theta \theta (\bar{F}^{-1})_\theta^\Theta \frac{r}{R} = (\bar{F}^{-1})_\Theta^\theta \frac{r}{R}. \quad (241)$$

Thermoelastic strain and hence conjugate stress components are equivalent between choices in Eqs. 217 and 236:

$$\begin{aligned} (e^E)_r^r &= (e^E)_R^R, & (e^E)_\theta^\theta &= (e^E)_\Theta^\Theta, & (e^E)_z^z &= (e^E)_Z^Z \\ \Rightarrow \quad \Sigma_r^r &= \Sigma_R^R, & \Sigma_\theta^\theta &= \Sigma_\Theta^\Theta, & \Sigma_z^z &= \Sigma_Z^Z. \end{aligned} \quad (242)$$

Remaining equations in Sections 4.4.1 and 4.4.2 are unchanged. However, as demonstrated for compressible neo-Hookean solids previously,⁸⁸ proposition Eq. 236 may be advantageous to Eq. 217 in the Eulerian description of isotropic materials, since in that case the stress-strain and equilibrium equations can be invoked without introduction of any specific reference basis $\{\mathbf{G}_K\}$. For anisotropic solids, attention should be given to proper formulation of strain energy potentials that account for a possible dependence of $(e^E)_j^i$ on spatial coordinates for arbitrary deformations. In contrast, $(e^E)_J^I$ are invariant under spatial rotations and hence may prove more convenient for analysis of anisotropic materials.

4.4.4 Linearization

The treatment of Sections 4.4.1 and 4.4.2, for a cylindrical specimen undergoing axisymmetric deformation, is tersely described in geometrically linear form corresponding to the general theory of Section 3. Displacement is of the form

$$u^R = u^R(R, t), \quad u^\Theta = 0, \quad u^Z = u^Z(Z, t). \quad (243)$$

Displacement gradients and thermoelastic strains follow as

$$\begin{aligned} \mathbf{h} &= \nabla_0 \mathbf{u} = h_R^R \mathbf{G}_R \otimes \mathbf{G}^R + h_\Theta^\Theta \mathbf{G}_\Theta \otimes \mathbf{G}^\Theta + h_Z^Z \mathbf{G}_Z \otimes \mathbf{G}^Z; \\ h_R^R &= \partial_R u^R, \quad h_\Theta^\Theta = \frac{u^R}{R}, \quad h_Z^Z = \partial_Z u^Z; \end{aligned} \quad (244)$$

$$\boldsymbol{\epsilon}^E = \mathbf{h}^E = \mathbf{h} - \mathbf{h}^\xi - \mathbf{h}^\eta; \quad (245)$$

$$\mathbf{h}^\xi(\xi) = \frac{\bar{\varphi}(\xi)}{3 - 3\bar{\varphi}(\xi)} \mathbf{G}_K \otimes \mathbf{G}^K, \quad \bar{\varphi}(\xi) = \phi(\xi) \cdot \bar{\varphi}_0 = (3\xi^2 - 2\xi^3)\bar{\varphi}_0; \quad (246)$$

$$\mathbf{h}^\eta(\eta) = \phi(\eta) \cdot [(e_0^\eta)_R^R \mathbf{G}_R \otimes \mathbf{G}^R + (e_0^\eta)_\Theta^\Theta \mathbf{G}_\Theta \otimes \mathbf{G}^\Theta + (e_0^\eta)_Z^Z \mathbf{G}_Z \otimes \mathbf{G}^Z]; \quad (247)$$

$$(e_0^\eta)_R^R = (e_0^\eta)_\Theta^\Theta = \frac{1}{3}(J_1^\eta - 1) \pm \frac{1}{2}\epsilon^\eta, \quad (e_0^\eta)_Z^Z = \frac{1}{3}(J_1^\eta - 1) \mp \epsilon^\eta; \quad (248)$$

$$\begin{aligned}
\bar{\mathbf{h}}^\eta(\eta) &= \mathbf{h}^\eta(\eta) - \frac{1}{3}\text{tr}[\mathbf{h}^\eta(\eta)] \\
&= \phi(\eta) \cdot \left[\pm \frac{1}{2}\epsilon^\eta(\mathbf{G}_R \otimes \mathbf{G}^R + \mathbf{G}_\Theta \otimes \mathbf{G}^\Theta) \mp \epsilon^\eta \mathbf{G}_Z \otimes \mathbf{G}^Z \right].
\end{aligned} \tag{249}$$

Scalar dislocation density of Eq. 227 is linearized as

$$\rho_G = \frac{1}{b_0} |\boldsymbol{\rho}_G : \boldsymbol{\rho}_G|^{1/2} = \frac{\sqrt{2}}{b_0} |6\eta(1-\eta)\epsilon^\eta \partial_Z \eta|. \tag{250}$$

Stresses are

$$\begin{aligned}
P_R^R &= \mathbf{B} \left[1 - \frac{1}{2}\beta'_0 \cdot (\text{tr} \boldsymbol{\epsilon}^E) \right] (\text{tr} \boldsymbol{\epsilon}^E) + 2\mathbf{G}(\epsilon'^E)_R^R - T_0 \gamma S, \\
P_\Theta^\Theta &= \mathbf{B} \left[1 - \frac{1}{2}\beta'_0 \cdot (\text{tr} \boldsymbol{\epsilon}^E) \right] (\text{tr} \boldsymbol{\epsilon}^E) + 2\mathbf{G}(\epsilon'^E)_\Theta^\Theta - T_0 \gamma S, \\
P_Z^Z &= \mathbf{B} \left[1 - \frac{1}{2}\beta'_0 \cdot (\text{tr} \boldsymbol{\epsilon}^E) \right] (\text{tr} \boldsymbol{\epsilon}^E) + 2\mathbf{G}(\epsilon'^E)_Z^Z - T_0 \gamma S.
\end{aligned} \tag{251}$$

Linear momentum conservation reduces to

$$\partial_R P_R^R + \frac{1}{R} (P_R^R - P_\Theta^\Theta) = \rho_0 \ddot{u}^R, \quad \partial_Z P_Z^Z = \rho_0 \ddot{u}^Z. \tag{252}$$

Mass conservation requires

$$-\dot{\rho}/\rho = \nabla_0 \cdot \dot{\mathbf{u}} = \frac{1}{R} \partial_R (R \dot{u}^R) + \partial_Z \dot{u}^Z. \tag{253}$$

Remaining Eqs. 232–235 in Section 4.4.2 are unchanged, with the exception that $\mathbf{e}^E \rightarrow \boldsymbol{\epsilon}^E$ in Eq. 235.

5. Uniaxial Stress Tension and Compression

Governing equations and boundary conditions are presented first in Section 5.1, followed by results for B_4C , TiB_2 , and the ceramic composite in Sections 5.2, 5.3, and 5.4, respectively.

5.1 Governing Equations and Boundary Conditions

Particular versions of equations derived in Section 4.4 are as follows. Steady extension or compression along the Z -axis is prescribed, where $\dot{\epsilon}$ is the constant nominal strain rate:

$$z(Z, t) = Z \cdot (1 \pm \dot{\epsilon}t) \text{ on } Z = 0, L; \quad \epsilon(t) = \int_0^t \dot{\epsilon} dt. \quad (254)$$

On the boundary of the closed cylinder $\partial\Omega_0$ with outward normal $\mathbf{N}$, mechanical traction components $t_{0k} = P_k^J N_J$ obey

$$t_{0r} = t_{0\theta} = 0 \forall \mathbf{X} \in \partial\Omega_0; \quad t_{0z} = 0 \text{ along } R = R_0, \quad t_{0z} = \pm P_z^Z \text{ at } Z = 0, L. \quad (255)$$

Furthermore, natural boundary conditions are imposed such that surface forces associated with order parameter gradients vanish everywhere:

$$t^\xi = \mathbf{s}^\xi \cdot \mathbf{N} = 0, \quad t^\eta = \mathbf{s}^\eta \cdot \mathbf{N} = 0 \quad (\forall \mathbf{X} \in \partial\Omega_0). \quad (256)$$

In the geometrically linear case, the first of Eq. 254 is replaced with $u^Z = \pm Z\dot{\epsilon}t$.

Spatially homogeneous solutions satisfy the above conditions in conjunction with the governing equations of Section 4.4. Thermoelastic strain and order parameter fields are independent of (R, Θ, Z) and are of the form

$$\mathbf{e}^E = \mathbf{e}^E(t), \quad \xi = \xi(t), \quad \eta = \eta(t). \quad (257)$$

Symmetries of material behaviors and loading demand $\sigma_\theta^\theta = \sigma_r^r \Rightarrow \Sigma_\Theta^\Theta = \Sigma_R^R \Rightarrow (e^E)_\Theta^\Theta = (e^E)_R^R$. Since $\bar{F}_\Theta^\Theta = \bar{F}_R^R$, it follows from Eqs. 216 and 219 that

$$\begin{aligned} \frac{r}{R} (F^E)_\Theta^\Theta &= \frac{r}{R} \frac{F_\Theta^\Theta}{\bar{F}_\Theta^\Theta} = \frac{r}{R} \frac{1}{\bar{F}_\Theta^\Theta} = \frac{r}{R} \frac{1}{\bar{F}_R^R} = (F^E)_R^r = \frac{F_R^r}{\bar{F}_R^R} = \frac{\partial_R r}{\bar{F}_R^R} \\ &\Rightarrow \partial_R r = \frac{r}{R} \Rightarrow P_\theta^\Theta = \frac{r}{R} P_r^R. \end{aligned} \quad (258)$$

The balance of linear momentum in Eq. 231 and boundary conditions in Eq. 255 then produce

$$\partial_R P_r^R = P_r^R = 0 = P_\theta^\Theta; \quad \partial_Z P_z^Z = 0 \Rightarrow P_z^Z = P_z^Z(t). \quad (259)$$

In other words, all stress components vanish except P_z^Z , where the latter is constant over Ω_0 at any time instant t . The axial true stress component is $\sigma_z^z = J\Sigma_Z^Z = (R^2/r^2)P_z^Z$. The same arguments hold for the geometrically linear theory when $P_z^Z(t)$ is replaced by $P_Z^Z(t)$. The microforce balances in Eq. 233 reduce to $\pi^\xi = \pi^\eta = 0$. Either adiabatic conditions in Eq. 234 or isothermal conditions are imposed, where the latter are used unless noted otherwise for uniaxial stress problems.

The solution procedure is as follows. Model complexity precludes closed-form analytical solutions. Hence, the essential boundary condition in Eq. 254 is imposed incrementally over a time period $t \in [0, t_0]$ with a fixed increment Δt . In each increment, the constitutive equations are solved for stress state and temperature, if applicable. Order parameter fields are updated via explicit integration of kinetic laws Eq. 201 or Eq. 204 for ξ and Eq. 210 for η . These become nonlinear ordinary differential equations in the present case of homogeneous fields since $\nabla_0^2 \xi = 0$ in $\tilde{\mathcal{R}}$ of Eq. 203 and $\nabla_0^2 \eta = 0$ in $\bar{\mathcal{R}}$ of Eq. 211. An iterative procedure determines the value of $F_R^r(t) = r(t)/R$ in each increment that ensures transverse stresses vanish in accordance with Eq. 259. In the adiabatic case, entropy is updated via explicit integration of Eq. 234.

Fracture is triggered ($\dot{\xi} > 0$) for the present kinetic models under homogeneous thermoelastic loading. Transformation ($\dot{\eta} > 0$) is not initiated naturally under homogeneous loading because $\eta = 0$ is always an admissible (trivial) solution of the governing equations, though above some threshold the trivial solution is not the minimum-energy solution.^{20,95} Thus, a small perturbation, whose magnitude does not affect the end result, is tested at each increment until transformation is triggered via $\dot{\eta} > 0$.

Viscosity parameters $\tilde{\beta}$ for evolution of ξ in Eq. 201 or Eq. 204 and $\bar{\beta}$ for evolution of η in Eq. 210 are varied among sets of calculations for each material and loading protocol. For 1D homogeneous conditions considered in Section 5 and later in Section 6, solutions depend only on the dimensionless products $\tilde{\beta}\dot{\epsilon}$ and $\bar{\beta}\dot{\epsilon}$, and not $\tilde{\beta}$, $\bar{\beta}$, and applied strain rate $\dot{\epsilon}$ individually.

Homogeneous problems are typically used to verify phase field energy functionals and kinetic laws, as well as to calibrate material parameters.^{26–28,35} In the present 1D calculations, the predicted response up to peak loading is of primary interest. For brittle solids, or for strain-softening ductile solids, localization of deformation can be energetically favorable in the strain softening regime, leading to abrupt specimen failure.^{28,35,95} In rate dependent solids, strain softening does not necessarily lead to ill-posed governing equations because of viscous regularization, but localization is often easily triggered by small perturbations in material properties, specimen geometry, or boundary conditions.¹⁵² When gradients of order parameters affect the material response as in phase field models, regularization ensues even in the rate-independent limit. However, localization is still often energetically favorable when a critical load is exceeded.^{11,35,95} For general 3D loading protocols and arbitrary constitutive models, strain softening is neither necessary nor sufficient to induce localization.^{152,153} In the present calculations, whereby spatial gradients of order parameters vanish by construction, the homogeneous solution is not necessarily a unique solution to the governing equations, but it is always an admissible solution.

As remarked in Section 4.1, the terminal stress-free state is identically described by the present model and standard quasi-static phase field theories of fracture so long as healing is suppressed. The transition path from homogeneous to localized deformation for the present nonlinear theory cannot be readily derived via analytical methods, and thus remains to be modeled in future numerical studies. However, in the quasi-static limit, the threshold-type model in Eq. 204 is very similar to the irreversible model with threshold in equations (54) and (70) of C Miehe,³⁵ whereby 1D numerical simulations of localized tensile fracture are reported in Figure 5(c) of that reference. The present model is thus expected to provide similar physically credible results as in that work,³⁵ with convergence to a sharp discontinuity attained as $l_\xi \rightarrow 0$.

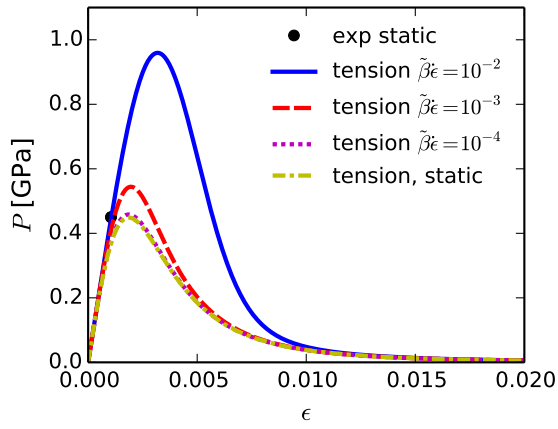
5.2 Results: Boron Carbide

In results of Section 5.2, driving forces are insufficient to enable $\dot{\eta} > 0$ according to Eq. 210 and parameters in Table 1. This agrees with experimental observations that report no evidence of amorphization of polycrystalline B_4C under uniaxial stress tension or uniaxial stress compression loading.^{73,74,78} Accordingly, B_4C behaves as an elastic-brittle solid at room temperature in the absence of high confining pressure.

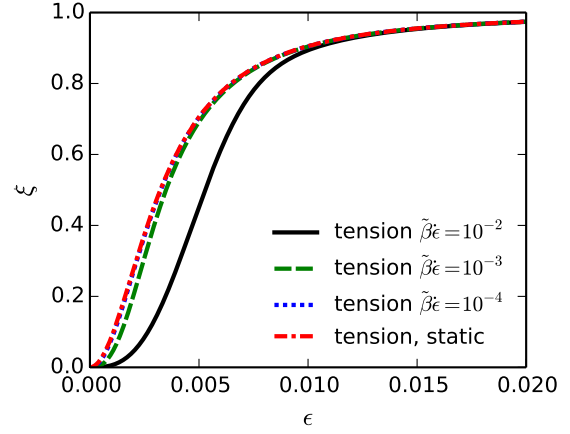
5.2.1 Tension

Predictions obtained using the TDGL-type fracture model of Eq. 201 are reported in Fig. 3. Axial true stress, positive in tension, is denoted by $P = \sigma_z^z$ (nonlinear theory) or $P = P_Z^Z$ (linear theory). Differences between linear and nonlinear models are negligible. Peak tensile strength P_T is matched accurately in Figs. 3a and 3c, but strain ϵ at peak loading is overpredicted: 1.86×10^{-3} versus 1.05×10^{-3} for observed elastic-brittle to failure behavior. This is an artifact of the kinetic model that enables $\dot{\xi} > 0$ immediately with $\epsilon > 0$, as evidenced by results in Figs. 3b and 3d. Flexure strength data is for PAD B₄C, for which only the static value is known. Dynamic data on SPS B₄C⁷⁸ show a near-negligible increase in tensile strength as the strain rate is increased by 6 orders of magnitude. Thus, to obtain a realistic response, results suggest crack viscosity should be constrained as $\tilde{\beta}\dot{\epsilon} \lesssim 10^{-4}$.

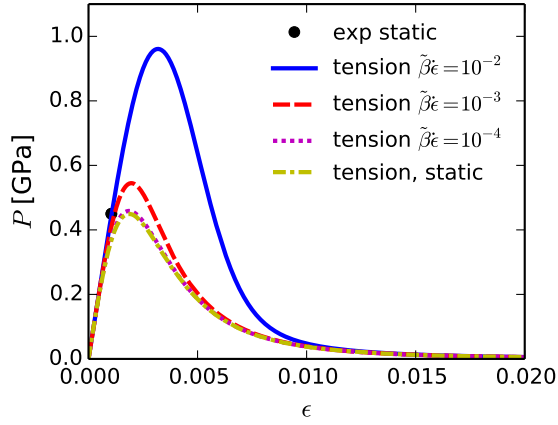
Predictions obtained using the threshold-type fracture model of Eq. 204 are reported in Fig. 4. Differences between linear and nonlinear models are again negligible. Peak tensile strength P_T is matched accurately in Figs. 4a and 4c, as is the corresponding strain at peak load for observed elastic-to-failure behavior. According to the threshold kinetic model, $\dot{\xi} > 0$ only when peak load is attained, as shown in Figs. 4b and 4d. The load drop after attainment of peak stress is steeper in Fig. 4 than the gradual stress decay in Fig. 3, and thus more physically realistic. However, in both models, admission of localization corresponding to a dominant crack would enable more abrupt stress drops excluded by homogeneous solutions more descriptive of distributed micro-cracking.^{35,124} Constraint $\tilde{\beta}\dot{\epsilon} \lesssim 10^{-4}$ is deduced to enable near rate-independent behavior in the uniaxial tensile loading regime. The value of $\tilde{\beta} = 10^{-7}$ s shown in Table 1, calibrated to shock rise times later in Section 7.2, fulfills this constraint for $\dot{\epsilon} \lesssim 10^3$ /s, a tensile strain rate 2 orders of magnitude larger than achieved in Rubink et al.⁷⁸



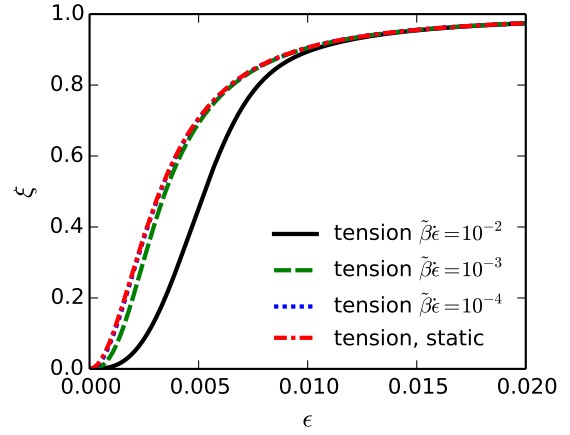
(a) stress, nonlinear



(b) fracture, nonlinear

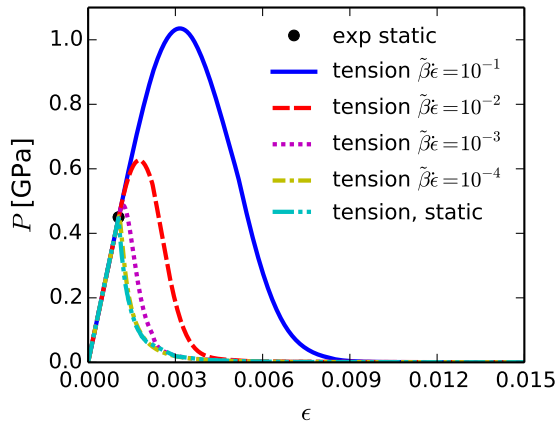


(c) stress, linear

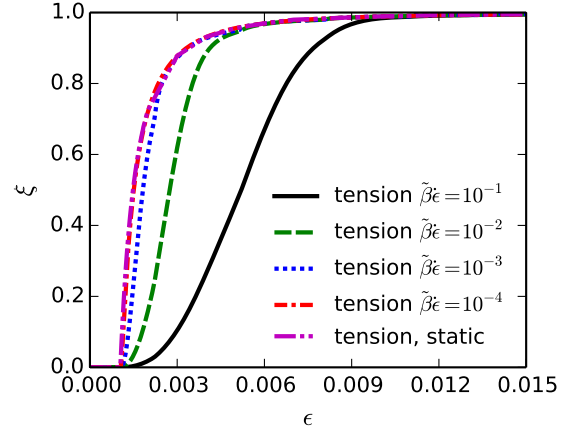


(d) fracture, linear

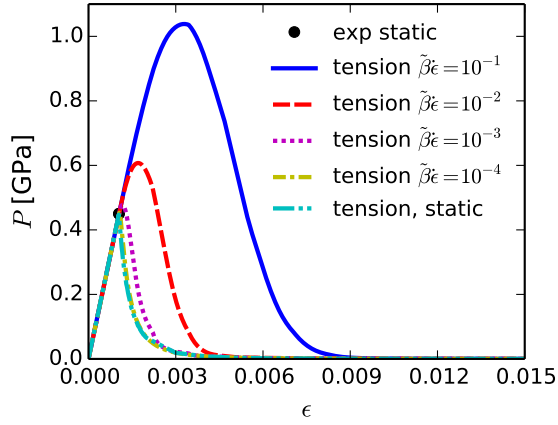
Fig. 3 Boron carbide: axial true stress and fracture order parameter versus axial strain predicted by TDGL-type fracture model of Eq. 201. Tensile loading at various dimensionless strain rates $\tilde{\beta}\dot{\epsilon}$, with experimental tensile strength data⁷³: (a) P , nonlinear theory (b) ξ , nonlinear theory (c) P , linear theory (d) ξ , linear theory



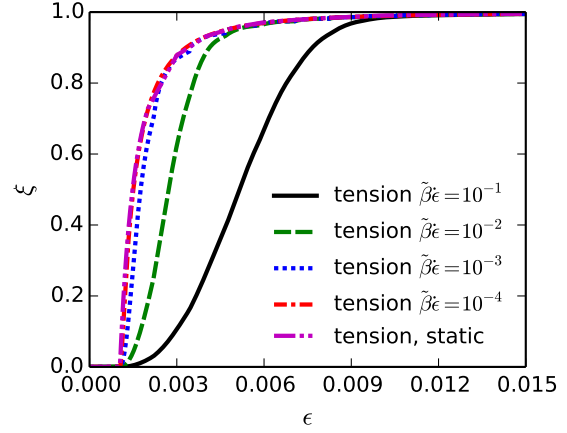
(a) stress, nonlinear



(b) fracture, nonlinear



(c) stress, linear



(d) fracture, linear

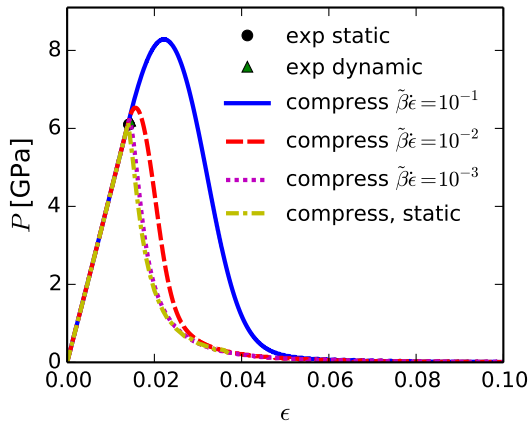
Fig. 4 Boron carbide: axial true stress and fracture order parameter versus axial strain predicted by threshold-type fracture model of Eq. 204. Tensile loading at various dimensionless strain rates $\tilde{\beta}\dot{\epsilon}$, with experimental tensile strength data⁷³: (a) P , nonlinear theory (b) ξ , nonlinear theory (c) P , linear theory (d) ξ , linear theory

5.2.2 Compression

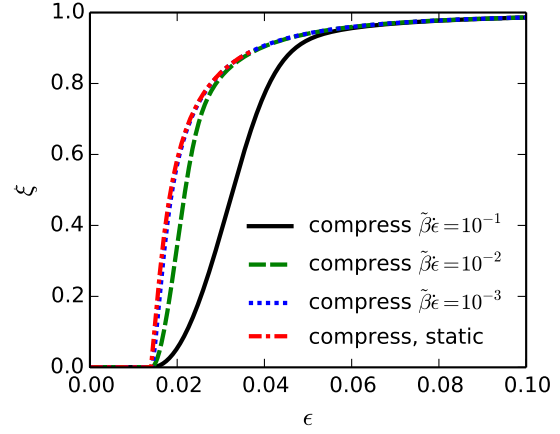
Results obtained from the TDGL-type kinetic model of Eq. 201, with parameters of Table 1, correlate poorly with experimental compressive strength data^{73,74,148} of the material. The standard TDGL model does not account for the drastic difference in strength properties of brittle solids under compression versus tension loading.^{28,35} In the present case, the TDGL model predicts a peak unconfined compressive strength of only 0.5 GPa, versus $P_C = 6.1$ GPa obtained experimentally.⁷³ The TDGL model also suffers from immediate softening upon any nonzero compressive strain, contradicting observed elastic-brittle behavior.^{73,148}

Thus, only results of the threshold-type model of Eq. 204 are reported for compression loading in Fig. 5. This model accounts for stress-state dependence of strength via inclusion of stress triaxiality in the kinetic equations, as explained in Section 4.1.3. Axial true stress, positive in compression, is $P = -\sigma_z^z$ (nonlinear theory) or $P = -P_Z^Z$ (linear theory). The static experimental strength is 6.1 GPa, at a rate of $\dot{\epsilon} \approx 10^{-4}/s$.^{73,148} The dynamic strength is 6.2 GPa, at $\dot{\epsilon} \approx 300 - 1600/s$.^{73,148} The constraint $\tilde{\beta}\dot{\epsilon} \lesssim 10^{-3}$ provides for the correct nearly rate-independent response in these regimes, consistent with the value of $\tilde{\beta}$ in Table 1. Linear and nonlinear models show indiscernible differences.

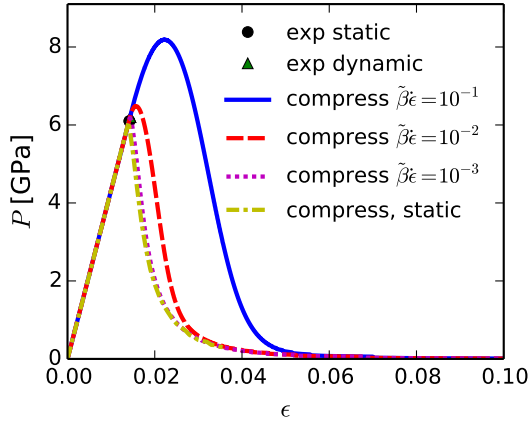
Prior results in Section 5.2 imposed isothermal conditions and omitted bulking, i.e., inelastic volume increase commensurate with fracture under pressure-shear loading. Effects of adiabatic conditions and nonzero bulking parameter $\bar{\varphi}_0$ are shown in Fig. 6 for the nonlinear theory. Adiabatic heating provides a negligible effect on stress P , and dilatation $\bar{\varphi}_0$ has a very small effect on stress for unconfined compressive loading in Fig. 6a. At a fast loading rate of $\tilde{\beta}\dot{\epsilon} = 10^{-2}$, evolution of ξ is relatively unaffected by thermal conditions or bulking in Fig. 6b. Temperature rise under adiabatic loading is shown for two strain rates, with or without inelastic volume change, in Fig. 6c. Results for $\gamma_0 = 0$ show that thermoelastic heating is nearly negligible. Rather, nearly all temperature rise manifests from entropy production due to crack phase kinetics. The higher the value of $\tilde{\beta}\dot{\epsilon}$, the greater the temperature increase due to viscous dissipation. For $\tilde{\beta}\dot{\epsilon} = 10^{-1}$, peak $T = 369K$ with $\bar{\varphi}_0 = 0$, and peak $T = 373K$ with $\bar{\varphi}_0 = 0.01$.



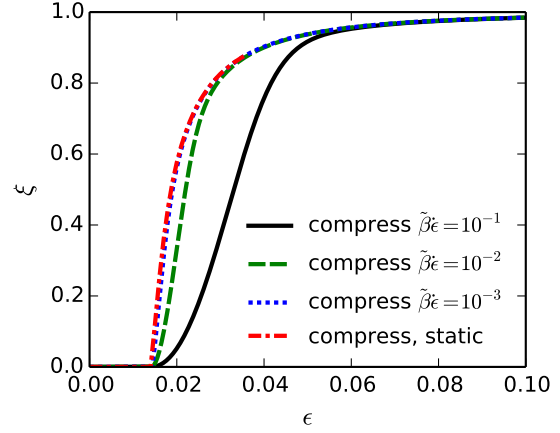
(a) stress, nonlinear



(b) fracture, nonlinear

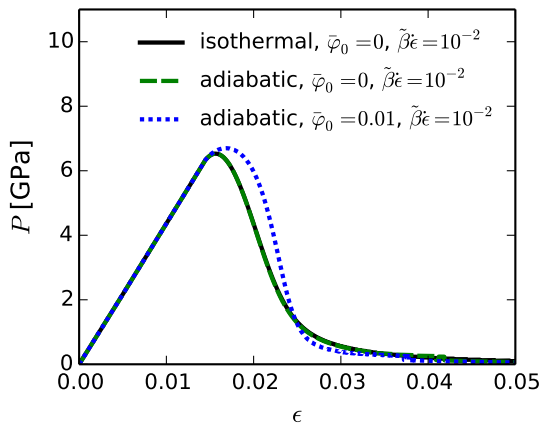


(c) stress, linear

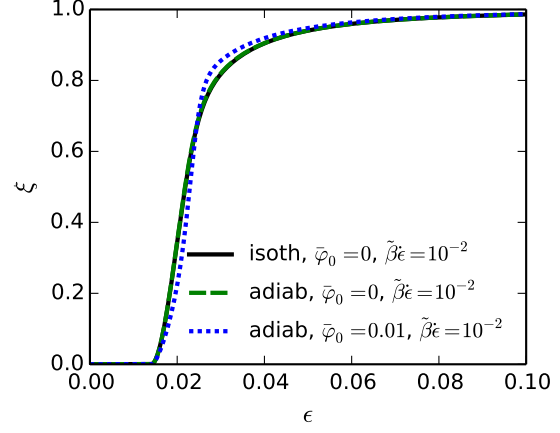


(d) fracture, linear

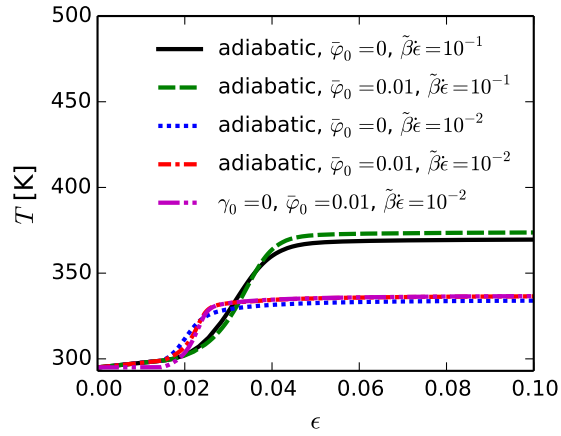
Fig. 5 Boron carbide: axial true stress and fracture order parameter versus axial strain predicted by threshold-type fracture model of Eq. 204. Unconfined compression at various dimensionless strain rates $\tilde{\beta}\dot{\epsilon}$, with experimental strength data^{73,148}: (a) P , nonlinear theory (b) ξ , nonlinear theory (c) P , linear theory (d) ξ , linear theory



(a) stress, nonlinear



(b) fracture, nonlinear



(c) temperature, nonlinear

Fig. 6 Boron carbide: effects of bulking parameter $\bar{\varphi}_0$ and thermal conditions, threshold-type fracture model of Eq. 204 and unconfined compressive loading at various dimensionless strain rates $\tilde{\beta}\dot{\epsilon}$: (a) P , nonlinear theory (b) ξ , nonlinear theory (c) T , nonlinear theory

5.3 Results: Titanium Diboride

In the results of Section 5.3, driving forces are insufficient to enable $\dot{\eta} > 0$ according to Eq. 210 and the parameters in Table 2. This agrees with experimental observations that report no evidence of dislocation slip in polycrystalline TiB₂ under uniaxial stress loading at room temperature.^{134,136} Polycrystalline TiB₂ behaves as an elastic-brittle solid in Section 5.3.

5.3.1 Tension

Results obtained from the TDGL-type kinetic model Eq. 201 are not shown since they suffer the same pathologies noted for B₄C in Section 5.2. Predictions the threshold-type fracture model of Eq. 204 are shown in Fig. 7. Differences between linear and nonlinear models are negligible, so only results of the nonlinear theory are shown. Peak tensile strength P_T is matched accurately in Fig. 7a along with the corresponding strain at peak load for brittle elastic-to-failure behavior. According to Eq. 204, $\dot{\xi} > 0$ commences only when peak load is attained, as is clear from Fig. 7b. The dynamic flexure strength of the material is unknown. However, $\tilde{\beta}\dot{\epsilon} \lesssim 10^{-4}$ provides for near rate-independent behavior. The value of $\tilde{\beta} = 10^{-7}$ s shown in Table 2 fulfills this constraint for tensile loading rates $\dot{\epsilon} \lesssim 10^3$ /s.

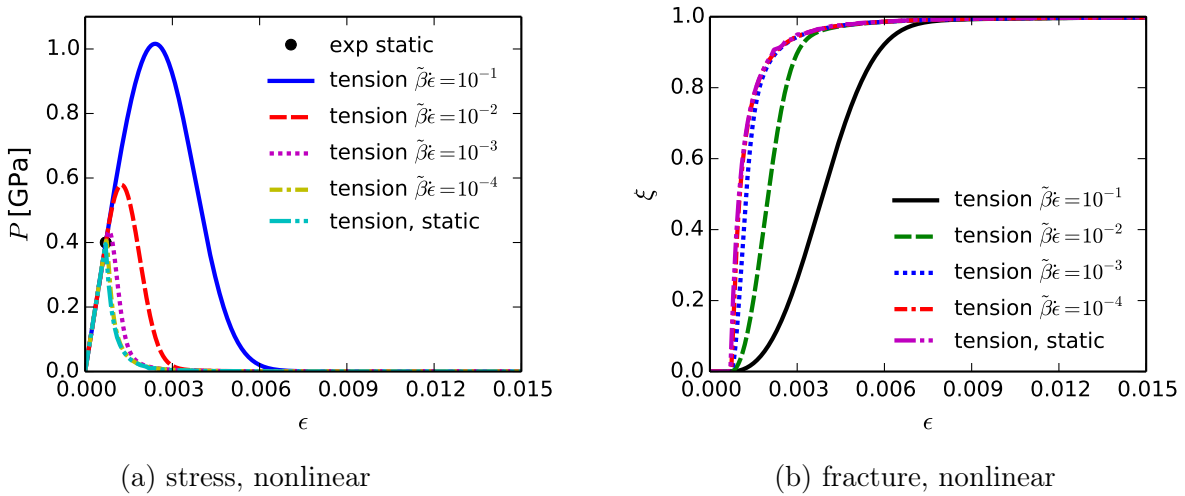


Fig. 7 Titanium diboride: axial true stress and fracture order parameter versus axial strain predicted by irreversible threshold-type fracture model of Eq. 204. Tensile loading at various dimensionless strain rates $\tilde{\beta}\dot{\epsilon}$, with experimental tensile strength data¹³⁶: (a) P , nonlinear theory (b) ξ , nonlinear theory

5.3.2 Compression

Outcomes of the threshold-type model of Eq. 204 are shown for uniaxial stress compression loading in Fig. 8. The static experimental strength P_C is 6.0 GPa, measured at a rate of $\dot{\epsilon} \approx 10^{-4}/\text{s}$, and the dynamic strength is 6.1 GPa, at $\dot{\epsilon} \approx 1200/\text{s}$.¹⁴⁸ The constraint $\tilde{\beta}\dot{\epsilon} \lesssim 10^{-3}$ provides for the correct dynamic response in this regime. This choice is consistent with the value of $\tilde{\beta}$ in Table 2. Linear and nonlinear models show only minute differences; nonlinear results are given here.

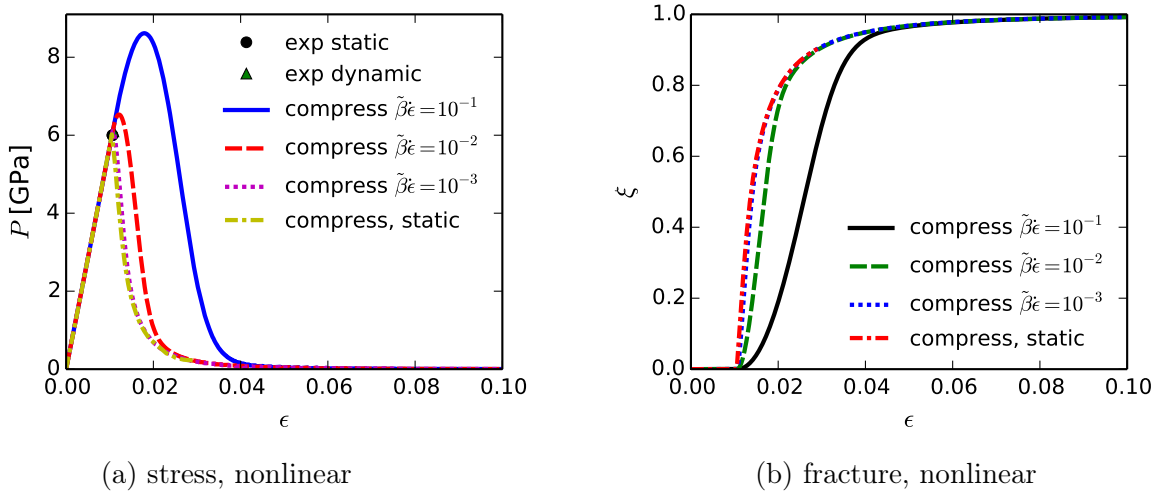


Fig. 8 Titanium diboride: axial true stress and fracture order parameter versus axial strain predicted by irreversible threshold-type fracture model of Eq. 204. Unconfined compression at various dimensionless strain rates $\tilde{\beta}\dot{\epsilon}$, with experimental compressive strength data¹⁴⁸: (a) P , nonlinear theory (b) ξ , nonlinear theory

5.4 Results: Ceramic Composite

As was the case for pure B_4C and TiB_2 polycrystals, no evidence of phase transformation or plastic slip exists for the ceramic composite when loaded under uniaxial stress in the absence of confinement at room temperature. The kinetic model Eq. 210 with the parameters in Table 3 correctly predicts $\dot{\eta} = 0$ for loading conditions reported in Section 5.4.

5.4.1 Tension

Predictions the threshold-type fracture model of Eq. 204 are given in Fig. 9. Differences between linear and nonlinear models are negligible; results of the nonlinear theory are shown. Peak tensile strength P_T is matched well in Fig. 9a, as is the strain

at peak load for elastic-to-failure behavior. Such behavior is enabled by the state-dependent initiation threshold built in to Eq. 204: $\dot{\xi} > 0$ in Fig. 9b initiates only when peak load is achieved. The dynamic flexure strength of the composite has been measured,⁷⁸ with a value about 10% higher at $\dot{\epsilon} \approx 10^1/\text{s}$ versus the quasi-static value at $\dot{\epsilon} \approx 10^{-5}/\text{s}$. The choice $\tilde{\beta} \approx 2 \times 10^{-4}\text{s}$ provides correct rate dependence^{67,78} for tensile loading.

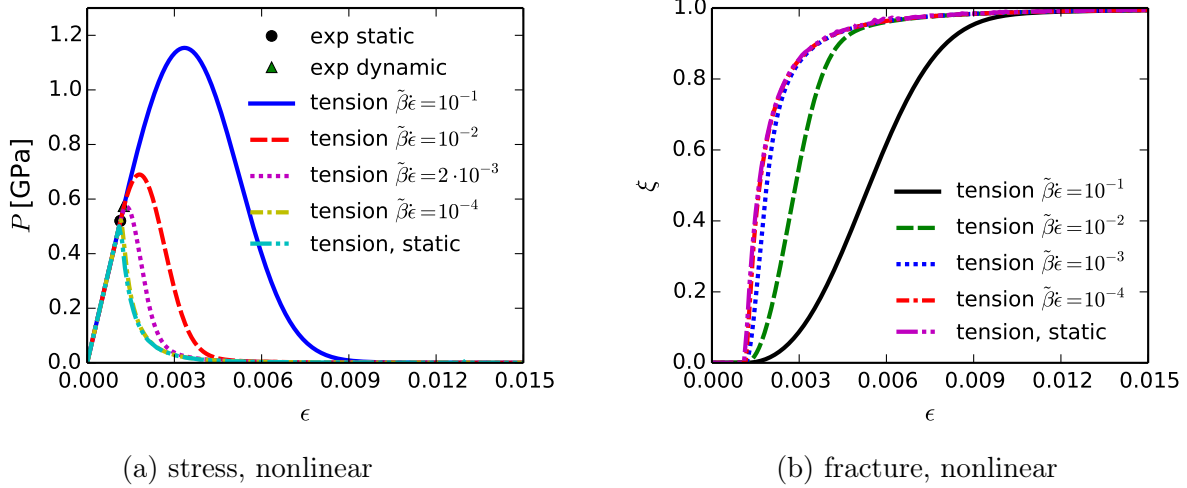


Fig. 9 Ceramic composite: axial true stress and fracture order parameter versus axial strain predicted by irreversible threshold-type fracture model of Eq. 204. Tensile loading at various dimensionless strain rates $\tilde{\beta}\dot{\epsilon}$, with experimental tensile strength data⁷⁸: (a) P , nonlinear theory (b) ξ , nonlinear theory

5.4.2 Compression

Reported in Fig. 10 are results from the threshold-type model of Eq. 204. The composite shows much stronger strain-rate dependence of compressive strength than either of its pure B_4C or pure TiB_2 constituents.^{67,68} The static experimental strength P_C is 5.3 GPa, measured at a rate of $\dot{\epsilon} \approx 10^{-3}/\text{s}$, and the dynamic strength is 8.9 GPa, at $\dot{\epsilon} \approx 700/\text{s}$.⁶⁷ These strength values have been corrected by a factor of $\frac{4}{3}$ to enable fair comparison with values for the other two ceramics tested using dumbbell-shaped specimens.^{73,148} The choice $\tilde{\beta}\dot{\epsilon} \approx 0.25$ produces a relatively accurate rate-dependent response versus the test data.⁶⁷ This choice, with the quoted dynamic strain rate, suggests $\tilde{\beta} \approx 3.6 \times 10^{-4}\text{s}$. The value listed in Table 3, $3 \times 10^{-4}\text{s}$, is a compromise accounting for the slightly smaller value needed to match tensile data for this material in Section 5.4.1. Again, since linear and nonlinear models give almost identical results, only nonlinear results are shown.

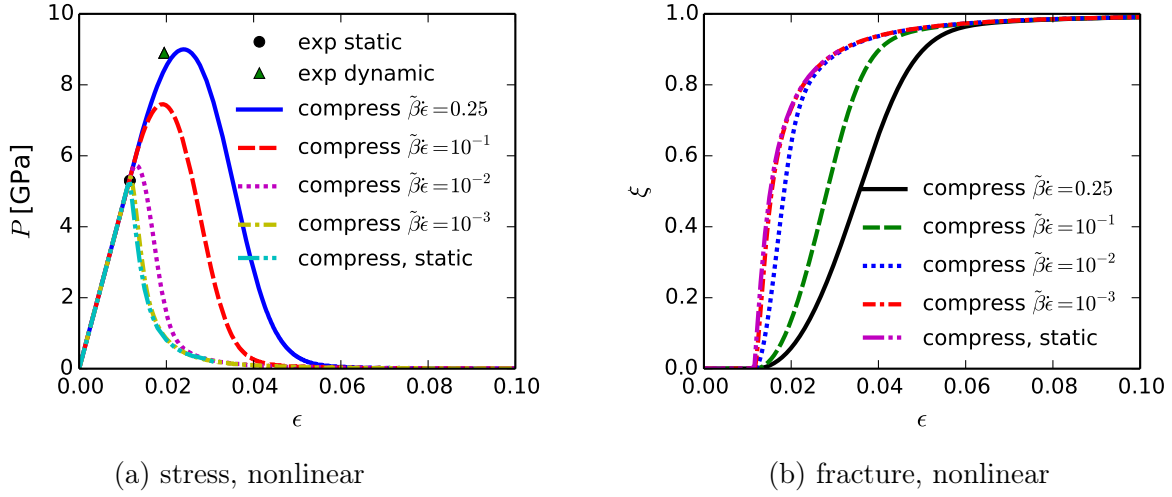
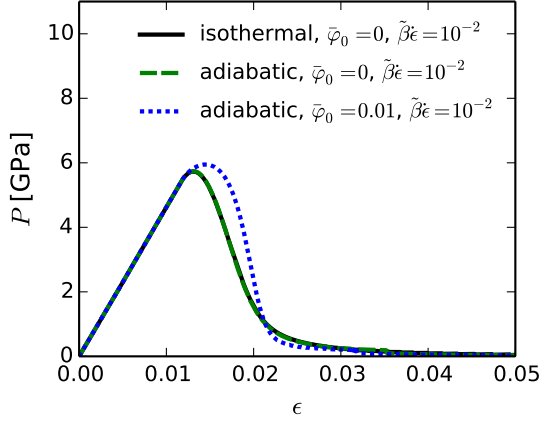
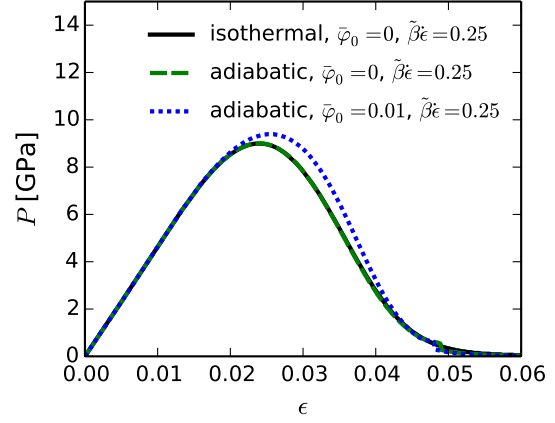


Fig. 10 Ceramic composite: axial true stress and fracture order parameter versus axial strain predicted by irreversible threshold-type fracture model of Eq. 204. Unconfined compression at various dimensionless strain rates $\tilde{\beta}\dot{\epsilon}$, with experimental compressive strength data⁶⁷: (a) P , nonlinear theory (b) ξ , nonlinear theory

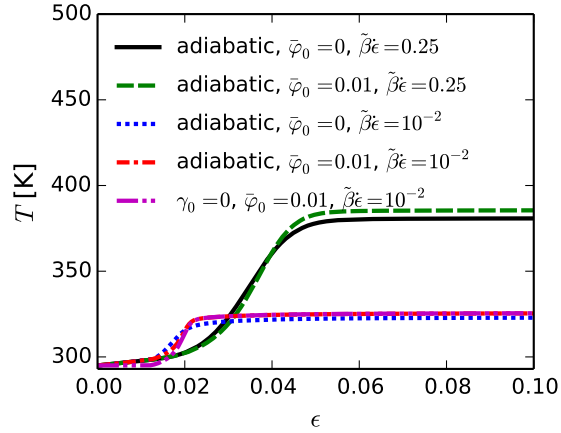
Prior results in Section 5.4 imposed isothermal conditions ($T = T_0 = 295\text{K}$) and omitted bulking ($\bar{\varphi}_0 = 0$). Effects of adiabatic conditions and nonzero $\bar{\varphi}_0$ are shown in Fig. 11 for the nonlinear theory. Adiabatic heating yields a negligible effect on stress P , and dilatation $\bar{\varphi}_0$ has a minor effect on stress for unconfined compressive loading in Figs. 11a and 11b, among which applied strain rates vary by a factor of 25 if viscosity is held fixed. Temperature rise is shown for two strain rates, with or without bulking, in Fig. 11c. Results for $\gamma_0 = 0$ show that thermoelastic heating is nearly negligible, in accordance with Fig. 6c for pure B_4C . Almost all temperature rise is due to dissipative crack kinetics, with higher temperatures attained as the product of strain rate and viscosity increases. For $\tilde{\beta}\dot{\epsilon} = 0.25$, peak $T = 386\text{K}$ with $\bar{\varphi}_0 = 0.01$. Temperature increases from adiabatic heating under unconfined compressive load are insufficient to notably relieve thermal residual stresses: the decrease in fracture toughness and crack growth resistance according to Eq. 214, based on the model of Taya et al.,¹⁰⁹ does not noticeably reduce compressive stress in these calculations.



(a) stress, lower rate, nonlinear



(b) stress, higher rate, nonlinear



(c) temperature, two rates, nonlinear

Fig. 11 Ceramic composite: effects of bulking parameter $\bar{\varphi}_0$ and thermal conditions, threshold-type fracture model of Eq. 204 and unconfined compressive loading at various dimensionless strain rates $\tilde{\beta}\dot{\epsilon}$: (a) P , nonlinear theory, lower strain rate (b) P , nonlinear theory, higher strain rate (c) T , nonlinear theory, both strain rates

6. Uniaxial Strain Compression

Governing equations and boundary conditions are briefly summarized in Section 6.1. Model results for B_4C , TiB_2 , and the ceramic composite follow in Sections 6.2, 6.3, and 6.4, respectively.

6.1 Governing Equations and Boundary Conditions

Equations are very similar to those of Section 5.1, where particular versions of those derived in Section 4.4 are as follows. Uniaxial strain compression along the Z -axis is prescribed, where $\dot{\epsilon}$ is the imposed nominal strain rate, positive in compression:

$$\begin{aligned} r &= R, \quad \theta = \Theta \quad (\forall \mathbf{X} \in \Omega); \\ z(Z, t) &= Z \cdot (1 - \dot{\epsilon}t) \text{ on } Z = 0, L; \quad \epsilon(t) = \int_0^t \dot{\epsilon} dt. \end{aligned} \quad (260)$$

The shifter of Eq. 237 reduces to $g_K^k = \delta_K^k$, and $J = \det \mathbf{F} = F_Z^z = \partial_Z z$. Lateral tractions $t_{0r} = P_r^R$ do not generally vanish at $R = R_0$, but other traction conditions in Eq. 255 still apply, as do free natural boundary conditions on surface microforces in Eq. 256.

Spatially homogeneous solutions, whereby field variables are of the form in Eq. 257, satisfy the imposed boundary conditions and momentum balances. The deformation gradient and Jacobian determinant, independent of Z in the homogeneous case, reduce to

$$\mathbf{F}(t) = \delta_K^k \mathbf{g}_k \otimes \mathbf{G}^K - \dot{\epsilon} t \mathbf{g}_z \otimes \mathbf{G}^Z, \quad J(t) = \det \mathbf{F}(t) = 1 - \dot{\epsilon} t = 1 - \epsilon(t). \quad (261)$$

Since $\mathbf{F}$, $\mathbf{F}^E$, and $\bar{\mathbf{F}}$ are all independent of R , the balance of linear momentum Eq. 231 produces, with $r/R = 1$,

$$\partial_R P_r^R = 0, \quad P_r^R = P_\theta^\Theta; \quad \partial_Z P_z^Z = 0 \Rightarrow P_z^Z = P_z^Z(t). \quad (262)$$

In other words, the stress tensor $\mathbf{P}$ is diagonal with two independent components P_z^Z and $P_r^R = P_\theta^\Theta$. Cauchy stress components are $\sigma_z^z = P_z^Z$, $\sigma_r^r = \sigma_\theta^\theta = J^{-1} P_r^R = (\partial_Z z)^{-1} P_r^R$. In the geometrically linear theory, $u^Z = -Z\dot{\epsilon}t$, $u^R = u^\Theta = 0$, and P_z^Z replaces P_z^Z . Also noteworthy is exact relation for volume change under uniaxial strain in the linear theory: $J = \det(\mathbf{1} + \nabla_0 \mathbf{u}) = 1 + \text{tr}(\mathbf{h})$, which affords accuracy of resolution of finite volume changes by the linear theory under 1D-strain conditions

studied in Section 6 and later in Section 7. Balances in Eq. 233 degenerate to $\pi^\xi = \pi^\eta = 0$. Isothermal or adiabatic conditions are enforced, with adiabatic results most often compared with high-rate, high-pressure experimental data.

As was the case in Section 5, solutions are obtained numerically, wherein kinetic equations Eq. 201 or Eq. 204 for $\dot{\xi}$ and Eq. 210 for $\dot{\eta}$ are integrated explicitly with a time increment Δt small enough for high accuracy and stability. Since all components of the deformation gradient are fully imposed under homogeneous uniaxial strain loading, an iterative procedure is not necessary to ensure equilibrium in the radial direction. Rate dependence enters solutions only via dimensionless products $\tilde{\beta}\dot{\epsilon}$ and $\bar{\beta}\dot{\epsilon}$ that are varied parametrically in subsequent calculations.

6.2 Results: Boron Carbide

A parameter study is undertaken first in Section 6.2.1 to enable understanding of influences of crack kinetic viscosity and inelastic free volume change, in the absence of phase transformation. Amorphization is enabled in Sections 6.2.2 and 7.2, whereby comparisons with high-pressure, high-rate experimental data^{60,67} are made. In all cases, the threshold-type fracture evolution model of Eq. 204 is invoked since it accounts for pressure-dependent kinetics via the stress triaxiality, as explained in Section 4.1.3. The TDGL-type model Eq. 201 produces immediate damage softening ($\epsilon > 0 \Rightarrow \dot{\xi} > 0$) and drastically under-predicts uniaxial compressive strength, as explained in Section 5.2.2, so it is abandoned for the present application.

6.2.1 Parameter Study

Axial compressive stress is defined for uniaxial strain compression as $P = -P_z^Z = -\sigma_z^z$ for the nonlinear theory and $P = -P_z^Z$ for the linear theory. Shown in Fig. 12 are effects of strain rate-viscosity product $\tilde{\beta}\dot{\epsilon}$ on homogeneous stress and fracture parameter kinetics for isothermal compression. Effects of viscous stiffening are small for $\tilde{\beta}\dot{\epsilon} = 10^{-2}$ and negligible for $\tilde{\beta}\dot{\epsilon} \lesssim 10^{-3}$, showing that the latter is a valid constraint to enable comparison with the equilibrium or quasi-static response. Trends are similar among nonlinear and linear predictions. Delineated in Fig. 13 are effects of bulking parameter $\bar{\varphi}_0$ for adiabatic quasi-static loading at $\tilde{\beta}\dot{\epsilon} = 10^{-3}$. In each case, the linear response is slightly stiffer than the nonlinear response, and $\bar{\varphi}_0 = 0.01$ produces higher compressive stress P , higher shear stress τ , but lower temperature T . The latter effect manifests from the additional energy consumed

by the material to overcome inelastic dilatation under compressive pressure. Shear stress, as is conventionally reported in shock physics literature,^{72,154} is defined as $\tau = \frac{1}{2}|\sigma_z^z - \sigma_r^r|$ for the nonlinear theory and $\tau = \frac{1}{2}|P_Z^Z - P_R^R|$ for the linear theory. For the present symmetry conditions, $\tau = \frac{1}{2}\sigma_V$, where σ_V is the von Mises effective stress.¹⁰⁸

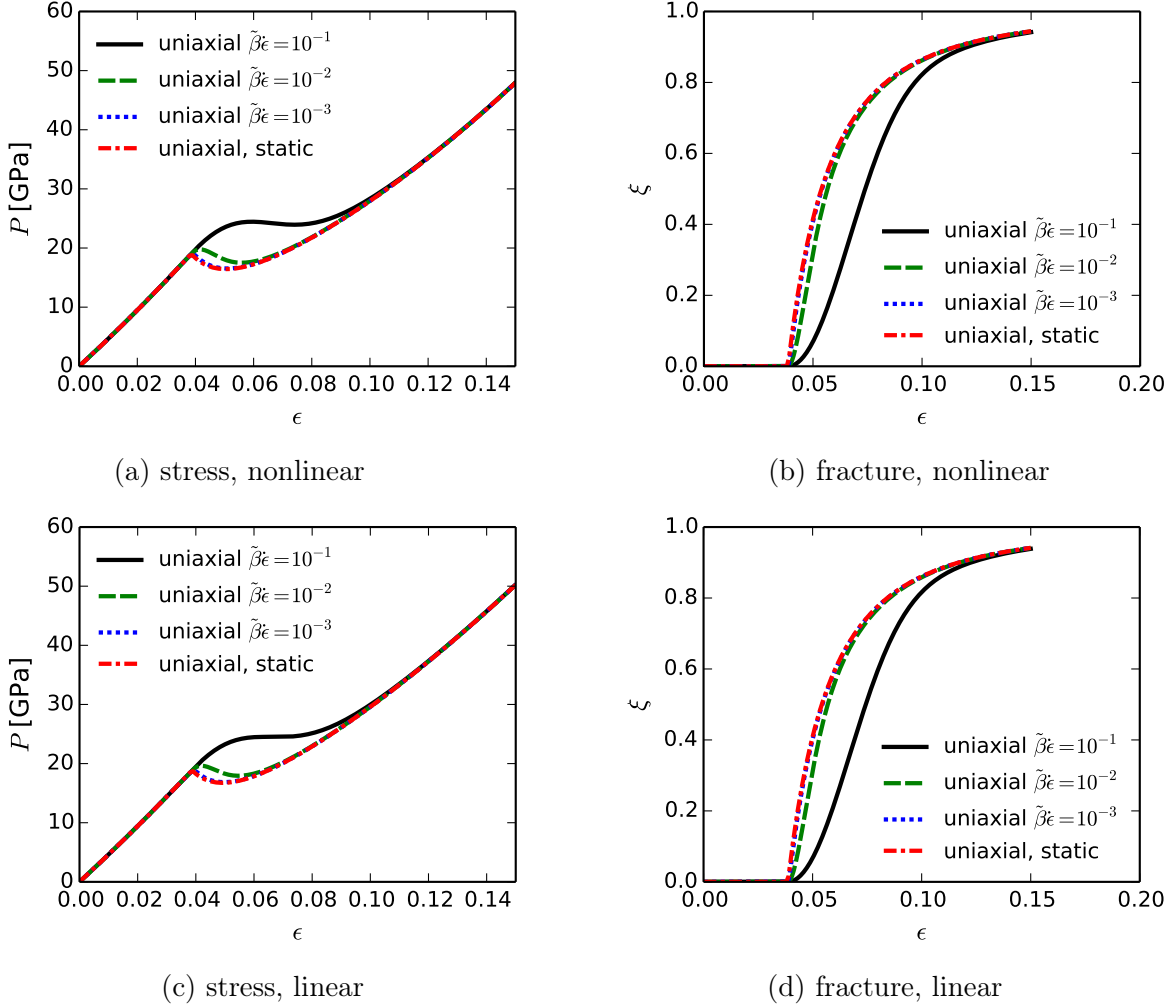
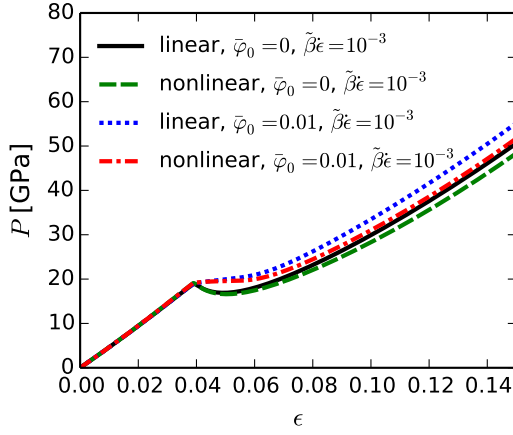
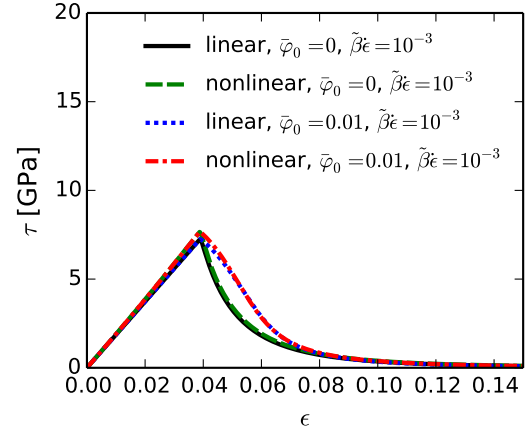


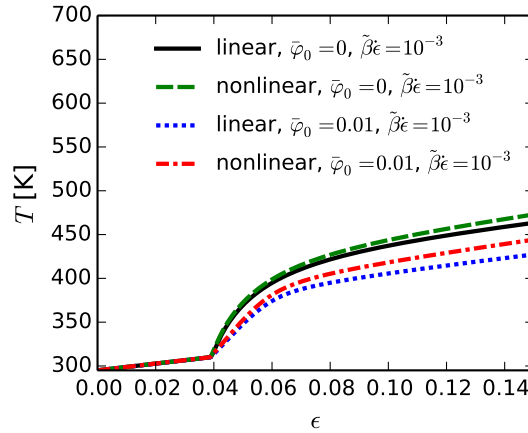
Fig. 12 Boron carbide: axial stress and fracture order parameter versus axial strain predicted by threshold-type fracture model of Eq. 204, with phase change and bulking suppressed ($\dot{\eta} = 0$, $\bar{\varphi}_0 = 0$). Isothermal uniaxial strain compressive loading at dimensionless strain rates $\tilde{\beta}\epsilon$: (a) P , nonlinear theory (b) ξ , nonlinear theory (c) P , linear theory (d) ξ , linear theory.



(a) longitudinal stress



(b) shear stress



(c) temperature

Fig. 13 Boron carbide: axial stress, shear stress, and temperature versus axial strain predicted by threshold-type fracture model of Eq. 204, with phase change kinetics Eq. 210 suppressed ($\dot{\eta} = 0$). Adiabatic uniaxial strain compressive loading at low dimensionless strain rate $\beta\dot{\epsilon}$, with different values of bulking parameter $\bar{\varphi}_0$: (a) P , nonlinear and linear theories (b) τ , nonlinear and linear theories (c) T , nonlinear and linear theories.

6.2.2 Predictions and Comparisons with Test Data

In the present section, phase transformation kinetics are enabled via $\dot{\eta} \geq 0$ in Eq. 210. In order to facilitate comparison with high-pressure data obtained from conventional plate impact^{60,75} and laser shock⁶² experiments, adiabatic conditions are assumed. Furthermore, bulking is enabled via $\bar{\varphi}_0 = 0.01$, which eliminates a drop in longitudinal stress (see Fig. 13b), at strains exceeding the HEL, that is inaccessible in Hugoniot data procured from plate impact testing. A known anomaly in the shock data of B₄C is that extrapolation of the hydrostat using only second- and third-order elastic coefficients produces a pressure-volume curve that exceeds the Hugoniot.^{60,115,145} As such, a fourth-order elastic constant is incorporated to best fit the high-pressure elastic response. Third-order strain energy function Eq. 93 is augmented with a bulk fourth-order isentropic elastic coefficient C_0'' :

$$\begin{aligned} W^U(\mathbf{e}^E, S, \eta, \xi) = & \frac{1}{2} B(\eta, \xi, \bar{\omega}) \cdot (\text{tr} \mathbf{e}^E)^2 \\ & \times \left[1 - \frac{1}{3} \{ B_0'(\eta) - 2 \} \cdot (\text{tr} \mathbf{e}^E) - \frac{1}{12} C_0''(\eta) \cdot (\text{tr} \mathbf{e}^E)^2 \right] \\ & + G(\eta, \xi) \cdot (\mathbf{e}'^E : \mathbf{e}'^E) - T_0 [\gamma(\eta, \xi, \bar{\omega}) \cdot (\text{tr} \mathbf{e}^E) \cdot S - h(S)] . \end{aligned} \quad (263)$$

Due to the lack of high-pressure data on the pure glassy solid, it is assumed that $C_0'' = \text{constant}$, independent of phase η . Elsewhere, a fourth-order constant was needed to model the high-pressure elasticity of quartz,^{155,156} and both fourth- and fifth-order constants were useful for modeling high-pressure phase transformations in silicon.¹⁵⁷ Effects of nonzero C_0'' with the specific value given in Table 1 manifest only at large compressive strain ($\epsilon \gtrsim 0.1$) and are inconsequential for the uniaxial stress response studied in Section 5.

Homogeneous, adiabatic uniaxial strain compression at constant strain rate enables a second-order accurate comparison with weak shock data such that certain model parameters can be calibrated and verified.^{154,158} A more realistic comparison is afforded later in Section 7, whereby the inhomogeneous material response along the Rayleigh line for a given steady shock velocity is computed explicitly. For comparison with conventional plate impact Hugoniot data, the material is assumed to reach an equilibrium state along the measured Hugoniot, such that adiabatic quasi-static response with $\tilde{\beta}\dot{\epsilon} = 10^{-3}$ provides a valid comparison. The time to reach steady state is on the order of microseconds. In contrast, laser shock probes much faster

kinetics, whereby experiments conclude in times on the order of nanoseconds.⁶² Thus, loading rates 3 orders of magnitude higher⁶² are prescribed for comparison with laser shock data, i.e., $\tilde{\beta}\dot{\epsilon} = 1$.

Wave propagation is monitored over time periods on the order of microseconds or longer for conventional plate impact experiments as well as Kolsky bar compression experiments, for which no evidence of amorphization is reported.^{73,74,159} As proposed in an experimental study,⁶² fractures dominate failure behavior at these loading rates. On the other hand, pulse durations on the order of several nanoseconds are too brief to enable crack growth and comminution during laser shock experiments.⁶² In laser shock experiments,⁶² intact samples can be recovered and show some fractures, but inelasticity is dominated by amorphization. Threshold impact stresses for amorphization are on the order of 25 GPa.^{62,123,160} To enable amorphization to occur at higher strain rates, at time scales on the order of nanoseconds or less, but fracture to dominate at lower strain rates, imposed for the present transformation kinetics is $\bar{\beta} = 10^{-2}\tilde{\beta} = 1$ ns, as given in Table 1. Then the value of A entering Eq. 200 is calibrated such that $\dot{\eta} > 0$ at the aforementioned stress thresholds for a steady dynamic loading rate of $\tilde{\beta}\dot{\epsilon} = 1$, or $\dot{\epsilon} = 10^7/\text{s}$ (e.g., attainment of 10% compression in only 10 ns). Fracture dominates over crystal-to-glass transformation for the model at lower average rates of $\dot{\epsilon} = 10^3 - 10^6/\text{s}$, closer to estimates for plate impact⁵⁴ or Kolsky bar loading.^{74,148}

Longitudinal stress, shear stress, temperature, and order parameter histories are shown in Fig. 14, for both aforementioned loading rates, all under adiabatic conditions. The lower-rate data, $\tilde{\beta}\dot{\epsilon} = 10^{-3}$ are intended for comparison with the shock Hugoniot data from.⁶⁰ The linear model provides a closer match to the experimental P data for $\epsilon \lesssim 0.12$, the nonlinear model a closer match for $\epsilon \gtrsim 0.15$. Linear and nonlinear models predict very similar histories of τ , T , ξ , and η at the lower strain rate, where T from the nonlinear theory slightly exceeds that from the linear theory, and $\eta = 0$ for both theories since amorphization does not occur at all for $\tilde{\beta}\dot{\epsilon} = 10^{-3}$. Shear stress τ drops rapidly at strains exceeding those for the HEL ($\epsilon \gtrsim 0.04$) as the tangent shear modulus $G = G_0 \cdot \chi(\xi)$ degrades with increasing fracture parameter ξ .

At the higher strain rate of $\tilde{\beta}\dot{\epsilon} = 1$, deemed more representative for achieving end states of laser shock, differences between predictions of nonlinear and linear mod-

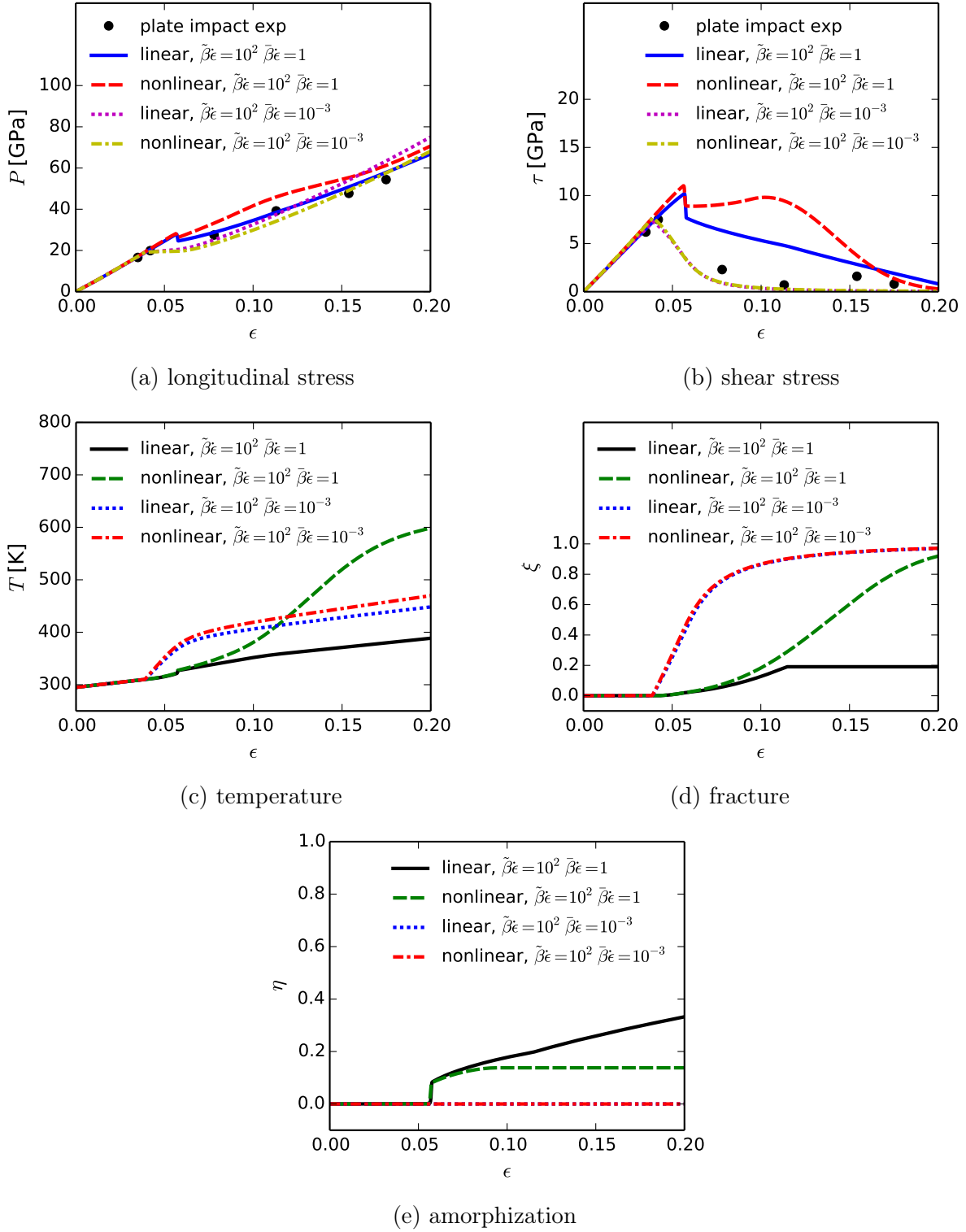


Fig. 14 Boron carbide: axial stress, shear stress, temperature and order parameters versus axial strain predicted by threshold-type fracture model of Eq. 204, with phase change kinetics Eq. 210 enabled ($\dot{\eta} \geq 0$). Adiabatic uniaxial strain compressive loading at dimensionless strain rates $\tilde{\beta}\dot{\epsilon}$, with experimental Hugoniot longitudinal and shear stress data⁶⁰: (a) P (b) τ (c) T (d) ξ (e) η .

els are pronounced. Both models provide for higher stress, especially shear stress in Fig. 14b, as the applied strain rate is increased by a factor of 10^3 . Amorphization dominates at the expense of fracture, as suggested by experiment.⁶² Both models produce a sharp drop in τ commensurate with a steep rise in η . From Figs. 14d and 14e, η plateaus at larger ϵ and fracture ensues in the nonlinear model, whereas η grows rather steadily with ϵ and fracture is suppressed in the linear model. Temperature rise is much greater for the nonlinear model in this case ($T \approx 600\text{K}$ at $\epsilon = 0.2$) since the viscosity parameter for crack kinetics is 2 orders of magnitude larger than that for phase transformation. Even so, T remains far below T_M such that the drop in apparent viscosity $\bar{\beta}_A$ through Eq. 210 does not appreciably affect model results. Experimental data are not sufficient to identify which of the nonlinear or linear predictions is most realistic at the higher loading rate.

6.3 Results: Titanium Diboride

The irreversible fracture kinetic model of Eq. 204 is used, since it accounts for pressure-dependent strength in the threshold for damage evolution. Adiabatic conditions and a strain rate-viscosity product of $\tilde{\beta}\dot{\epsilon} = 10^{-4}$ are imposed to facilitate comparison with shock Hugoniot data.^{65,66,76,135,147,161} Elastic constants in Table 2 corresponding to the formerly Cercom (now CoorsTek) material^{65,147} are used for the same reason, rather than those quoted for ceramics from other manufacturers.¹³⁶ The fourth-order constant of Eq. 263 is not needed (i.e., $C_0'' = 0$ for TiB_2). Under planar shock compression, polycrystalline TiB_2 demonstrates an unusual “double-yield” behavior evidenced by inflection points in the particle velocity history profiles and a concave downward region of the stress-volume Hugoniot.^{65,66,76,161} Depending on impact stress, multiple plastic waves may arise for the under-driven case, as opposed to the usual two-wave structure observed for weak shocks in metals and most ceramics.^{72,154} The concave downward region between the two yield points also suggests simple wave spreading¹⁵⁴ that should inhibit steady steep shocks for plane waves in this stress region.

As proposed in prior works on shock wave dynamics of the polycrystalline material,^{56,76} the first yield point, which occurs at $P_H \approx 7\text{ GPa}$, is attributed to fracture in the form of micro-cracking, and the second at $P \approx 17\text{ GPa}$ to slip of partial and/or full dislocations, as supported by experimental evidence of mobile dislocation loops in the basal plane of shock-recovered material.⁶⁴ The first yield point manifests from the kinetic relation Eq. 204 for fracture ultimately via P_H in Eq. 208. The value of

A in Eq. 200 is obtained for TiB_2 such that $\dot{\eta} \gg 0$ at the second yield point, wherein $P \approx 17$ GPa. Time scales for fracture and dislocation slip are assumed comparable, with local crack velocities limited by the Raleigh wave speed and local dislocation velocities limited by the shear wave speed. Thus, kinetic viscosities $\tilde{\beta}$ and $\bar{\beta}$ should agree within an order of magnitude. Both such viscosity values are calibrated later in Section 7.3 to observed shock rise times via comparison with results of steady wave analyses. The value of $\tilde{\beta} = 10^{-7}$ s is assumed the same as for B_4C , while the value of $\bar{\beta} = 5 \times 10^{-7}$ s is slightly larger to account for longer rise times observed in TiB_2 for shocks in which plastic flow is assumed to occur, versus those in B_4C that is elastic-brittle.

Titanium diboride also demonstrates an unusual (for a brittle ceramic) shear strength increase when shock compressed to stresses exceeding the HEL.^{65,147} The physical reason for this behavior is unknown from experimental evidence. Here, it is assumed that fracture is suppressed above a pressure limit, corresponding to a drastic increase in viscosity $\tilde{\beta}$, perhaps due to sliding friction or other mechanisms that cause cracks to arrest or that inhibit granular flow of comminuted material. Fracture suppression is achieved in the present model via setting $p \geq p_L \Rightarrow \tilde{\beta} \rightarrow 10^4 \tilde{\beta} \Rightarrow \dot{\xi} \rightarrow 0$, where p is the local transient Cauchy pressure (negative mean stress) and p_L is the locking pressure, above which the fracture phase field evolves at a negligibly low rate under dynamic uniaxial strain compression. For the present material and loading conditions $p_L = 4$ GPa (Table 2) provides realistic results for resulting longitudinal and shear stresses. Note that p_L is substantially lower than peak pressure obtained in uniaxial stress compression ($p \lesssim \frac{1}{3}P_C = 2$ GPa), so the analysis of unconfined compression in Section 5.3.2 is unaffected by this incorporation of pressure-dependent viscosity for micro-crack kinetics.

Reported in Fig. 15 are longitudinal stress, shear stress, temperature, and order parameter histories obtained under adiabatic conditions at $\tilde{\beta}\dot{\epsilon} = 10^{-3}$. Results are compared with shock Hugoniot data tabulated by DP Dandekar.⁶⁵ The nonlinear model provides a slightly closer match to the experimental P data for $\epsilon \gtrsim 0.05$. The abrupt drop in P and τ corresponds to the second yield point at stress levels on the order of 17 GPa. This correlates with the sharp rise in η reflective of inelastic slip in Fig. 15e. Such load drops would be inaccessible in classic Hugoniot experiments (load control), but could be resolved under deformation-controlled testing. The linear model more closely agrees with the experimental τ data, but the higher-

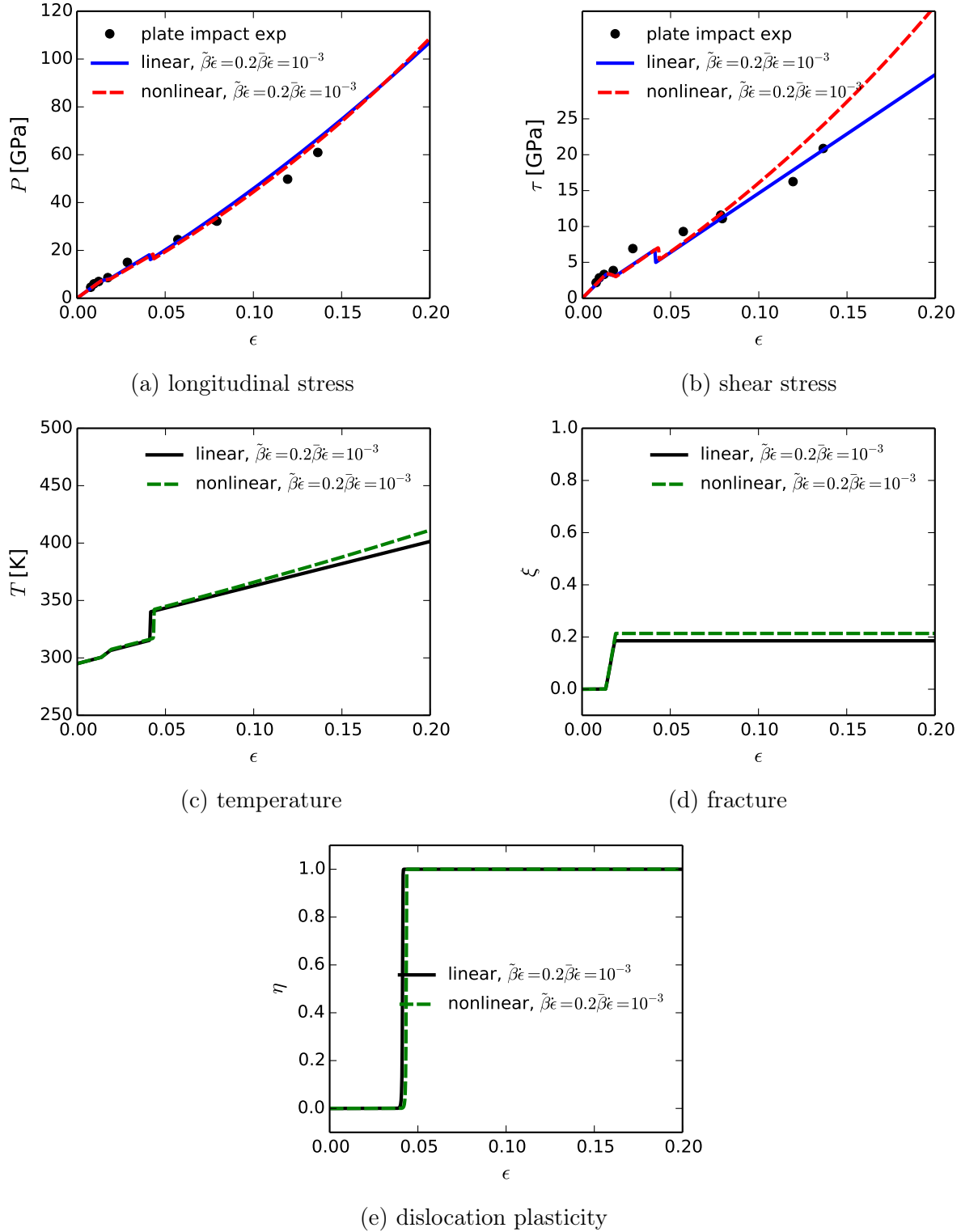


Fig. 15 Titanium diboride: axial stress, shear stress, temperature and order parameters versus axial strain predicted by threshold-type fracture model of Eq. 204, with phase change kinetics Eq. 210 enabled ($\dot{\eta} \geq 0$). Adiabatic uniaxial strain compressive loading at dimensionless strain rate $\tilde{\beta}\dot{\epsilon}$, with experimental Hugoniot longitudinal and shear stress data⁶⁵: (a) P (b) τ (c) T (d) ξ (e) η .

strain data points suggest a nonlinear rise in strength, which if extrapolated, would provide better accuracy of the nonlinear model for $\epsilon \gtrsim 0.15$. The data thus do not clearly indicate superiority of the nonlinear model over the linear model, or vice versa.

The locking pressure p_L restricts ξ to maxima on the order of 0.2 at $\epsilon \gtrsim 0.0185$, which enables shear strength to continue to increase with increasing compression as observed for TiB_2 , rather than degrade to zero as observed for B_4C . Linear and nonlinear models show similar histories for T , ξ , and η , where T from the nonlinear theory slightly exceeds the linear result. At 20% compression, $T = 411$ K for the nonlinear theory, which is lower than the 470 K attained by B_4C at the same strain rate, and is also insufficient to induce a drop in $\bar{\beta}_A$ in Eq. 210, indicating increased dislocation mobility,¹³⁴ large enough to affect model results.

6.4 Results: Ceramic Composite

The irreversible fracture kinetic model of Eq. 204 is used for consistency with former studies of B_4C and TiB_2 . No model parameters are fitted explicitly for analysis of uniaxial strain compression of the composite. Viscosity for crack kinetics $\tilde{\beta}$ has already been calibrated to results in Section 5.4. Viscosity for slip, $\bar{\beta}$, is assumed the same as that for TiB_2 since dislocation generation and motion only occur in grains of the TiB_2 phase of the composite. Mixture rules are deemed appropriate for other parameters, as explained in Section 4.3. However, limited available shock compression data⁶⁸ do not provide high-pressure shear strength of the composite, and thus are insufficient to allow one to deduce a suitable value of p_L , if applicable at all. Two assumptions are considered here. The first, $p_L \rightarrow \infty$, corresponds to no pressure locking and total strength loss due to fracture similar to pure B_4C analyzed in Section 6.2. The second, $p_L = 10$ GPa, preserves some post-HEL strength similar to TiB_2 in Section 6.3.

Longitudinal stress, shear stress, temperature, and order parameter histories predicted under adiabatic conditions at $\tilde{\beta}\dot{\epsilon} = 10^{-3}$ are given in Fig. 16. Shock Hugoniot data on P from experiments⁶⁸ is shown for comparison. This reference⁶⁸ reports the HEL for the composite material (65% by volume B_4C , 35% by volume TiB_2 , $\rho_0 = 3.2$ g/cc) as $P_H \approx 16$ GPa. Both linear and nonlinear models provide similar results that agree with shock data in the elastic regime. However, the two experimental data points corresponding to impact stresses exceeding the HEL appear anomalous. Shock velocities for these data points quoted from that study⁶⁸ over 14 km/s exceed the precursor velocity (elastic wave speed at the HEL), indicating overdriven, i.e., strong, shocks. Compression ϵ , calculated using the Hugoniot relations Eq. 271 and particle velocities tabulated in that reference,⁶⁸ appears too small. Even when a nonlinear elastic model is used, wherein no strength decrement is possible from fracture or slip, P is severely under-predicted relative to the test data. The large discrepancy persists when either set of ultrasonically measured elastic constants^{68,149} for these B_4C - TiB_2 materials of slightly different mass densities is used.

Linear and nonlinear results are very similar for P , T , ξ , and η . When $p_L = 10$ GPa is enforced, then τ for the nonlinear theory increases more rapidly with compression than for the linear theory, similarly to pure TiB_2 . Temperature rise is greater when $p_L \rightarrow \infty$ since dissipation from fracture is unrestricted. In the nonlinear case, $T =$

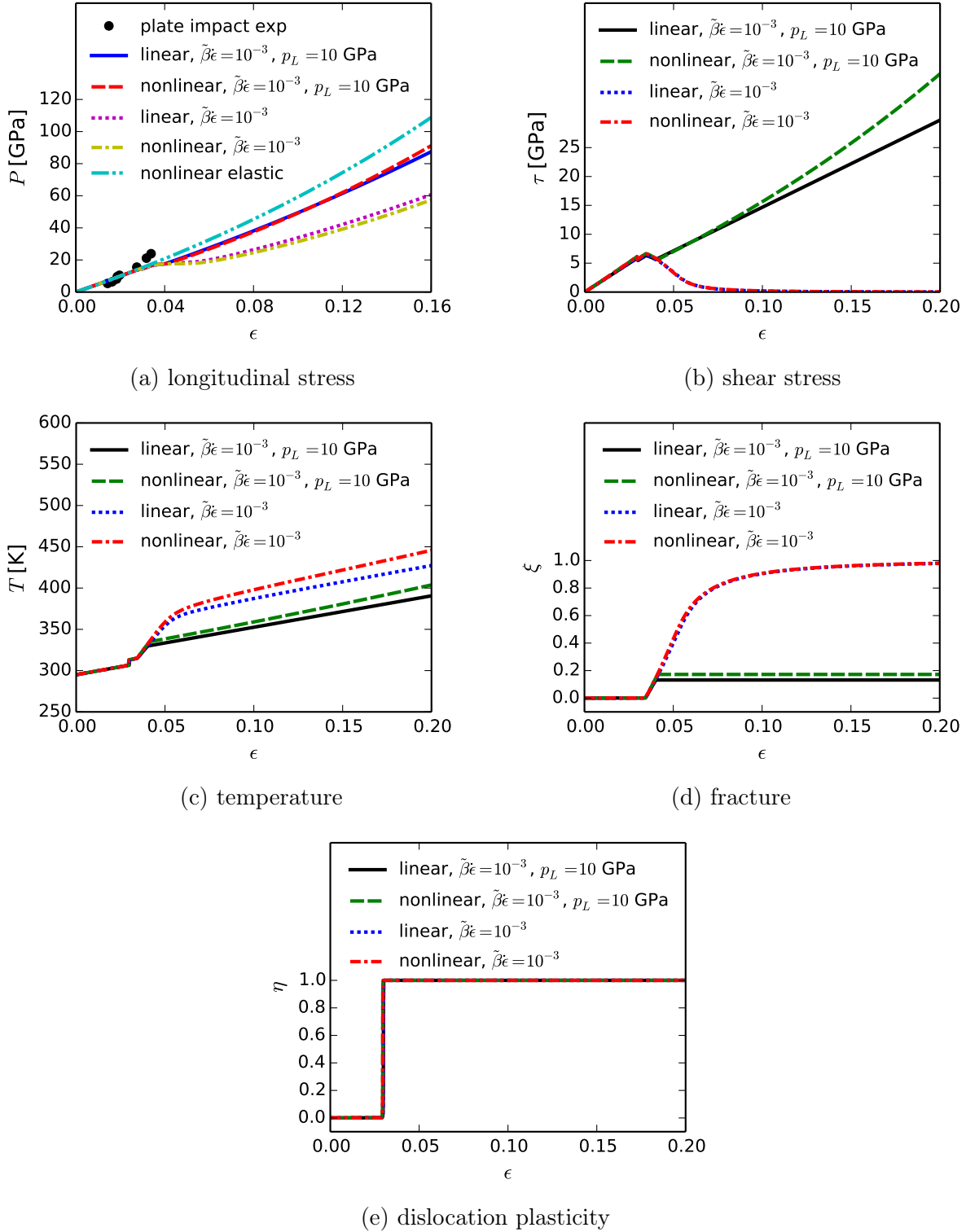


Fig. 16 Ceramic composite: axial stress, shear stress, temperature and order parameters versus axial strain predicted by threshold-type fracture model of Eq. 204, with phase change kinetics Eq. 210 enabled ($\tilde{\eta} \geq 0$). Adiabatic uniaxial strain compressive loading at dimensionless strain rate $\tilde{\beta}\dot{\epsilon}$, with experimental Hugoniot longitudinal stress data⁶⁸: (a) P (b) τ (c) T (d) ξ (e) η .

446 K at 20% compression. This temperature change is not enough to affect crack growth resistance or gross model predictions according to Eq. 214.

7. Structured Steady Shock Waves

The analysis in the present section admits spatially heterogeneous order parameter fields. A plane shock wave propagates through the cylindrical domain, here of infinite length, at steady Lagrangian velocity D in the Z -direction. The shock is treated as a continuous process in space and time, and is said to be “structured”, whereby the shape, including finite width, of the waveform is dictated by the rate-dependent constitutive laws for the material. This is in contrast to simpler treatments of shock waves as discontinuities of infinitesimal thickness, as analyzed in prior works^{56,58,61,72} for B_4C and TiB_2 ceramics. Others analyzed the steady structured shock wave problem for viscoplastic metals.^{154,162–165} These prior works invoked conventional continuum constitutive relations for inelastic response. In the present work, determination of the structure of steady inelastic shock waves is undertaken using phase field theory, in what appears to be first documented treatment of the problem with the phase field method. The phase field approach introduces additional length scale(s) associated with gradient regularization besides the length scale(s) associated with viscous regularization. Only pure B_4C and TiB_2 polycrystals are analyzed, in respective Sections 7.2 and 7.3.

7.1 Governing Equations and Boundary Conditions

The general governing equations of Section 4.4 are specialized as follows. Uniaxial strain conditions apply, where axial deformation and order parameter fields vary with axial coordinate Z and time t :

$$r = R, \quad \theta = \Theta, \quad z = z(Z, t); \quad \xi = \xi(Z, t), \quad \eta = \eta(Z, t). \quad (264)$$

The particle velocity vector is

$$\mathbf{v}(Z, t) = v(Z, t)\mathbf{G}^Z = \dot{z}(Z, t)\mathbf{G}^Z. \quad (265)$$

Acceleration $\dot{v}(Z, t)$ need not vanish. The deformation gradient and scalar com-

pressive strain are, respectively,

$$\begin{aligned}\mathbf{F}(Z, t) &= \delta_K^k \mathbf{g}_k \otimes \mathbf{G}^K - \epsilon(Z, t) \mathbf{g}_z \otimes \mathbf{G}^Z; \\ \epsilon(Z, t) &= 1 - F_Z^z(Z, t) = 1 - J(Z, t) = 1 - \rho_0/\rho(Z, t),\end{aligned}\tag{266}$$

where $J = \det \mathbf{F}$. In the geometrically linear theory, $u^R = u^\Theta = 0$, $v = \dot{u}^Z$, and $\mathbf{h} = -\epsilon \mathbf{G}_Z \otimes \mathbf{G}^Z$. From symmetry, stresses obey the following conditions as in Section 6: $\mathbf{P}$ is diagonal with two independent components P_z^Z and $P_r^R = P_\theta^\Theta$, and Cauchy stress components are $\sigma_z^z = P_z^Z$, $\sigma_r^r = \sigma_\theta^\theta = J^{-1} P_r^R = (\partial_Z z)^{-1} P_r^R$. In the linear theory, P_Z^Z is equivalent to P_z^Z .

Define $P = -P_z^Z = -\sigma_z^z$ as the longitudinal compressive stress. The mass conservation (i.e., continuity) equation in Eq. 230 and the momentum conservation equation in the Z -direction in Eq. 231 reduce to

$$\begin{aligned}\dot{F}_Z^z &= \frac{\partial}{\partial t} \frac{\partial z}{\partial Z} = \frac{\partial^2 z}{\partial Z \partial t} = \frac{\partial z}{\partial Z} \frac{\partial v}{\partial z} = \frac{\partial v}{\partial Z} \Rightarrow \frac{\partial \epsilon}{\partial t} = -\frac{\partial v}{\partial Z}; \\ \frac{\partial P_z^Z}{\partial Z} &= \rho_0 \dot{v} \Rightarrow \frac{\partial P}{\partial Z} = -\rho_0 \frac{\partial v}{\partial t}.\end{aligned}\tag{267}$$

In a steady waveform traveling at Lagrangian velocity $D > 0$, field variables depend on the moving coordinate $Y = Z - Dt$ rather than Z and t independently:

$$\begin{aligned}v(Z, t) &= v(Z - Dt) = v(Y), & \epsilon(Z, t) &= \epsilon(Z - Dt) = \epsilon(Y); \\ \xi(Z, t) &= \xi(Z - Dt) = \xi(Y), & \eta(Z, t) &= \eta(Z - Dt) = \eta(Y); \\ P(Z, t) &= P(Z - Dt) = P(Y), & S(Z, t) &= S(Z - Dt) = S(Y).\end{aligned}\tag{268}$$

Similar expressions apply for temperature, internal energy, and lateral stress fields. Note the general identities for a differentiable function $f(Z, t) = f(Z - Dt) = f(Y)$:

$$\frac{\partial f}{\partial Z} = \frac{df}{dY} \frac{\partial Y}{\partial Z} = \frac{df}{dY}, \quad \frac{\partial f}{\partial t} = \frac{df}{dY} \frac{\partial Y}{\partial t} = -D \frac{df}{dY}.\tag{269}$$

Application of Eqs. 268 and 269 to Eq. 267 produces conservation equations for a steady planar waveform:

$$\frac{d\epsilon}{dY} = \frac{1}{D} \frac{dv}{dY}, \quad \frac{dP}{dY} = \rho_0 D \frac{dv}{dY} \Rightarrow \frac{dP}{dY} = \rho_0 D^2 \frac{d\epsilon}{dY}.\tag{270}$$

The rightmost equation is the differential form of the Raleigh line stress-strain equation, where the slope of the Rayleigh line is the constant stiffness $\rho_0 D^2$ for a given steady shock velocity. The equations in Eq. 270 can be integrated to give the Hugoniot relations for the jump $[[(\cdot)]] = (\cdot)^- - (\cdot)^+$ between any two points associated with different values of (Y^+, Y^-) immediately preceding, within, or immediately following the waveform:

$$[[v]] = D[[\epsilon]], \quad [[P]] = \rho_0 D[[v]] = \rho_0 D^2[[\epsilon]]. \quad (271)$$

For a compressive wave, if Y^+ and Y^- are coordinates preceding and following the waveform, then $[[\epsilon]] > 0$, $[[v]] > 0$, and $[[P]] > 0$. For a structured wave, rigorous use of Eq. 271 requires that $D = \text{constant}$. However, the same equations hold for a shock of infinitesimal thickness (i.e., moving surface of discontinuity), whether steady or unsteady.^{72,154} Similar jump equations can be derived for energy conservation and the dissipation inequality,^{58,72,154,166} but these are not needed in the present investigation. Adiabatic conditions are assumed, as is standard practice for analysis of shock waves.^{72,154}

From Eq. 228 or Eq. 251 with Eq. 268, constitutive equations for longitudinal stress in total and incremental form along the Rayleigh line can be expressed as follows:

$$\begin{aligned} P &= P(\epsilon(Y), S(Y), \xi(Y), \eta(Y)) \\ \Rightarrow \quad \frac{dP}{dY} &= \frac{\partial P}{\partial \epsilon} \frac{d\epsilon}{dY} + \frac{\partial P}{\partial S} \frac{dS}{dY} + \frac{\partial P}{\partial \xi} \frac{d\xi}{dY} + \frac{\partial P}{\partial \eta} \frac{d\eta}{dY}. \end{aligned} \quad (272)$$

Equating Eq. 272 with the rightmost expression in Eq. 270, the following nonlinear ordinary differential equation is obtained for the rate of change of compressive strain with respect to moving coordinate Y along the Rayleigh line:

$$\frac{d\epsilon}{dY} = \frac{1}{(\rho_0 D^2 - C_l^t)} \left[\frac{\partial P}{\partial S} \frac{dS}{dY} + \frac{\partial P}{\partial \xi} \frac{d\xi}{dY} + \frac{\partial P}{\partial \eta} \frac{d\eta}{dY} \right]. \quad (273)$$

The tangent longitudinal stiffness C_l^t is defined as follows and must exceed the shock stiffness $\rho_0 D^2$ in the present analysis that excludes both overdriven and rarefaction shocks (note $d\epsilon/dY \leq 0$ as $Y : +\infty \rightarrow -\infty$):

$$C_l^t = \partial P(\epsilon, S, \xi, \eta) / \partial \epsilon > \rho_0 D^2. \quad (274)$$

Entropy is assumed to arise only from order parameter kinetics, as in the adiabatic representation Eq. 234, and not from any other dissipative processes not included in the continuum theory:

$$\frac{dS}{dY} = -\frac{1}{D} \frac{\mathfrak{D}}{T}. \quad (275)$$

Dissipation depends on order parameter rates, where from application of Eq. 269 to the irreversible fracture model with threshold in Eq. 204 and the TDGL-type phase kinetic model in Eq. 210 modified for strict irreversibility,

$$\frac{d\xi}{dY} = -\frac{1}{D\tilde{\beta}} \langle \tilde{\mathcal{F}} - \tilde{\mathcal{R}} \rangle, \quad \frac{d\eta}{dY} = -\frac{1}{D\bar{\beta}_A} \langle \bar{\mathcal{F}} - \bar{\mathcal{R}} \rangle. \quad (276)$$

Expressions introduced in Section 4 for state-dependent driving forces $\tilde{\mathcal{F}}$ and $\bar{\mathcal{F}}$ apply verbatim. Resistances to structural transformations depend on divergences of order parameters. For the present case of fields of the form in Eq. 268, application of Eq. 269 to Eqs. 203 and 211 produces

$$\begin{aligned} \tilde{\mathcal{R}} &= 2 \left[\xi - (\kappa_\xi l_\xi)^2 \frac{d^2 \xi}{dY^2} \right], \\ \bar{\mathcal{R}} &= 6\eta(1-\eta) + \frac{A}{\Xi} \left[2\eta(1-\eta)(1-2\eta) - \frac{1}{8} (\kappa_\eta l_\eta)^2 \frac{d^2 \eta}{dY^2} \right]. \end{aligned} \quad (277)$$

New parameters $\kappa_\xi \geq 0$ and $\kappa_\eta \geq 0$ are introduced to enable changes in gradient regularization (e.g., enabling or disabling it) in subsequent parameter studies, without affecting other features of the models. Unless stated otherwise, $\kappa_\xi = \kappa_\eta = 1$ by default. Setting $\kappa_\xi = \kappa_\eta = 0$ in Eq. 277 produces “scale-free” versions of the phase field model wherein gradients of order parameters are omitted in the thermodynamics and kinetic laws.^{167,168}

For the geometrically nonlinear theory of Section 2 for an isotropic solid, the tangent longitudinal modulus and other partial derivatives of the axial stress entering Eq. 273 are derived as follows:

$$\begin{aligned} C_l^t &= \frac{1}{J^2} \left(\frac{4}{3} G + B \left[1 - \frac{1}{2} (B'_0 - 2) (\text{tre}^E) - \frac{1}{6} C''_0 (\text{tre}^E)^2 \right] \right. \\ &\quad \left. - B \left[\frac{1}{2} (B'_0 - 2) + \frac{1}{3} C''_0 (\text{tre}^E) \right] (\text{tre}^E) + JP \right), \end{aligned} \quad (278)$$

$$\partial P / \partial S = T \gamma / J, \quad (279)$$

$$\frac{\partial P}{\partial \xi} = \frac{1}{J} \left(\frac{4}{3} \frac{d\chi}{d\xi} G_0 [(e^E)_R^R - (e^E)_Z^Z] + B \left[1 - \frac{1}{2}(B'_0 - 2)(\text{tre}^E) - \frac{1}{6}C''_0(\text{tre}^E)^2 \right] \frac{6\xi(1-\xi)\bar{\varphi}_0}{1-\xi^2(3-2\xi)\bar{\varphi}_0} \right), \quad (280)$$

$$\begin{aligned} \frac{\partial P}{\partial \eta} = \frac{1}{J} & \left(\left\{ \frac{4}{3}G + B \left[1 - \frac{1}{2}(B'_0 - 2)(\text{tre}^E) - \frac{1}{6}C''_0(\text{tre}^E)^2 \right] \right\} \frac{6\eta(1-\eta)(e^\eta_Z)^Z}{1+\eta^2(3-2\eta)(e^\eta_Z)^Z} \right. \\ & \left. - 2 \left\{ \frac{2}{3}G - B \left[1 - \frac{1}{2}(B'_0 - 2)(\text{tre}^E) - \frac{1}{6}C''_0(\text{tre}^E)^2 \right] \right\} \frac{6\eta(1-\eta)(e^\eta_R)^R}{1+\eta^2(3-2\eta)(e^\eta_R)^R} \right). \end{aligned} \quad (281)$$

For the geometrically linear theory of Section 3, the analogous terms are derived as

$$C_l^t = \frac{4}{3}G + B \left[1 - \frac{1}{2}\beta'_0(\text{tre}^E) - \frac{1}{6}C''_0(\text{tre}^E)^2 \right] - B \left[\frac{1}{2}\beta'_0 + \frac{1}{3}C''_0(\text{tre}^E) \right] (\text{tre}^E), \quad (282)$$

$$\partial P / \partial S = T\gamma, \quad (283)$$

$$\begin{aligned} \frac{\partial P}{\partial \xi} = \frac{4}{3} \frac{d\chi}{d\xi} G_0 & [(\epsilon^E)_R^R - (\epsilon^E)_Z^Z] \\ & + B \left[1 - \frac{1}{2}\beta'_0(\text{tre}^E) - \frac{1}{6}C''_0(\text{tre}^E)^2 \right] \frac{6\xi(1-\xi)\bar{\varphi}_0}{1-\xi^2(3-2\xi)\bar{\varphi}_0}, \end{aligned} \quad (284)$$

$$\begin{aligned} \frac{\partial P}{\partial \eta} = & \left\{ \frac{4}{3}G + B \left[1 - \frac{1}{2}(B'_0 - 2)(\text{tre}^E) - \frac{1}{6}C''_0(\text{tre}^E)^2 \right] \right\} \{6\eta(1-\eta)(e^\eta_Z)^Z\} \\ & - 2 \left\{ \frac{2}{3}G - B \left[1 - \frac{1}{2}(B'_0 - 2)(\text{tre}^E) - \frac{1}{6}C''_0(\text{tre}^E)^2 \right] \right\} \{6\eta(1-\eta)(e^\eta_R)^R\}. \end{aligned} \quad (285)$$

Equations 273–276 are integrated numerically along the Rayleigh line, from $Y = +\infty$ to $Y = -\infty$. The steady shock velocity D is input as the loading condition. A second-order backward difference approximation is used to calculate the derivatives on the right sides of Eq. 277. The steady state of the material ahead of the shock (e.g., the precursor state) is labeled $(\cdot)^+$, that behind the shock (i.e., the Hugoniot state) is labeled $(\cdot)^-$. Free natural boundary conditions on order parameters are $d\xi/dY = d\eta/dY = 0$ as $Y \rightarrow \pm\infty$. Assignment of the $(\cdot)^+$ state is approached differently for B_4C and TiB_2 as detailed in Sections 7.2 and 7.3, respectively, since the first plastic wave is analyzed in the former and the second plastic wave in the latter. In each case, the terminal Y^- coordinate is effectively attained as the argument of $d\epsilon(Y)/dY = 0$ for a given imposed D . If the particle velocity ahead of the shock front $v(Y^+)$ is known a priori along with solution of Eq. 273, then the

Rankine–Hugoniot equation in Eq. 271 for continuity can be used to obtain particle velocity anywhere else in the structured shock or at the terminal state:

$$v(Y) = v(Y^+) + D[\epsilon(Y) - \epsilon(Y^+)]. \quad (286)$$

When η indicates plastic slip, as in TiB_2 , then the scalar GND density in a steady wave is calculated from Eq. 227 as

$$\rho_G = \frac{\sqrt{2}}{b_0} [(\bar{F}^\eta)_Z^Z]^{-3/2} \left| (\bar{e}_0^\eta)_Z^Z \frac{d\phi}{d\eta} \frac{d\eta}{dY} \right|. \quad (287)$$

The geometrically linear counterpart of Eq. 287 is Eq. 250 with $\partial_Z \eta \rightarrow d\eta/dY$.

7.2 Results: Boron Carbide

For analysis of the sole plastic wave in B_4C , the upstream $(\cdot)^+$ state corresponds to the HEL, i.e., the thermoelastically deformed material in the elastic precursor wave. Order parameters $\xi = \eta = 0$ for $P < P_H$. The isentropic uniaxial strain solution is used to estimate strain and temperature at the $(\cdot)^+$ state. This is considered a highly accurate approximation since prior works^{55,155} have shown that entropy production from the precursor/elastic shock in ceramics and minerals produces an increase in P of less than 1%.

For B_4C , given an imposed shock velocity D , the shock structure, including 5-95% rise time t_R and corresponding shock width δ_R , are controlled primarily by the fracture kinetic viscosity $\tilde{\beta}$ and the effective gradient regularization length $\kappa_\xi l_\xi$. Viscous regularization imposes a dissipative penalty for short rise times: the larger the value of $\tilde{\beta}$, the longer the time required for micro-crack nucleation, extension, and percolation in the waveform leading to comminution. Gradient regularization induces an energetic penalty for a steep wavefront. The larger the value of $\kappa_\xi l_\xi$, the larger the geometric resistance $\tilde{\mathcal{R}}$ when $d\xi^2/dY^2 < 0$ in Eq. 277. Both kinds of regularization constrain the solution such that a discrete jump from a pristine state ($\xi^+ = 0$) to a comminuted state ($\xi^- = 1$) is forbidden. The transition region with $\xi \in (0, 1)$ physically represents a partially degraded material with some residual strength, wherein micro-cracks have nucleated but not saturated the medium.^{54,61} The present analysis does not resolve the geometry or velocity of individual cracks. In polycrystalline ceramics, cracks tend to propagate at speeds significantly below

Table 4 Boron carbide: predicted 5 – 95% shock rise time t_R from particle velocity profiles and normalized shock front width δ_R from nonlinear and linear models. Plate impact experiments⁶⁰ suggest $t_R \approx 10 - 100$ ns for $D \approx 9.9 - 11.8$ km/s. Rise times and shock widths decrease with increasing D in both model and experiment.

Shock velocity D [km/s]	Viscosity $\tilde{\beta}$ [s]	t_R [ns] linear	t_R [ns] nonlinear	δ_R/l_ξ linear	δ_R/l_ξ nonlinear	$\eta^- > 0$ linear	$\eta^- > 0$ nonlinear
10	10^{-8*}	5.6	4.5	36	28	no	no
	10^{-7}	57	42	355	261	no	no
	10^{-6}	564	413	3543	2595	no	no
11	10^{-8*}	3.5	3.1	24	21	no	no
	10^{-7}	31	23	215	162	no	no
	10^{-6}	311	234	2150	1616	no	no
12	10^{-8*}	1.2	2.3	9.2	17	yes	no
	10^{-7}	6.8	12	52	90	yes	no
	10^{-6}	154	120	1159	906	no	no

*gradient regularization from $l_\xi^2 \nabla_0^2 \xi$ inhibits steady wave solution when $\kappa_\xi = 1$

the Rayleigh wave speed,⁷⁴ which in turn is usually lower than the shock velocity D . The analogy for an elastic-plastic material is that a continuum flow rule does not resolve the motions of individual dislocations in a plastic waveform, which in turn tends to travel faster than the shear wave velocity that limits dislocation glide velocities.

Comparison of rise times from particle velocity histories with experimental wave profiles enables calibration of $\tilde{\beta}$. Listed in Table 4 are t_R and normalized shock width δ_R/l_ξ for three imposed shock velocities $D = 10, 11, 12$ km/s and three viscosities $\tilde{\beta} = 10^{-8}, 10^{-7}, 10^{-6}$ s. The occurrence of amorphization in model predictions, $\eta^- > 0$, is also noted in Table 4. Rise times and shock widths are $\approx 20\%$ larger for the linear theory relative to the nonlinear theory. Experimental data,⁶⁰ to the extent afforded by figure resolution, suggest rise times of $10 - 100$ ns for shock velocities in this range. Thus, the value of $\tilde{\beta} = 10^{-7}$ s provides best agreement, as prescribed already in Table 1. Amorphization is predicted for $D = 12$ km/s in the linear model, but not the nonlinear model. For both linear and nonlinear theories, t_R decreases with increasing D , in general agreement with experimental trends for B_4C .⁶⁰

Effects of viscous and gradient regularization on particle velocity profiles are resolved in Fig. 17 for a steady plastic shock of Lagrangian velocity $D = 11$ km/s.

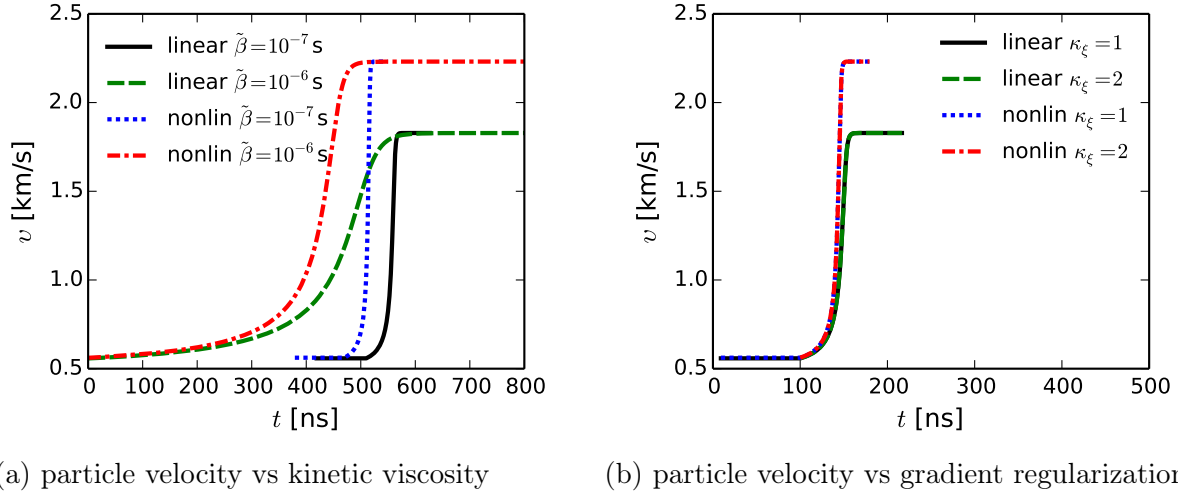
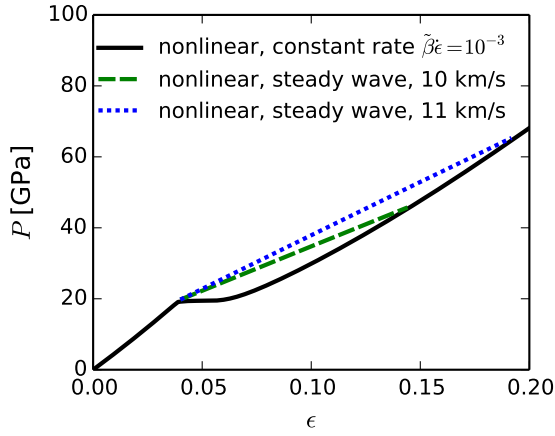


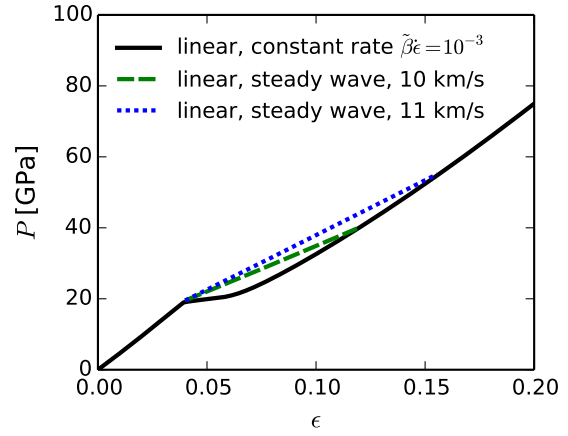
Fig. 17 Boron carbide: effects of viscosity and effective regularization length $\kappa_\xi l_\xi$ on particle velocity v versus time t in steady structured waveform of speed $D = 11$ km/s: (a) v , $\kappa_\xi = 1$, variable $\tilde{\beta}$ in Eq. 276 (b) v , $\tilde{\beta} = 10^{-7}$ /s, variable κ_ξ in Eq. 277. Steady wave profiles staggered with respect to t to enable visualization.

Broadening of the waveform with increasing $\tilde{\beta}$ is evident in Fig. 17a. Gradient regularization has a near-negligible effect on waveforms for $\kappa_\xi \leq 2$ and $\tilde{\beta} = 10^{-7}$ s. However, if a smaller viscosity, $\tilde{\beta} = 10^{-8}$ s, is used, then gradient regularization with $l_\xi = 1$ prevents the formation of a steady structured plastic waveform, as indicated in the footnote of Table 4. In that case, the steep velocity and stress rise dictated by the low dynamic viscosity is incompatible with the minimum shock width permitted by gradient regularization. The incompatibility arises when $\delta_R/l_\xi \lesssim 35$, setting a constraint on the minimum permissible dynamic viscosity. Remaining results in Section 7.2 are obtained from the recommended values $\tilde{\beta} = 10^{-7}$ s and $\kappa_\xi = 1$.

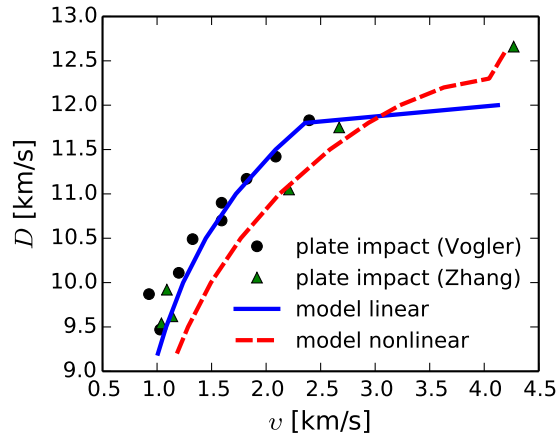
Shown in Figs. 18a and 18b are Rayleigh lines (dotted or dashed lines) generated in analyses of steady shocks for nonlinear and linear theories. Rayleigh lines terminate on the predicted Hugoniot, which clearly is close to the uniaxial steady-rate predictions of Section 6.2 (solid curves). Slopes of Rayleigh lines for each imposed D are identical for linear and nonlinear theories, but termination points at the Hugoniot stress corresponding to each D differ between the theories. Shock velocity is reported versus particle velocity in Fig. 18c. Discrete data points are those published by Vogler et al.⁶⁰ (Table I, median HEL ≈ 16 GPa for comparable v^+) and Zhang



(a) shock stress, nonlinear



(b) shock stress, linear



(c) shock velocity vs particle velocity

Fig. 18 Boron carbide: Rayleigh lines with predicted terminal Hugoniot states from steady wave analysis, uniaxial strain steady rate compression curves from Section 6.2.2, predicted shock velocity versus particle velocity, and plate impact Hugoniot data^{60,75}: (a) P , nonlinear model (b) P , linear model (c) $D - v$

et al.⁷⁵ (Table II, HEL ≈ 19.5 GPa). The geometrically linear model provides better agreement with experiment than the nonlinear model for $D \lesssim 11$ km/s. This is also reflected in the closer agreement of steady-rate response with Hugoniot stress-strain data for $\epsilon \lesssim 0.12$ in Fig. 14a, whereby P predicted by the nonlinear theory is low relative to experimental data of TJ Vogler.⁶⁰ However, the linear model predicts amorphization and a notable stiffness decrement for $\epsilon \gtrsim 0.15$ or $D \gtrsim 11.8$ km/s, a phenomenon which is not apparent in aggregated data for the shock response of B₄C.¹¹⁵ The $D \gtrsim 11$ km/s data of the second reference⁷⁵ (triangles in Fig. 18c) is also better captured by the nonlinear theoretical results; both model and experiment show kinks due to changing compressibility at high pressure. Thus, in accordance with observations of Section 6.2, the linear model may be a suitable replacement for the nonlinear model for uniaxial compression wherein $\epsilon \lesssim 0.12$ and $P \lesssim 50$ GPa, but should be used with caution at much higher pressures.

Longitudinal stress, shear stress, temperature, axial strain rate, and order parameter profiles within steady waveforms are shown in Fig. 19 for $D = 10, 11, 12$ km/s. In most cases, P , τ , T , $\dot{\epsilon}$, and ξ rise more strongly for the nonlinear model than the linear model. An exceptional result is the prediction of amorphization, with $\eta > 0$, for the linear model at $D = 11$ km/s. In that case, fracture is suppressed as amorphization accommodates shear deformation, lowering the driving force for shear-induced fracture. Peak strain rates increase dramatically with increasing shock stress, with maximum values of $\dot{\epsilon}$ reaching $10^7 - 10^8$ /s in the plastic wavefront in Fig. 19d. Maximum strain rate is notably highest for the linear simulation that demonstrates amorphization, in agreement with the prescribed viscosities that favor phase transformation over fracture at sub-nanosecond rise-time scales. Temperature rise for shock compression in Fig. 19c exceeds that for steady-rate compression to the same ϵ in Fig. 14c. For the strongest shocks studied here, $T \approx 0.5T_M$ for $P \approx 100$ GPa in the nonlinear theory. Whether or not this temperature rise would be sufficient to induce strain localization and/or amorphization, as posited in earlier analysis⁷⁷ and from atomic simulations,⁶³ is unresolved by the current study.

Recall from Section 7.1 that in a steady wave, field variables depend only on moving coordinate $Y = Z - Dt$, such that independent variables Z and t are related by a linear transformation. In other words, profiles of field variables with respect to t at fixed Z (as in Figs. 17 and 19) or with respect to Z at fixed t provide similar information. Shown in Fig. 20 are profiles with respect to the latter, showing how

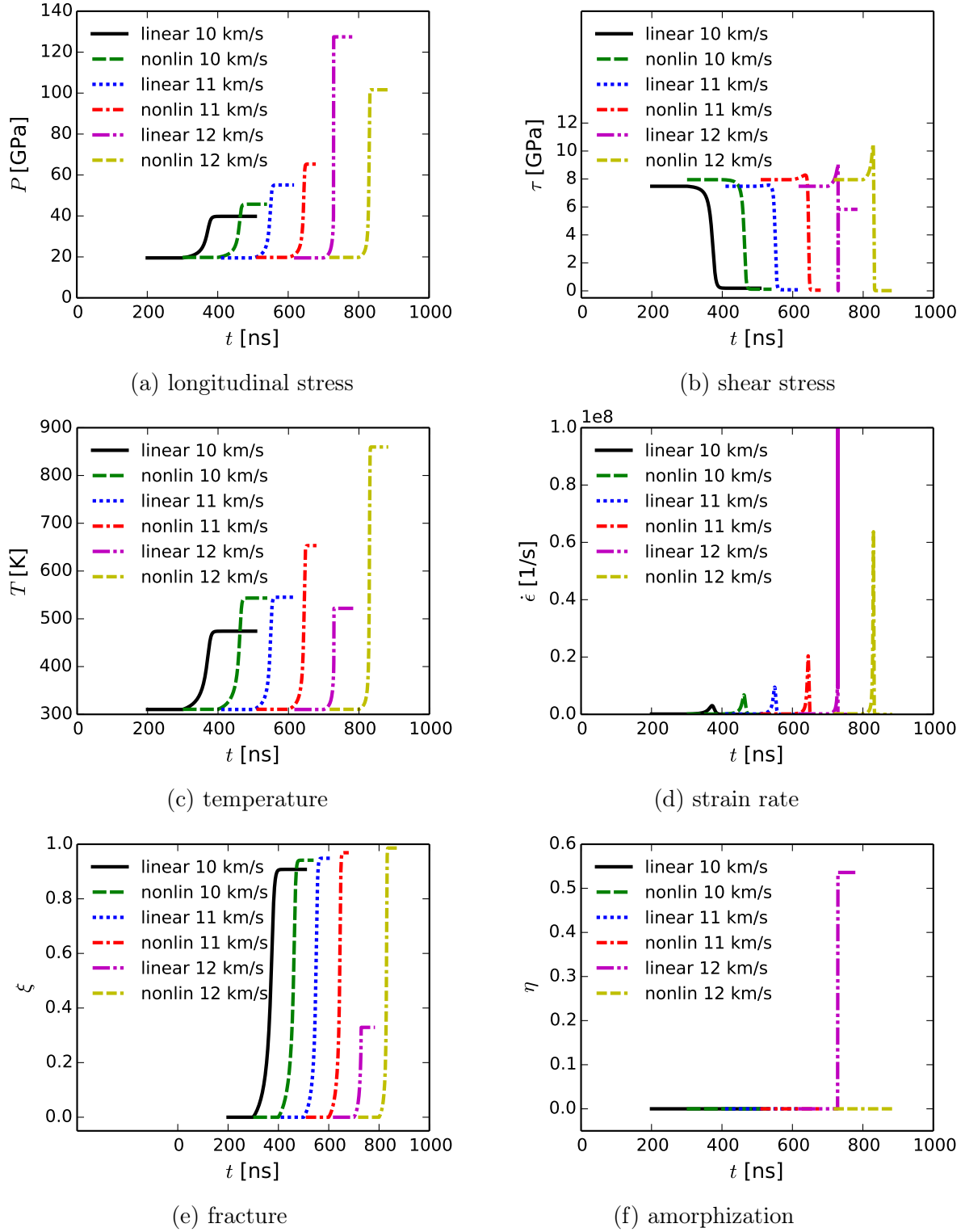
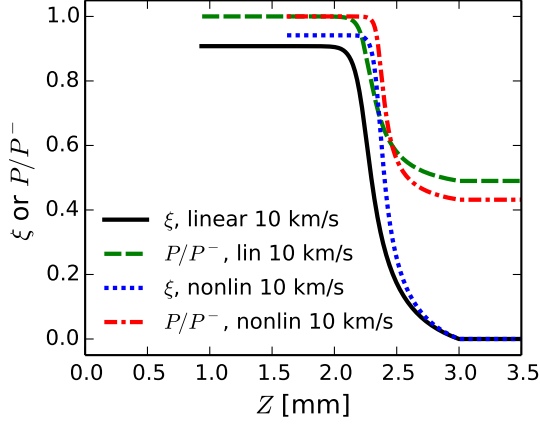
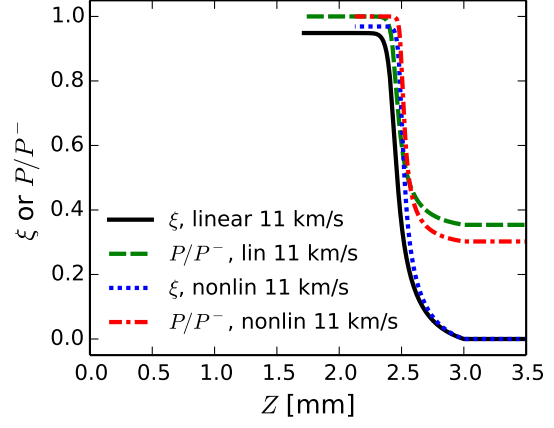


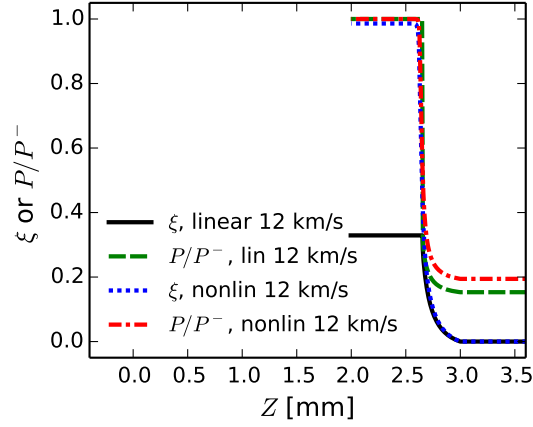
Fig. 19 Boron carbide: longitudinal stress, shear stress, temperature, strain rate, and order parameters in steady structured shock waves, $\tilde{\beta} = 10^{-7}$ s: (a) P (b) τ (c) T (d) $\dot{\epsilon}$ (e) ξ (f) η . Profiles staggered in t to enable visualization.



(a) $D = 10$ km/s



(b) $D = 11$ km/s



(c) $D = 12$ km/s

Fig. 20 Boron carbide: normalized longitudinal stress and fracture phase field parameter versus material position Z at fixed t in steady structured shock waves, $\tilde{\beta} = 10^{-7}$ s, shock velocities of (a) 10 km/s (b) 11 km/s (c) 12 km/s

longitudinal stress P , normalized by end state Hugoniot stress P^- , and fracture phase field variable $\xi \in [0, 1]$ simultaneously vary with position. Results indicate that waveforms for longitudinal stress and the order parameter coincide closely in space, meaning that the moving phase boundary does not lag the stress wave, or vice-versa. (Such a lag could be possible, even if both mechanisms propagate at the same speed D .) Steepening of waveforms is apparent as D increases, in agreement with experimental data on B_4C .⁶⁰

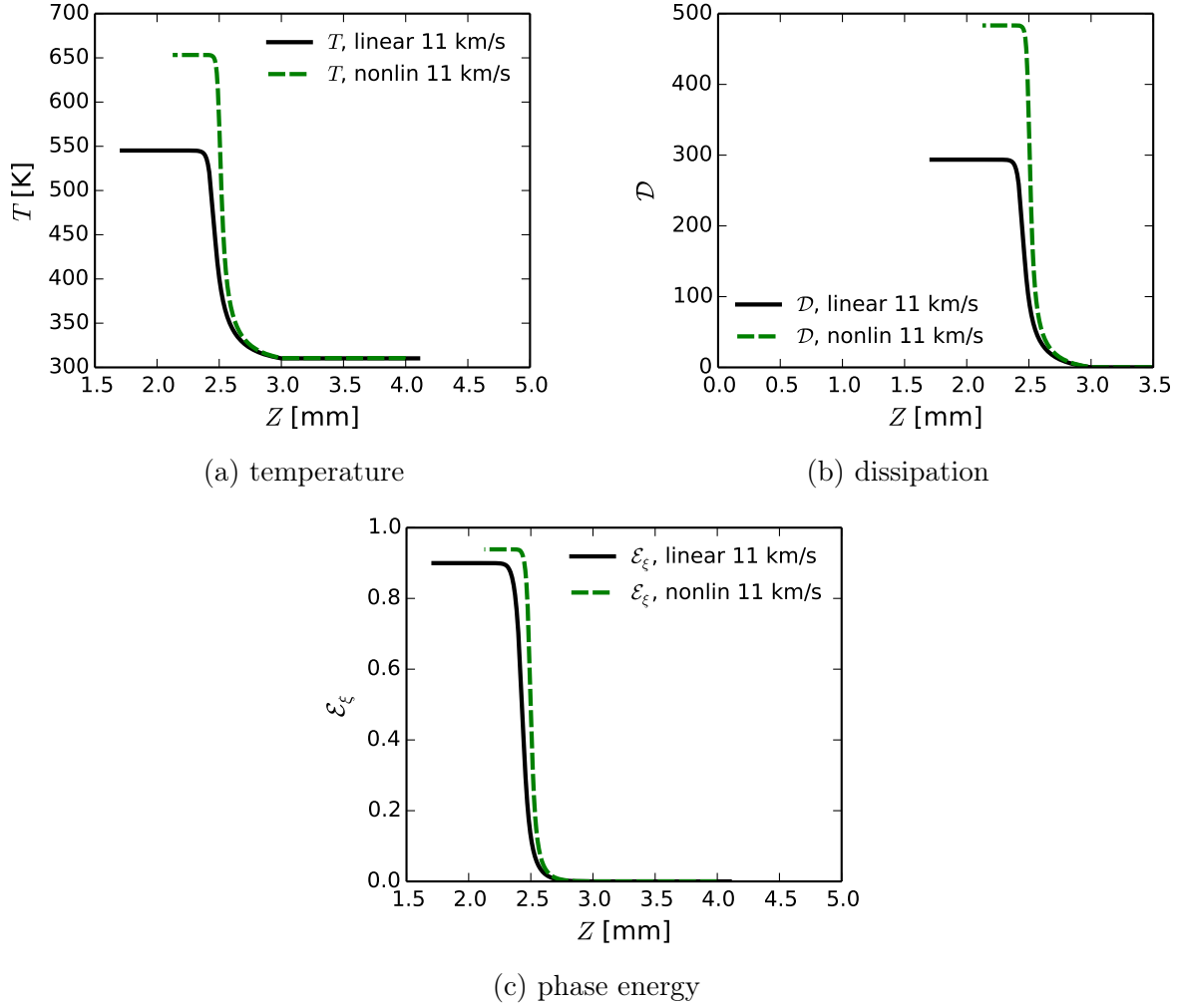


Fig. 21 Boron carbide: thermodynamic quantities versus material position Z at fixed t in steady structured shock waves, $\tilde{\beta} = 10^{-7}$ s, shock velocity of 11 km/s: (a) T (b) $\mathcal{D}$ (c) $\mathcal{E}_\xi$

Given in Fig. 21 are thermodynamic quantities versus Z at fixed t for a shock velocity of 11 km/s: temperature, cumulative dissipation, and phase energy, where the

latter two are normalized by energy per unit volume Υ/l_ξ :

$$\mathcal{D}(Z, t) = \frac{l_\xi}{\Upsilon} \int_0^t \mathfrak{D}(Z, \tau) d\tau, \quad \mathcal{E}_\xi(Z, t) = \frac{l_\xi}{\Upsilon} f_\xi^U(Z, t) = [\xi(Z, t)]^2 + \left[l_\xi \frac{\partial \xi(Z, t)}{\partial Z} \right]^2. \quad (288)$$

In a steady waveform, these fields depend only on moving coordinate Y rather than (Z, t) independently; coordinate transformations are given in Section 7.1. Profiles of T and $\mathcal{D}$ are of similar width, each closely tracking profiles of ξ in Fig. 20b. Trends are expectedly similar given the contribution of dissipated energy to temperature rise for adiabatic shocks. Viscous dissipation and temperature rise are notably larger in the nonlinear theory compared to the linear theory, with narrower profiles in the nonlinear case. Differences among predicted waveforms from linear and nonlinear models for phase energies in Fig. 21c are much less prominent, and such waveforms have narrower widths than those in Figs. 21a and 21b. In the Hugoniot state, the ratio of dissipated energy to phase energy is $\mathcal{D}^-/\mathcal{E}_\xi^- \approx 300\text{-}500$.

7.3 Results: Titanium Diboride

Analysis of the second plastic wave, corresponding to dislocation nucleation and plastic slip, is undertaken, with shock stresses $P^- \gtrsim 17$ GPa. The first plastic wave, associated with shock stresses in the range $P_H \leq P^- \lesssim 17$ GPa, cannot be studied using the present steady-wave approach due to an inflection and downward concavity of the stress-volume Hugoniot in that range. The first wave is attributed to fracture that initiates at the (first) HEL for $P \geq P_H = 7$ GPa. For analysis of the second wave, the upstream $(\cdot)^+$ state is approximated as that corresponding to the adiabatic uniaxial strain solution from Section 6.3 at $\tilde{\beta}\dot{\epsilon} = 10^{-3}$, at the second yield point at $P \approx 17$ GPa. The upstream particle velocity v^+ is unknown according to this approach, but the thermo-mechanical field variables can still be calculated throughout a steady waveform using the procedure of Section 7.1. Since $p^+ > p_L$, the fracture order parameter is frozen at $\xi(Y) = \xi^+$ throughout and following the second plastic wave. Inelastic deformation and dissipation arise solely from $\dot{\eta}$ in the second wave. The transition region with $\eta \in (0, 1)$ and $|\nabla_0 \eta| > 0$ physically represents a partially slipped and dislocated material in the plastic rise of the waveform. Therein, stacking fault energy and transient elastic energy from dislocations (including geometrically necessary) prohibit a discrete jump to a fully slipped equilibrium state whereby $\eta = \eta^-$ on the Hugoniot.

Table 5 Titanium diboride: predicted 5–95% shock rise time t_R from stress wave profiles and normalized shock front width δ_R from nonlinear and linear models for second plastic wave. Plate impact experiments⁷⁶ suggest $t_R \approx 60$ ns for $D \approx 8 - 9$ km/s from particle velocity histories. Correlation between t_R and D unknown from experiment.

Shock velocity D [km/s]	Viscosity $\tilde{\beta}$ [s]	t_R [ns] linear	t_R [ns] nonlinear	δ_R/l_η linear	δ_R/l_η nonlinear
8	$1 \times 10^{-7*}$	12	12	7.6	7.3
	5×10^{-7}	58	58	36	37
	1×10^{-6}	116	114	73	72
9	$1 \times 10^{-7*}$	12	11	9.0	7.6
	5×10^{-7}	54	53	38	38
	1×10^{-6}	106	105	76	75

*gradient regularization from $l_\eta^2 \nabla_0^2 \eta$ inhibits steady wave solution when $\kappa_\eta = 1$

Similarly to the calibration of $\tilde{\beta}$ for B_4C in Section 7.2 for ξ -dominated mechanisms in the waveform, comparison of rise times from particle velocity histories with experimental wave profiles enables calibration of $\tilde{\beta}$ for η -dominated inelastic-

ity in TiB_2 . Table 5 gives t_R and normalized shock width δ_R/l_η for two imposed shock velocities $D = 8$ and 9 km/s and three phase viscosities $\bar{\beta} = 10^{-7}$, 5×10^{-7} , and 10^{-6} s. Rise times and shock widths are very similar according to linear and nonlinear theories. Limited experimental data⁷⁶ suggest rise times around 60 ns for shock velocities in this range. The value of $\bar{\beta} = 5 \times 10^{-7}$ s provides the closest calibration, as listed already in Table 2. Subsequently discussed results apply this value.

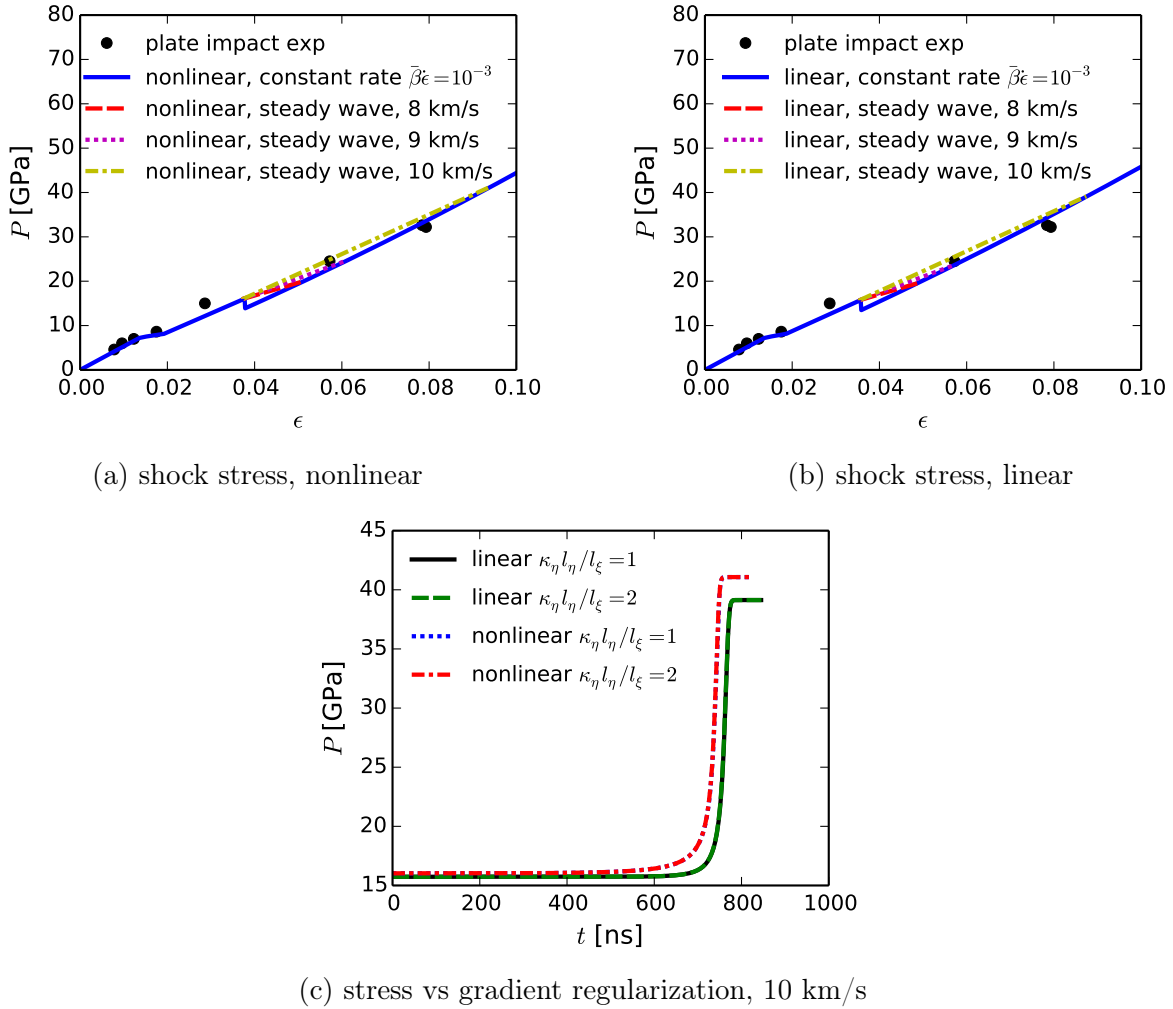
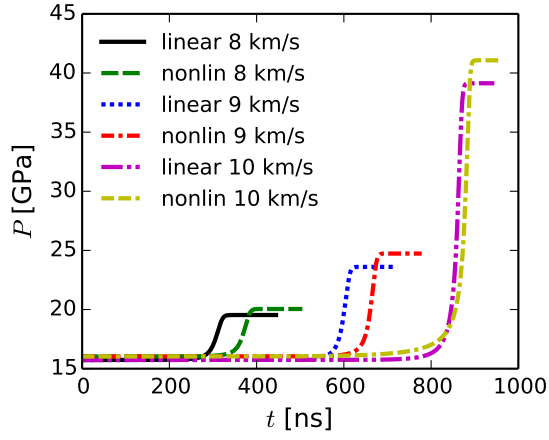


Fig. 22 Titanium diboride: Rayleigh lines with predicted terminal Hugoniot states from steady wave analysis, uniaxial strain steady rate compression curves from Section 6.3, and plate impact Hugoniot data⁶⁵ (a) P , nonlinear model (b) P , linear model; and (c) influence of effective regularization length $\kappa_\eta l_\eta$ in Eq. 277 on axial stress P versus time t in steady structured wave-form of speed $D = 10$ km/s. Results shown obtained with $\bar{\beta} = 5 \times 10^{-7}$ s.

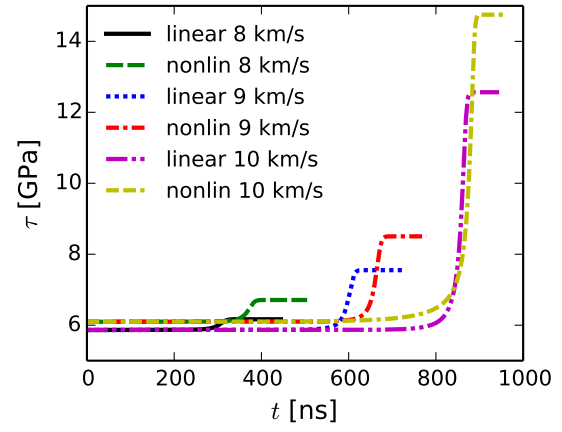
Dotted or dashed lines in Fig. 22a and Fig. 22b are Rayleigh lines created in analysis of steady shocks for respective nonlinear and linear theories. Rayleigh lines terminate on the predicted Hugoniot, which in turn closely matches the uniaxial steady-rate predictions of Section 6.3 given by the solid curves. Effects of gradient regularization on longitudinal stress histories are resolved in Fig. 22c for a steady plastic shock of Lagrangian velocity $D = 10$ km/s. Gradient regularization has no visible effect on predicted waveforms for $\kappa_\eta l_\eta \leq 2l_\xi$ and $\bar{\beta} = 5 \times 10^{-7}$ s. But if a smaller phase viscosity, $\bar{\beta} = 1 \times 10^{-7}$ s, is used, then gradient regularization with $\kappa_\eta l_\eta = l_\xi$ precludes existence of a steady structured plastic waveform, as noted in the footnote of Table 5. In such an instances, the lower dynamic viscosity promotes a steeper waveform that is incompatible with the minimum shock width permitted by gradient regularization of the η -field. The incompatibility occurs when $\delta_R/l_\eta \lesssim 35$, constraining $\bar{\beta}$ to a permissible minimum if l_η is imposed with the standard thermodynamic prescription of $\kappa_\eta = 1$, which is used henceforth.

The associated constraint on the width of the plastic waveform dictated by the dynamic viscosity, $\delta_R/l_\eta \gtrsim 35$, matches that obtained for boron carbide in Section 7.2. In both materials, the shock width afforded by the corresponding kinetic viscosity ($\tilde{\beta}$ for fracture in B_4C , $\bar{\beta}$ for slip in the second wave in TiB_2) should exceed around 35 corresponding gradient regularization lengths to enable steady-wave solutions using the rate-dependent phase field method.

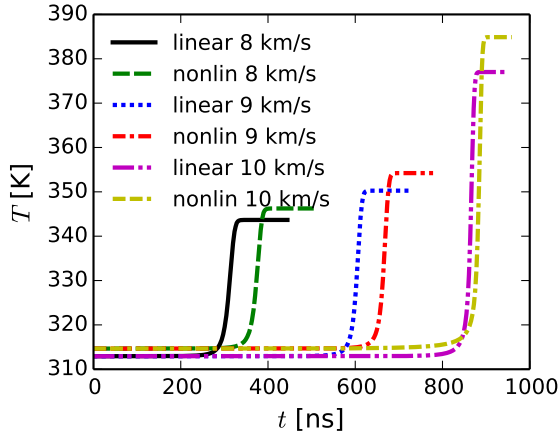
Finally, longitudinal stress, shear stress, temperature, strain rate, slip order parameter, and GND profiles within steady waveforms are shown in Fig. 23 for $D = 8, 9, 10$ km/s. In all cases, peak and Hugoniot values for P , τ , T , and $\dot{\epsilon}$ are larger for the nonlinear model than the linear model. Profiles of η , on the other hand, are nearly indistinguishable among the two theories. Temperature increase for shock compression in Fig. 23c exceeds that for steady-rate compression to the same ϵ in Fig. 15c but remains insufficient to affect dislocation motion according to the model of Eq. 210 or the lower-rate, higher-temperature data.¹³⁴ Peak strain rates are an order of magnitude lower in Fig. 23d than those predicted for B_4C in Fig. 19d, in accordance with the fivefold larger pertinent dynamic viscosity in the former. Following trends similar to $\dot{\epsilon}$, geometrically necessary dislocation densities in Fig. 23f are comparable for 8 and 9 km/s shocks, and somewhat larger for $D = 10$ km/s shocks. Values of similar magnitude have been predicted for weaker steady plastic waves ($P^- \approx 5$ GPa) in polycrystalline metals,¹⁰⁸ which in turn were estimated



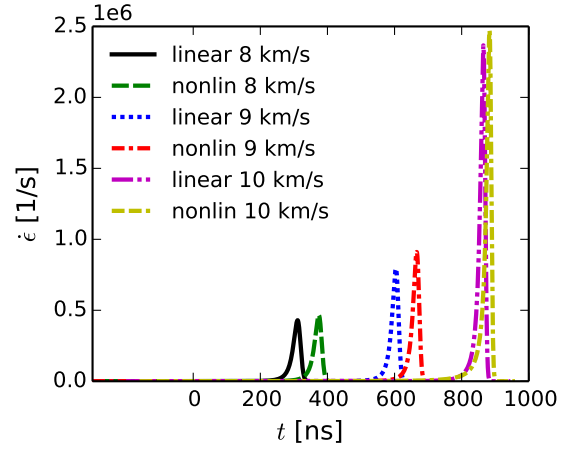
(a) longitudinal stress



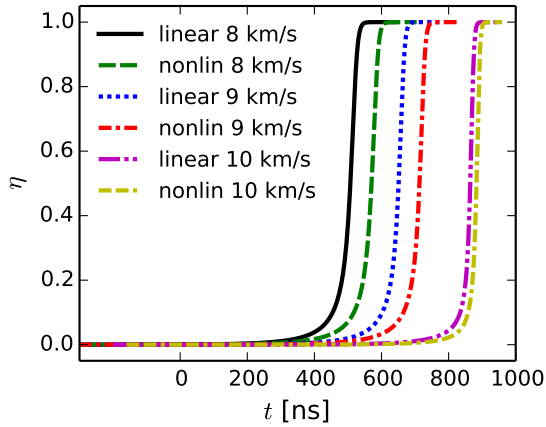
(b) shear stress



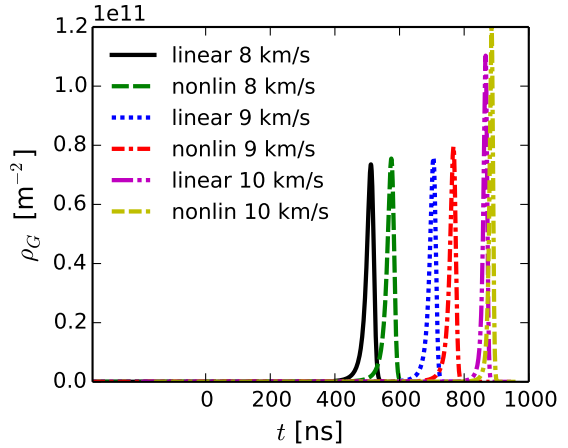
(c) temperature



(d) strain rate



(e) dislocation plasticity



(f) geometrically necessary dislocations

Fig. 23 Titanium diboride: longitudinal stress, shear stress, temperature, strain rate, slip order parameter, and geometrically necessary dislocation density versus time in steady structured shock waves, $\bar{\beta} = 5 \cdot 10^{-7}$ s: (a) P (b) τ (c) T (d) $\dot{\epsilon}$ (e) η (f) ρ_G . Profiles staggered in t to enable visualization.

3–4 orders of magnitude smaller than the total dislocation density. Note that $\rho_G^- = 0$ since $\nabla_0 \eta^- = 0$ at any shocked homogeneous equilibrium state on the Hugoniot: GND density so resolved is transient at material point Z , rather than permanent.

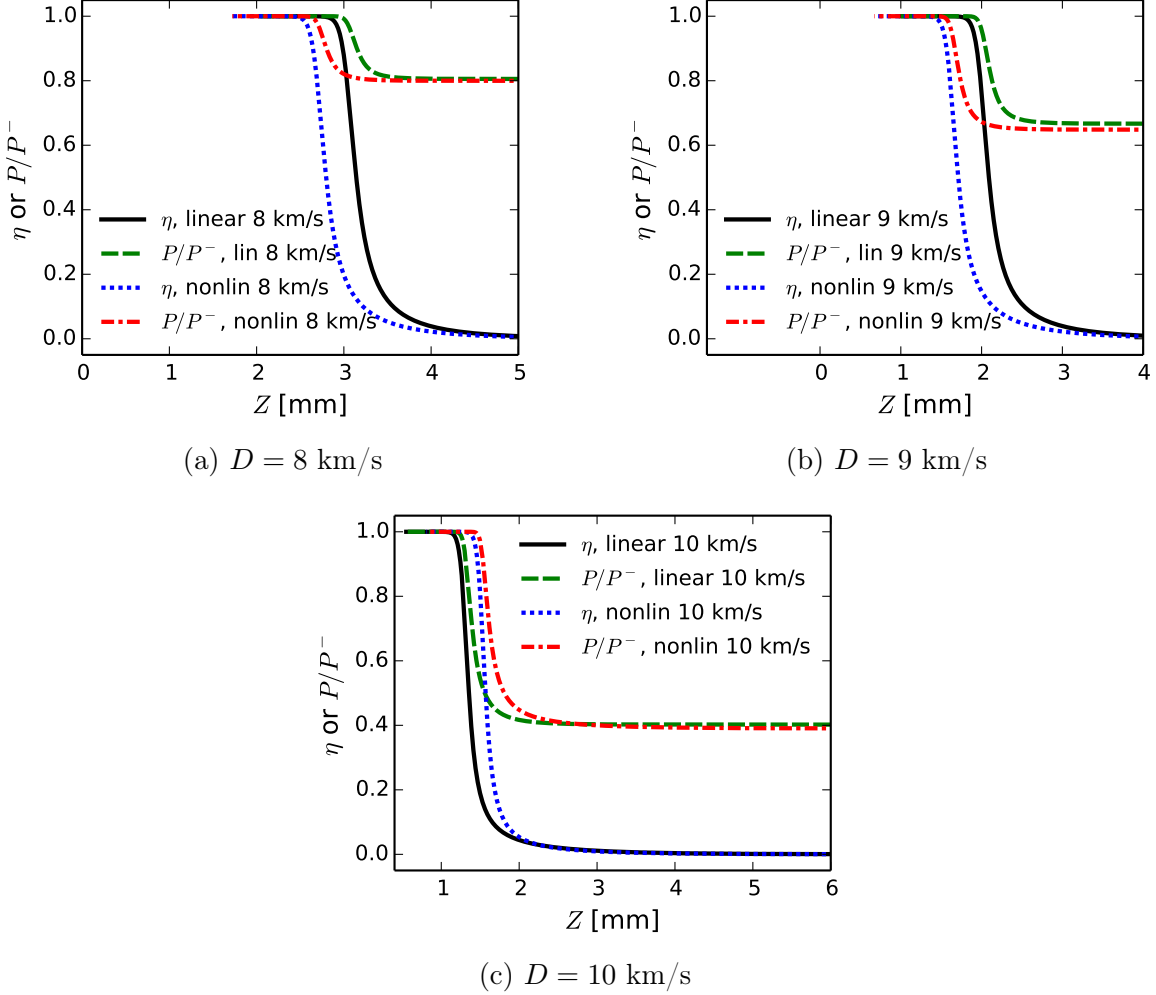


Fig. 24 Titanium diboride: normalized longitudinal stress and slip phase field parameter versus material position Z at fixed t in steady structured shock waves, $\bar{\beta} = 5 \times 10^{-7}$ s, shock velocities of (a) 8 km/s (b) 9 km/s (c) 10 km/s

Shown in Fig. 24 are profiles stress and phase fields with respect to position Z , at a snapshot fixed in time t . Longitudinal stress P is again normalized by end state Hugoniot stress P^- , and the slip phase field variable $\eta \in [0, 1]$. Results compare stress and phase fields concurrently such that any differences can be identified among stress waves and moving phase interfaces. Center coordinates of waveforms for longitudinal stress and the order parameter coincide closely in space, without

appreciable lag between the two for any of the shock velocities shown. However, the initial rise in phase field variable η appears to slightly lead that of P for the lower shock velocities of 8 and 9 km/s. Steepening of the η -waveforms is evident as D increases. Comparing Figs. 20a and 24c, shock widths in TiB_2 (Hugoniot stresses above second yield, dislocation mediated) are larger than those in B_4C (fracture mediated) at $D = 10$ km/s, in general agreement with data^{60,76} and understood by the fivefold larger kinetic viscosity for the former.

8. Conclusions

Phase field theory accounting for simultaneous fracture and other structural transformations in solids has been advanced to study rate-dependent thermo-mechanical phenomena at high loading rates, high pressures, and high temperatures. The following unique collection of features has been incorporated:

- Nonlinear logarithmic thermoelasticity referred to a locally relaxed intermediate configuration of the body;
- Consistent system of micro-forces and dissipative kinetics enabling unconditional satisfaction of accepted laws of continuum mechanics and thermodynamics;
- Geometric linearization, with higher-order corrective terms retained in strain energy, enabling accurate resolution of high pressure response for uniaxial strain compression loading to moderate volume reductions;
- Fracture kinetic model with stress-state dependent threshold to account for pressure-dependent strength and elastic-to-failure behaviors of brittle solids;
- General formulations admitting unlimited order parameters and anisotropy, with specializations to isotropy.

Performance of the theory has been verified for three polycrystalline ceramics: B_4C , TiB_2 , and a composite mixture of B_4C and TiB_2 . Both the nonlinear model and the corrected linear model, with threshold-based fracture kinetics, accurately resolve experimental stress-strain data for these materials up to peak load. The former cases consider homogeneous uniaxial stress tension and compression, at low and

high strain rates, initiated at room temperature, wherein elastic-brittle behavior is observed with no phase changes or slip.

The high-pressure shock response is likewise well-represented by theoretical calculations for steady-rate adiabatic compression, and for inhomogeneous adiabatic compression in steady planar waveforms. Experimentally measured rise times of the latter enable calibration of phase viscosities associated with dynamic fracture, amorphization, or dislocation mechanisms. Gradient regularization constrains minimum viscosities such that the 1D steady plastic waveform must be wide enough to contain on the order of 35 order-parameter regularization lengths. Otherwise, the energetic and kinetic barriers imposed by order parameter gradients in the phase field formulation prevent formation of steeper structured steady waves.

Results for shock wave loading provide fundamental insight into phenomena not available from experimental works that report particle velocity histories but supply no quantitative data on thermodynamics or structural transformations, since ceramic samples, pulverized upon plate impact loading at stresses far exceeding the HEL, are not recoverable for post-mortem characterization. New information revealed by the present study includes steady wave profiles of temperature rise, strain rate, dissipated energy, and surface energy of micro-cracks. Relationships among shock intensity, profile widths, and maxima attained in these profiles have been quantified. For B_4C , the volume fraction of amorphization under uniaxial strain has been predicted, while for TiB_2 , the density of geometrically necessary dislocations in the shock front has been quantified.

In B_4C , amorphization occurs in the model for very fast shock loading as in laser-driven experiments, or for extreme plastic wave velocities wherein peak strain rates exceed $\approx 10^8/s$. Shear-driven fractures are evidently responsible for strength loss in B_4C at lower compressive strain rates, for example in Kolsky bar tests or weaker shocks in conventional plate impact experiments. In TiB_2 , inelastic behavior is explained by fracture initiation at the first yield point and activity of dislocation mechanisms at the second, higher-pressure, yield point. A locking pressure, above which fracture and comminution are impeded under dynamic compression via a sharp increase in viscosity for fracture kinetics, provides an accurate depiction of high-pressure strength maintenance in shock-compressed TiB_2 .

The present work has focused on homogeneous stress-deformation states for model

development and calibration, followed by 1D planar shocks to study the high-rate, high-pressure response. Deformation is non-uniform in the latter (i.e., localized within the structured waveform), but overall dynamic stiffness of the material remains positive due to viscous stiffening and decreasing compressibility with increasing pressure. Upon future implementation of the irreversible theory with nucleation threshold within a finite element setting, a study of the quasi-static, localized failure response—e.g., whereafter the tangent stiffness becomes negative—while not necessary for understanding of the shock problem, should be undertaken for completeness. Analysis of robustness and stability of the model¹²⁷ to include 2D and 3D loading protocols, is likewise warranted for future work. Numerical methods should also examine sensitivity to model parameters whose baseline values have been obtained in the present study.

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List of Symbols, Abbreviations, and Acronyms

TERMS:

1D – one-dimensional

2D – two-dimensional

3D – three-dimensional

B₄C – boron carbide

EOS – equation of state

GND – geometrically necessary dislocation

HEL – Hugoniot elastic limit

TDGL – time-dependent Ginzburg–Landau

TiB₂ – titanium diboride

MATHEMATICAL SYMBOLS:

t – time

$\mathbf{X}, X^K$ – reference coordinates

$\mathbf{x}, x^k$ – spatial coordinates

η^i – transformation or slip order parameters

ξ^j – fracture order parameters

$\mathbf{F}, F_J^i$ – deformation gradient

$\mathbf{e}^E, e_{\alpha\beta}^E$ – logarithmic thermoelastic strain

ρ – mass density

U – internal energy density

Ψ – Helmholtz free energy density

S – entropy density

T – absolute temperature

$\mathbf{P}, P_i^J$ – first Piola–Kirchhoff stress

$\mathbf{v}, v^k$ – particle velocity

D – Lagrangian shock velocity

MATHEMATICAL OPERATORS:

$(\dot{})$ – the overdot denotes a material time derivative of a quantity

$\nabla()$ – the spatial gradient of a quantity

REFERENCE INDICATOR:

$()_0$ – a quantity associated with an initial, reference, or constant condition, unless otherwise noted

1 DEFENSE TECHNICAL
(PDF) INFORMATION CTR
DTIC OCA

FCDD RLW TF
P JANNIOTTI
D MALLICK

1 DEVCOM ARL
(PDF) FCDD RLD DCI
TECH LIB

ABERDEEN PROVING GROUND

36 DEVCOM ARL
(PDF) FCDD RLC HC
J CRONE
J KNAP
FCDD RLW B
R BECKER
P GILLICH
C HOPPEL
A TONGE
FCDD RLW MB
G GAZONAS
J LIGDA
D MAGAGNOSC
FCDD RLW ME
A DIGIOVANNI
M GUZIEWSKI
M KORNECKI
N KU
J LASALVIA
W SHOULDERS
J SWAB
FCDD RLW TA
M GREENFIELD
FCDD RLW TB
J MCDONALD
S SATAPATHY
FCDD RLW TC
J BERRY
D CASEM
J CAZAMIAS
J CLAYTON
M FERMEN-COKER
A FREED
R LEAVY
J LLOYD
C MEREDITH
R REGUEIRO
T SCHARF
S SEGLETES
L SHANNAHAN
S TURNAGE
C WILLIAMS