Finsler-Geometric Continuum Mechanics and the Micromechanics of Fracture in Crystals

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Weapons and Materials Research Directorate (ARL)


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A continuum theory for the mechanical response of solid bodies subjected to potentially finite deformation is further developed and applied to solve several new problems in the context of the micromechanics of crystalline solids. The theory invokes concepts from Finsler differential geometry, and it provides a diffuse interface description of fracture surfaces. The director or internal state vector is associated with an order parameter describing degradation of the solid. Here, the deformation gradient between pseudo-Finsler reference and spatial configuration spaces is decomposed into a product of two terms, neither necessarily integrable to a vector field. The first is the recoverable elastic deformation, the second is the residual deformation attributed to changes in free volume in failure zones. The latter is restricted to spherical or isotropic symmetry; resulting Euler–Lagrange equations for mechanical and state variable equilibrium are derived. Metric tensors and volume elements depend on the internal state via a conformal transformation, i.e., Weyl scaling. This version of the theory is first applied to tensile fracture of magnesium. Analytical solutions demonstrate the models capability to predict ductile versus brittle fracture depending on incorporation of Weyl scaling, with results aligned with molecular dynamics (MD) simulations. The second application is shear fracture in boron carbide: solutions depict weakening and tensile pressure in conjunction with structural collapse in shear transformation zones, as suggested by experiments, quantum mechanics, and/or MD simulations.
Finsler-geometric continuum mechanics and the micromechanics of fracture in crystals

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Abstract A continuum theory for the mechanical response of solid bodies subjected to potentially finite deformation is further developed and applied to solve several new problems in the context of the micromechanics of crystalline solids. The theory invokes concepts from Finsler differential geometry, and it provides a diffuse interface description of fracture surfaces. The director or internal state vector is associated with an order parameter describing degradation of the solid. Here, the deformation gradient between pseudo-Finsler reference and spatial configuration spaces is decomposed into a product of two terms, neither necessarily integrable to a vector field. The first is the recoverable elastic deformation, the second is the residual deformation attributed to changes in free volume in failure zones. The latter is restricted to spherical or isotropic symmetry; resulting Euler–Lagrange equations for mechanical and state variable equilibrium are derived. Metric tensors and volume elements depend on the internal state via a conformal transformation, i.e., Weyl scaling. This version of the theory is first applied to tensile fracture of magnesium. Analytical solutions demonstrate the model’s capability to predict ductile versus brittle fracture depending on incorporation of Weyl scaling, with results aligned with molecular dynamics (MD) simulations. The second application is shear fracture in boron carbide: solutions depict weakening and tensile pressure in conjunction with structural collapse in shear transformation zones, as suggested by experiments, quantum mechanics, and/or MD simulations.

Keywords Continuum mechanics; differential geometry; non-linear elasticity; fracture; microstructure; phase field.

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1. Introduction

Predictive modeling of failure of solids under general mechanical loading has remained a challenging endeavor for decades, with incremental progress involving research in diverse branches of engineering mechanics, condensed matter physics, applied mathematics and materials science. Failure in this context refers to the action of damage mechanisms — fractures, voids, shear bands and so forth — on the loss of stiffness and load bearing capacity of the solid. A micromechanics model is herein termed as predictive if it represents observed physics without prescription of ad hoc equations or excessive parameter fitting.

Methods of analysis of fracture are the present focus. Analytical solutions for most boundary value problems tend to be restricted to the domain of linear elastic fracture mechanics, for which mathematical tools have been developed to a high level of rigor [Rice, 1968; Freund, 1990]. Numerical methods may invoke sharp interface type theories, wherein jumps in displacement are explicitly resolved. Perhaps the most popular such method developed over the past three decades is the cohesive finite element method [Needleman, 1987]. This technique, though suffering from the drawback that fracture paths follow element boundaries when Lagrangian elements are used, has been implemented with some success to address failure in the context of elastodynamics [Xu and Needleman, 1994; Espinosa and Zavattieri, 2003], thermoelasticity [Ortiz and Suresh, 1993], static [Xu and Needleman, 1993] and dynamic [Clayton, 2005] crystal plasticity and multiscale mechanics [Li and Wang, 2004; Zeng and Li, 2010]. Diffuse interface approaches have also become prominent in the context of modeling fracture, for example phase field methods [Jin et al., 2001; Karma et al., 2001]. Phase field approaches have been used to study static and dynamic problems [Borden et al., 2012], including non-linear and anisotropic material responses [Clayton and Knap, 2014, 2015b]. Typical advantages of diffuse interface models are that relatively few parameters are necessary, with equilibrium or kinetics dictated by principles of energy minimization, and that conventional, continuous finite element meshes can be invoked. Both cohesive zone models and phase field models are regularized via introduction of length scales, either explicitly or implicitly. In the former, solid meshes must be fine enough to resolve cohesive zone lengths; in the latter, meshes or finite difference grids must be fine enough to resolve order parameter gradients.

The theory developed and exercised in the present work differs from others noted above, though it may reduce to a phase field type description under certain degenerate assumptions. In the context of geometrically non-linear representations, the present theory treats the body manifold in its referential and spatial configurations as a Finsler space, as opposed to a Euclidean space of conventional continuum mechanics. In Finsler geometry, the metric tensor and its derivative quantities functionally depend on an internal state vector or director vector. In the present theory, more precisely each configuration corresponds to pseudo-Finsler geometry since the internal state vector need not be of unit length and the metric tensor

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need not be homogeneous of degree zero with respect to internal state [Minguzzi, 2014]. Early work in this area includes the ferromagnetic theory of [Amari, 1962], the purely kinematic descriptions in Bejancu [1990], and the more complete and elaborate thermomechanical theory in Saczuk [1996] and Stumpf and Saczuk [2000]. The latter [Saczuk, 1996; Stumpf and Saczuk, 2000] feature the first known numerical solutions to a problem in Finsler geometric continuum mechanics, dealing with shear localization in a metal rod under tensile extension. A more extensive review is given in Clayton [2015c].

The theory implemented in the present paper extends recent prior developments [Clayton, 2016a,b,c]. Initial theoretical mathematical ideas were sketched in Clayton [2016a] with the first known analytical solutions reported: tensile fracture, shear fracture, and cavity expansion, all for isotropic non-linear elastic solids with generic properties. It was also demonstrated how the theory reduces to a non-linear phase field description [Clayton and Knap, 2015a] under the assumptions of null dependence of the metric and macroscopic motion function on the order parameter. The theory was subsequently refined in Clayton [2016c], which considered shear localization and cavitation problems in magnesium (Mg) crystals. Further, albeit optional, enhancements were introduced in Clayton [2016b], including additive and multiplicative decompositions of the Finsler deformation gradient and ensuing ramifications to the Euler–Lagrange equations. Analytical solutions for tensile fracture on the basal plane and stress-induced amorphization under uniaxial compression along the \( c \)-axis were obtained, with both solutions applying specifically for boron carbide single crystals.

The theory invoked in this paper uses a more detailed kinematic description than that of the multiplicative case introduced in Clayton [2016b]. In particular, here the deformation gradient, a two-point tensor between pseudo-Finsler reference and spatial configuration spaces, is separated into a product of two terms. The first is the recoverable elastic deformation conjugate to mechanical stress, and the second is the residual deformation attributed to microscopic changes in volume. Physically, the latter correspond to changes in density of voids or pores in the microstructure, or to changes in free volume (e.g., vacancies) in the atomic structure. A brief treatment of anholonomicity [Clayton, 2012a, 2014b] (i.e., compatibility) equations and geometric implications is given. Specific forms of Euler–Lagrange equations for equilibrium of stress and conjugate force to the order parameter are obtained. As first invoked in Clayton [2016a,c], a conformal transformation, i.e., Weyl scaling [Weyl, 1952], provides dependence of the metric on internal state.

Materials considered in prior work are revisited, specifically the crystalline solids Mg and boron carbide. Mg is a low density metal of hexagonal symmetry whose failure may be ductile or brittle depending on loading rate, temperature and processing [Armstrong, 1968; Kubota et al., 1999; Kondori and Benzerger, 2014]. Single crystal cleavage planes are thought to the basal and prismatic planes [Yoo, 1979, 1981]; polycrystals may fail along these and/or along grain boundaries.
Boron carbide ($B_4C$) is a low density ceramic of high hardness and low ductility. An interesting failure mechanism is stress-induced amorphization, whereby collapse of the rhombohedral unit cell is promoted by compression along the $c$-axis ([0001] in hexagonal Miller indices) and exacerbated by shear [Taylor et al., 2012; Clayton, 2012b, 2013a, 2014c; Taylor, 2015; An and Goddard, 2015]. In this paper, the refined Finsler theory is newly applied towards physical problems of tensile extension of a cylindrical rod of Mg and simple shearing of a semi-infinite slab of $B_4C$. Failure modes are described in each case. The Finsler theory is demonstrated to be capable of describing brittle versus ductile failure mechanisms as well as pressure-shear coupling without supplementation of fitting equations or unphysical calibration parameters.

The layout of the paper is as follows. Section 2 describes the general theory, including differential geometry, kinematics, thermodynamics and balance laws. Section 3 presents the application of the theory towards tensile rupture of Mg. Section 4 presents the application of the theory towards shear transformation and failure of $B_4C$. Section 5 concludes the paper.

Notation of continuum physics and Finsler geometry is used. When coordinate-free descriptions are invoked, bold type is used for vectors and tensors, italic type for scalars and scalar components. When index notation is invoked, the usual Einstein convention applies for summation over repeated contravariant and covariant pairs.

2. Theory

A terse presentation of mathematical aspects of Finsler-geometric continuum mechanics developed and justified physically in prior recent work [Clayton, 2016b,c] is given next. Several theoretical features are newly introduced; these are emphasized as they first appear in the forthcoming text.

2.1. Pseudo-Finsler geometry

The Finsler geometric representations of the reference and spatial configurations of a material body are discussed in Secs. 2.1.1 and 2.1.2. Mappings or differential transformations between such configurations are presented in Sec. 2.1.3. New refinements to the multiplicative kinematics are included in Secs. 2.1.4 and 2.1.5.

2.1.1. Reference configuration geometry

Let $\mathcal{M}$ be a differential manifold of spatial dimension 3. This manifold is physically identified with a material body embedded in ambient Euclidean three-space. Let $X \in \mathcal{M}$ denote a material point, and let $\{X^A\}(A = 1, 2, 3)$ denote a coordinate chart covering part or all of $\mathcal{M}$. Each point is assigned a vector $D$ that is, for the moment, a generic descriptor of material microstructure. Coordinates $\{D^A\}(A = 1, 2, 3)$ are the entries of $D$, the former of which can be associated with a second manifold $\mathcal{U}$.
of dimension 3. The vector \( \mathbf{D} \), referred to here as a state vector or internal state vector, need not be of unit length. Regarding notation, dependence of a function on \( (X, D) \) implies dependence on reference charts \( \{X^A\}, \{D^A\} \).

Similar to the geometric models of Bejancu [1990], the reference state is now described in terms of pseudo-Finsler geometry. Let \( \mathcal{Z} = (\mathfrak{Z}, \Pi, \mathfrak{M}, \Omega) \) be a fiber bundle of total space \( \mathfrak{Z} \) (dimension 6), where \( \Pi : \mathfrak{Z} \rightarrow \mathfrak{M} \) is the projection and \( \mathfrak{M} \) the fiber. A coordinate chart on \( \mathfrak{Z} \) is the set \( \{X, D\} \). Holonomic basis vectors on \( \mathfrak{Z} \) are the fields \( \{\frac{\partial}{\partial X^A}, \frac{\partial}{\partial D^A}\} \). Let \( N^A_B(X, D) \) denote non-linear connection coefficients whose possible origin will be discussed more later. A non-holonomic basis whose entries transform between coordinate systems as typical vectors is

\[
\delta X^A = \frac{\partial}{\partial X^A} - N^B_A\frac{\partial}{\partial D^B}, \quad \delta D^A = dD^A + N^A_B dX^B. \tag{2.1}
\]

The set \( \{\frac{\partial}{\partial X^A}, \frac{\partial}{\partial D^A}\} \) is thus logically used for a local basis on \( T \mathfrak{Z} \), and the reciprocal set \( \{dX^A, \delta D^A\} \) for \( T^* \mathfrak{Z} \). The Sasaki metric is

\[
G(X, D) = G_{AB}(X, D) dX^A \otimes dX^B + G_{AB}(X, D) \delta D^A \otimes \delta D^B. \tag{2.2}
\]

Components \( G_{AB} \) are used to lower (raise) indices. The determinant of the covariant metric is \( G(X, D) = \text{det}[G_{AB}(X, D)] \). Partial coordinate differentiation and delta-differentiation are the respective operations

\[
\partial_A(\cdot) = \frac{\partial(\cdot)}{\partial X^A}, \quad \bar{\partial}_A(\cdot) = \frac{\partial(\cdot)}{\partial D^A}, \quad \delta A(\cdot) = \frac{\partial(\cdot)}{\partial X^A} = \partial A(\cdot) - N^B_A \bar{\partial}_B(\cdot). \tag{2.3}
\]

The Christoffel symbols of the second kind for the Levi-Civita connection on \( \mathfrak{M} \) are

\[
\gamma^A_{BC} = \frac{1}{2} G^{AD}(\partial_C G_{BD} + \partial_B G_{CD} - \partial_D G_{BC}) = G^{AD} \gamma_{BCD}. \tag{2.4}
\]

Cartan’s tensor referred to material space is

\[
C^A_{BC} = \frac{1}{2} G^{AD}(\partial_C G_{BD} + \partial_B G_{CD} - \partial_D G_{BC}) = G^{AD} C_{BCD}. \tag{2.5}
\]

The horizontal coefficients of the Chern–Rund and Cartan connections are the following equivalent quantities:

\[
\Gamma^A_{BC} = \frac{1}{2} G^{AD}(\delta_C G_{BD} + \delta_B G_{CD} - \delta_D G_{BC}) = G^{AD} \Gamma_{BCD}. \tag{2.6}
\]

The spray and its canonical non-linear connection coefficients, the latter an example of those in (2.1) when \( N^A_B = G^A_B \), are

\[
G^A = \frac{1}{2} \gamma^A_{BC} B^B D^C, \quad G^A_B = \partial_B G^A. \tag{2.7}
\]

Let \( \nabla \) be the covariant derivative. Horizontal gradients of basis vectors are

\[
\nabla_{\delta/\delta X^B} \frac{\delta}{\delta X^C} = H^A_{BC} \frac{\delta}{\delta X^A}, \quad \nabla_{\delta/\delta X^B} \frac{\partial}{\partial D^C} = K^A_{BC} \frac{\partial}{\partial D^A}. \tag{2.8}
\]
with the momentarily generic coefficients \( H_{BC}^A \) and \( K_{BC}^A \). Vertical gradients of basis vectors are analogously computed from generic coefficients \( V_{BC}^A \) and \( Y_{BC}^A \):

\[
\nabla_{\partial/\partial x^B} \frac{\partial}{\partial D^B} = V_{BC}^A \frac{\partial}{\partial D^A}, \quad \nabla_{\partial/\partial D^B} \delta_{\delta X^B} = Y_{BC}^A \frac{\delta}{\delta X^A}.
\]

(2.9)

The above descriptions pertain to both pseudo-Finsler space and Finsler space. The latter type of space is a subset of the former. A Finsler space is further characterized by existence of a \( C^\infty \) fundamental scalar function \( \mathcal{L}(X, D) \) at every point of \( \Omega(0) \), homogeneous of degree one in \( D \). The metric tensor, spray connection coefficients and Cartan tensor are all obtained from differentiation of this function:

\[
G_{AB} = \frac{1}{2} \partial_A \partial_B (\mathcal{L}^2), \quad G_B^A = \gamma_{BC}^A D^C - C_{BC}^A \gamma_{DE}^D D^E D^F = \Gamma_{BC}^A D^C,
\]

\[
C_{ABC} = \frac{1}{4} \partial_A \partial_B \partial_C (\mathcal{L}^2).
\]

(2.10)

Two specific connections often encountered in the literature are [Minguzzi, 2014]


Let \( (\cdot)|_C \) denote horizontal covariant differentiation in a coordinate chart \( \{X^C\} \). Then when either of these two connections is used, the horizontal covariant derivative \( G_{ABC} = 0 \). Finsler space reduces to Riemannian space when \( G_{AB}(X, D) \rightarrow G_{AB}(X) \). Finsler space reduces to locally Minkowskian space when \( \mathcal{L}(X, D) \rightarrow \mathcal{L}(D) \) [Minguzzi, 2014].

Denote by \( dX \) a differential line element on \( \mathcal{M} \) and \( dD \) a corresponding element on \( \mathcal{M} \). Squared differential line lengths with respect to (2.2) are

\[
|dX|^2 = \langle dX, GdX \rangle = G_{AB} dX^A dX^B,
\]

\[
|dD|^2 = \langle dD, GdD \rangle = G_{AB} dD^A dD^B.
\]

(2.11)

Scalar volume elements and volume forms of \( \mathcal{M} \) are [Rund, 1975]

\[
dV = \sqrt{G} dx^1 dx^2 dx^3, \quad d\Omega = \sqrt{G} dx^1 \wedge dx^2 \wedge dx^3;
\]

(2.12)

the differential area form corresponding to a compact region of \( \mathcal{M} \) is

\[
\Omega = \sqrt{\beta} du^1 \wedge du^2; \quad \left[ X^A = X^A(U^\alpha), (\alpha = 1, 2); \beta^A_\alpha = \frac{\partial X^A}{\partial U^\alpha}, \beta = \det(\beta^A_\alpha G_{AB} \beta^B_\beta) \right].
\]

(2.13)

The following identities hold:

\[
\delta_A (\ln \sqrt{G}) = \Gamma_{AB}^B, \quad (\sqrt{G})_A = \delta_A (\sqrt{G}) - N^B_A \delta_B (\sqrt{G}) - \sqrt{G} H^B_{AB}.
\]

(2.14)

Let \( V^A(X, D) \Omega(X, D) \) be a 2-form, and let \( V^A \) be contravariant components of vector field \( V = V^A \frac{\delta}{\delta x^A} \). Let the horizontal connection be one for which \( H_{AB}^B =
or holonomic basis on $\pi$: coefficients, non-holonomic basis vectors are $\Gamma^d_{\alpha \beta}$.

The Levi-Civita connection coefficients on $\mathcal{M}$ are 

\[ \Gamma^B_{AB} = (\sqrt{g})_{|A} = 0. \]

Then in a coordinate chart $\{X^A\}$, a version of Stokes’ theorem is [Rund, 1975]

\[ \int_{\partial \mathcal{M}} [V^A_A + (V^A C^C_{BC} + \partial_B V^A) D^B_A] d\Omega = \oint_{\partial \mathcal{M}} V^A N_A \Omega. \quad (2.15) \]

Here, $N_A$ is the unit outward normal to $\partial \mathcal{M}$, $V^A_A = \delta_A V^A = \delta_A H^B_A$ and $D^B_A = \partial_A D^B + N^B_A$.

### 2.1.2. Deformed configuration geometry

The current configuration or spatial configuration corresponds to a time instance at which the solid is deformed. A pseudo-Finsler geometric framework is constructed in exact parallel to that of Sec. 2.1.1. Notation differs in that deformed coordinates and their indices, etc., are written in lower-case rather than capitals.

A differential manifold $\mathfrak{m}$ of spatial dimension 3 is identified with the body embedded in ambient Euclidean three-space. Let $x \in \mathfrak{m}$ denote a spatial point, and let $\{x^a\} \ (a = 1, 2, 3)$ denote a chart on $\mathfrak{m}$. Attached to each point is the internal state vector $\mathbf{d}$, with secondary coordinates $\{d^a\} \ (a = 1, 2, 3)$, which can be associated with manifold $\mathfrak{u}$ of dimension 3. Herein, $\mathbf{d}$ need not be of unit length. Define $\tilde{\mathfrak{z}} = (\mathfrak{z}, \pi, \mathfrak{m}, \mathfrak{u})$ as a fiber bundle of total (pseudo-Finsler) space $\mathfrak{z}$ (dimension 6), with $\pi : \mathfrak{z} \rightarrow \mathfrak{m}$ the projection and $\mathfrak{u}$ the fiber. A chart on $\mathfrak{z}$ is $\{x, d\}$. The natural or holonomic basis on $\mathfrak{z}$ is $\{\frac{\partial}{\partial x^a}, \frac{\partial}{\partial d^a}\}$. With $n^a_b(x, d)$ spatial non-linear connection coefficients, non-holonomic basis vectors are

\[ \frac{\delta}{\delta x^a} = \frac{\partial}{\partial x^a} - n^a_b \frac{\partial}{\partial d^b}, \quad \delta d^a = d d^a + n^a_b d^b. \quad (2.16) \]

The set $\{\frac{\partial}{\partial x^a}, \frac{\partial}{\partial d^a}\}$ will be used as a local basis for $T\mathfrak{z}$; $\{dx^a, \delta d^a\}$ for $T^*\mathfrak{z}$. The spatial Sasaki metric is the tensor

\[ g(x, d) = g_{ab}(x, d) dx^a \otimes dx^b + g_{ab}(x, d) \delta d^a \otimes \delta d^b \quad (2.17) \]

with $g(x, d) = \det[g_{ab}(x, d)]$. Spatial differentiation in coordinates is

\[ \partial_a(\cdot) = \frac{\partial}{\partial x^a}, \quad \partial_a(\cdot) = \frac{\partial}{\partial d^a}, \quad \delta_a(\cdot) = \frac{\delta}{\delta d^a} = \partial_a(-) - n^a_b \partial_b(\cdot). \quad (2.18) \]

The Levi-Civita connection coefficients on $\mathfrak{m}$ are

\[ \gamma^a_{bc} = \frac{1}{2} g^{ad} (\partial_c g_{bd} + \partial_b g_{cd} - \partial_d g_{bc}) = g^{ad} \gamma_{bcd}. \quad (2.19) \]

Cartan’s tensor is

\[ C^a_{bc} = \frac{1}{2} g^{ad} (\partial_c g_{bd} + \partial_b g_{cd} - \partial_d g_{bc}) = g^{ad} C_{bcd}. \quad (2.20) \]

Equivalent horizontal coefficients of Chern–Rund and Cartan connections are

\[ \Gamma^a_{bc} = \frac{1}{2} g^{ad} (\partial_c g_{bd} + \partial_b g_{cd} - \partial_d g_{bc}) = g^{ad} \Gamma_{bcd}. \quad (2.21) \]
The spray and canonical non-linear connection coefficients ($n^a_b = g^a_b$) are

$$g^a = \frac{1}{2} \gamma^d_{bc} d^b d^c, \quad g^a_b = \partial_b g^a.$$  \hspace{1cm} (2.22)

Horizontal gradients of basis vectors are, in terms of connection coefficients $H^a_b$ and $K^a_{bc}$:

$$\nabla_{\delta/\delta x^b} \delta/\delta x^c = H^a_{bc} \delta/\delta x^a, \quad \nabla_{\partial/\partial d^b} \partial/\partial d^c = K^a_{bc} \partial/\partial d^a.$$  \hspace{1cm} (2.23)

Similarly, in terms of vertical connection coefficients $V^a_{bc}$ and $Y^a_{bc}$:

$$\nabla_{\partial/\partial d^b} \partial/\partial d^c = V^a_{bc} \partial/\partial d^a, \quad \nabla_{\delta/\delta x^b} \delta/\delta x^c = Y^a_{bc} \delta/\delta x^a.$$  \hspace{1cm} (2.24)

Classifications regarding strict Finsler versus pseudo-Finsler space of Sec. 2.1.1 hold for the spatial manifold, as do definitions for spatial Chern–Rund and Cartan connections. Descriptions of line and volume elements analogous to those in Sec. 2.1.1 also apply, an area form like that in (2.13) can be introduced, and spatial versions of Stokes’ theorem and Rund’s divergence theorem in (2.15) apply.

2.1.3. Deformation Kinematics

The motion (and its inverse) from $\mathfrak{M}$ to $\mathfrak{m}$ (and vice versa) are the $C^2$ functions

$$x^a(X,D) = \varphi^a[X,D(X)], \quad X^A(x,d) = \Phi^A[x,d(x)].$$  \hspace{1cm} (2.25)

The variational theory in the present paper, like those in [Clayton, 2016b,c], is quasi-static, with incremental equilibrium conditions to be presented later; time does not enter as an explicit independent variable. Incorporation of the internal state ($D$ or $d$) in these motion functions distinguishes Finsler kinematics [Bejancu, 1990; Saczuk, 1996; Stumpf and Saczuk, 2000; Clayton, 2016c] from classical finite kinematics in Riemannian geometry. State vector mappings are

$$d^a(X,D) = \Theta^a[X,D(X)], \quad D^A(x,d) = \Theta^A[x,d(x)].$$  \hspace{1cm} (2.26)

This generalizes definitions of prior work [Bejancu, 1990; Clayton, 2016a,b,c] to possibly non-affine transformations.

The deformation gradient is defined as the partial derivative of motion, referred to the non-holonomic basis [Clayton, 2016c]:

$$F(X,D) = F^a_A(X,D) \frac{\delta}{\delta x^a} \otimes dX^A = \frac{\partial \varphi^a(X,D)}{\partial X^A} \frac{\delta}{\delta x^a} \otimes dX^A$$

$$= \frac{\partial x^a(X,D)}{\partial X^A} F^a_A = \partial_A \varphi^a.$$  \hspace{1cm} (2.27)

Mapping from spatial to referential tangent spaces analogously obeys

$$f(x,d) = f^A_a(x,d) \frac{\delta}{\delta X^A} \otimes dx^a = \frac{\partial \Phi^A(x,d)}{\partial x^a} \frac{\delta}{\delta X^A} \otimes dx^a$$

$$= \frac{\partial X(x,d)}{\partial x} f^A_a = \partial_a \Phi^A = \partial_a X^A.$$  \hspace{1cm} (2.28)
Deformation gradients $F$ and $f$ are invertible with positive determinants, and are inverses of one another at coincident points on $\mathbb{R}$ or $m$:

$$F_a^b[X, D(X)]f_b^a[x(X, D), d(x(X, D))] = \delta_a^b,$$  \hspace{1cm} (2.29)

$$f_a^b[x, d(x)]F_b^a[X(x, d), D(X(x, d))][X(x, d), D(X(x, d))] = \delta_a^b.$$  \hspace{1cm} (2.30)

Newly introduced in this work are the director deformation gradients, defined as the following partial derivatives of (2.26) with components referred to the non-holonomic basis:

$$\vartheta(X, D) = \vartheta_A^a(X, D) \frac{\partial}{\partial d^a} \otimes \delta D^A = \frac{\partial \vartheta^a(X, D)}{\partial D^A} \frac{\partial}{\partial d^a} \otimes \delta D^A$$

$$\Xi(X, D) = \Xi^A(x, d) \frac{\partial}{\partial D^A} \otimes \delta d^a = \frac{\partial \Xi^A(x, d)}{\partial D^A} \frac{\partial}{\partial D^A} \otimes \delta d^a$$

$$\vartheta_A^a[X, D(X)][\Xi^A(x, D), d(x(X, D))] = \delta_a^b,$$  \hspace{1cm} (2.31)

$$\Xi^A[x, d(x)][\vartheta_a^b[X(x, d), D(X(x, d))][X(x, d), D(X(x, d))] = \delta_A^a.$$  \hspace{1cm} (2.32)

Transformation equations for differential line elements and volume elements/forms are [Clayton, 2016a,b,c]:

$$dx = \frac{\partial x}{\partial X} dX \Leftrightarrow dx^a = F_a^b dX^b, \quad dX = \frac{\partial X}{\partial x} dx \Leftrightarrow dX^a = f_a^b dx^b;$$  \hspace{1cm} (2.33)

$$dv = JdV = [\det(F_a^b)]\sqrt{g/G}dV,$$

$$dV = jdv = [\det(F_a^b)]\sqrt{G/g}dv, \quad dw = Jd\Omega, \quad d\Omega = jdw.$$  \hspace{1cm} (2.34)

Lengths of deformed line elements relative to lengths of initial line elements are quantified by the symmetric deformation tensor $C$:

$$|dx|^2 = F_a^b F_b^c g_{ab} dX^a dX^b = C_{AB} dX^A dX^B = \langle dX, CdX \rangle,$$  \hspace{1cm} (2.35)

$$C = C_{AB} dX^A \otimes dX^B = F_a^b F_b^c dX^A \otimes dX^B.$$  \hspace{1cm} (2.36)

Note that $\det(C_{ij}^j) = \det(C_{AB})/G = J^2$. Gradients of non-holonomic bases are obtained using (2.3), (2.23) and (2.27):

$$\nabla_{\delta/dx^A} \frac{\delta}{\delta x^A} \nabla_{\delta/dx^A} \frac{\delta}{\delta x^A} = (F_a^b - N_{AB}^b \partial_B x^a) \nabla_{\delta/dx^A} \frac{\delta}{\delta x^A}$$

$$= (F_a^b - N_{AB}^b \partial_B x^a) H_{bc}^a \frac{\delta}{\delta x^A}.$$  \hspace{1cm} (2.36)
2.1.4. Multiplicative kinematics

A multiplicative decomposition of the Finsler-geometric deformation gradient of (2.27) is invoked. Let $F$ be decomposed into a product of two non-singular two-point tensors:

$$F = F^E F^D,$$

$$F^E = (F^E)^\alpha_\alpha (F^D)^\alpha_\alpha.$$  (2.37)

By construction, both the elastic or mechanically recoverable deformation, $F^E$, and the residual or inelastic deformation associated with changes of internal state, $F^D$, have positive determinants. Functional forms are [Clayton, 2016b]

$$(F^E)^\alpha_\alpha = (F^E)^\alpha_\alpha (X), \quad (F^D)^\alpha_\alpha = (F^D)^\alpha_\alpha [D(X)],$$  (2.38)

where the inelastic two-point tensor $F^D$ may have further dependence on $X$ only through possible dependence of its basis vectors on $X$. Greek indices correspond to a generally anholonomic space [Clayton, 2012a, 2014b] labeled the intermediate configuration. Local integrability conditions for the total deformation gradient, an application of Poincaré’s lemma, are

$$\partial_B \partial_A \varphi^\alpha = \partial_A \partial_B \varphi^\alpha \Leftrightarrow (F^E)^\alpha_\alpha [\partial_A (F^D)^\alpha_\beta _B - \partial_B (F^D)^\alpha_\beta _A]$$

$$= (F^D)^\alpha_\beta \partial_B (F^E)^\alpha_\beta - (F^D)^\alpha_\beta \partial_A (F^E)^\alpha_\beta.$$  (2.39)

Neither $F^E$ nor $F^D$ need be integrable. However, when they are, the following local compatibility conditions hold:

$$\partial_A (F^D)^\alpha_\beta = \partial_B (F^D)^\alpha_\beta, \quad \partial_A (F^E)^\alpha_\beta = (F^D)^\beta_\beta \partial_B (F^E)^\alpha_\beta.$$  (2.40)

and the motion becomes a composition of mappings:

$$\varphi = \varphi^E \circ \varphi^D; \quad F^D = \partial \varphi^D / \partial X, \quad (F^D)^\alpha_\alpha = \partial_A (\varphi^D)^\alpha_\alpha.$$  (2.41)

Though further details are outside the scope of the present paper, a lack of integrable kinematics may be associated with the presence of structural defects in a (crystalline) material [Lazar and Maugin, 2007; Clayton et al., 2005, 2006; Clayton, 2011; Steinmann, 2015].

A multiplicative split of the director gradient function $\theta$ of (2.30) is newly introduced:

$$\theta = \theta^E \theta^D, \quad \theta^E = (\theta^E)^\alpha_\alpha (\theta^D)^\alpha_\alpha.$$  (2.42)

Both the recoverable mapping $\theta^E$ and the residual mapping $\theta^D$ generally may be functions of $X$ and $D$; physically, the intermediate configuration implied by (2.42) is meant to correspond with the elastically unloaded intermediate state implied by (2.37). Local integrability conditions for total state gradient $\theta$ are

$$\partial_B \partial_A \theta^\alpha = \partial_A \partial_B \theta^\alpha \Leftrightarrow (\theta^E)^\alpha_\alpha [\partial_A (\theta^D)^\alpha_\beta _B - \partial_B (\theta^D)^\alpha_\beta _A]$$

$$= (\theta^D)^\alpha_\beta \partial_B (\theta^E)^\alpha_\beta - (\theta^D)^\alpha_\beta \partial_A (\theta^E)^\alpha_\beta.$$  (2.43)

Neither $\theta^E$ nor $\theta^D$ need be integrable to a vector field. However, should these functions be integrable, then equations analogous to (2.39) and (2.40) then would...
A metric tensor is likewise introduced for the intermediate configuration. Information is assumed to be spherical, i.e., volumetric only. In this situation, in subsequent applications, beginning with derivations in Sec. 2.2.2, inelastic deformation is assumed to be spherical, i.e., volumetric only. In this situation, $F^D$ of

$$G_{AB}(X, D) = \tilde{G}_{AC}(X)\tilde{G}^C_B(D), \quad G^{AB}(X, D) = \tilde{G}^{AC}(X)(\tilde{G}^{-1})^B_C(D).$$

Analogous decompositions into position- and microstructure-dependent parts apply for the spatial Sasaki metric and its inverse components:

$$g_{ab}(x, d) = \tilde{g}_{a\gamma}(x)\tilde{g}^\gamma_b(d), \quad g^{ab}(x, d) = \tilde{g}^{a\gamma}(x)(\tilde{g}^{-1})^\gamma_b.$$  (2.45)

For the choice (2.47), $\tilde{g}^{a\beta}(X, D) = \delta^{a\beta}$; for (2.48), $\tilde{g} = g$.  

$\tilde{g} = \det(g_{a\beta}) = 1/\det(g^{a\beta}).$

For the total intermediate metric and intermediate structure-independent metric at a material point $X \in \mathfrak{M}$ or for the total intermediate metric at spatial point $x \in \mathfrak{m}$, two possibilities [Clayton et al., 2004] are considered in further detail:

$$g_{\alpha\beta}(X, D) = \delta_{\alpha}^A G_{AB}(X, D)\delta^B_\beta = \delta_{\alpha}^A \tilde{G}_{AB}(X)\tilde{g}^\gamma_b(D)\delta^B_\gamma,$$

or

$$g_{\alpha\beta}[x(X, D), d(X, D)] = \delta_a^{\alpha} g_{ab}[x(X, D), d(X, D)]\delta^b_\beta. \quad (2.48)$$

Extending the theoretical developments of the present work, the local volume element $d\tilde{v}$ and volume form $d\tilde{\omega}$ on the intermediate space are obtained by analogy with those in (2.34):

$$d\tilde{v} = \{\det[(F^D)^a_b]\sqrt{\tilde{g}/G}\}dV = J^D dV, \quad d\tilde{v} = \{\det[(F^{E-1})^a_b]\sqrt{\tilde{g}/g}\}dv = J^E dv;$$

$$d\tilde{\omega} = J^D d\Omega = J^E d\omega.$$  (2.49)

Jacobian determinants are

$$J^D = \frac{1}{J^D} = \{\det[(F^D)^a_b]\sqrt{\tilde{g}/G}\} = \frac{d\tilde{v}}{dV}, \quad (2.50)$$

$$J^E = \frac{1}{J^E} = \{\det[(F^{E-1})^a_b]\sqrt{\tilde{g}/g}\} = \frac{d\tilde{v}}{dv}.$$  

For the choice (2.47), $\tilde{g} = G$; for (2.48), $\tilde{g} = g$.  

2.1.5. **Spherical inelastic kinematics**

In subsequent applications, beginning with derivations in Sec. 2.2.2, inelastic deformation is assumed to be spherical, i.e., volumetric only. In this situation, $F^D$ of
(2.37) and (2.38) becomes
\[ \mathbf{F}^{D}[D(X)] = \{J^{D}[D(X)]\}^{1/3}g_{\alpha}^{A} \otimes dX^{A}, \]  
(2.51)
with \( g_{\alpha} \) generic basis vectors for the intermediate state, and with \( g_{\alpha}^{A} \) the shifter components from reference to intermediate configurations [Clayton, 2014b]. Noting that
\[ \det \mathbf{F}^{D} = J^{D} \det (g_{\alpha}^{A}) = J^{D} \sqrt{G/\tilde{g}}, \]  
(2.52)
(2.51) is consistent with (2.49) and (2.50). Let the scalar field \( \chi = \chi(D) \) denote the dilatation or volume fraction of spherical defects per unit volume in the intermediate configuration [Clayton et al., 2005]:
\[ \chi = (\delta \tilde{v} - \delta V)/\delta \tilde{v} = 1 - J^{D} = (J^{D} - 1)/J^{D} \Rightarrow J^{D} = 1/(1 - \chi), \]  
(2.53)
\[ (F^{D})_{A}^{\alpha} = (1 - \chi)^{-1/3}g_{\alpha}^{A}. \]
For consistency with the particular but inessential choice of coincident referential and intermediate metric tensors in (2.47),
\[ g_{\alpha} = \delta_{A}^{\alpha}, \quad g_{\alpha}^{A} = \delta_{\alpha}^{A}, \quad \det(g_{\alpha}^{A}) = 1. \]  
(2.54)

2.2. Thermodynamics and balance laws

The variational framework for quasi-static equilibrium in pseudo-Finsler geometry developed in Clayton [2016b,c] is reviewed in brief. New extensions to the theory are described in Sec. 2.2.2.

The action integral for a compact region of \( \mathcal{M} \) with boundary \( \partial \mathcal{M} \) is \( \Psi \). Denote by \( p = p_{\alpha}dx^{\alpha} \) a mechanical load vector, specifically a force per unit reference area. Denote by \( z = z_{A}\delta D^{A} \) a thermodynamic force conjugate to the internal state vector. A variational principle is set forth:
\[ \delta \int_{\mathcal{M}} \psi d\Omega = \oint_{\partial \mathcal{M}} (\langle p, \delta x \rangle + \langle z, \delta D \rangle)\Omega. \]  
(2.55)
Denote by \( \psi \) the potential energy density. Then (2.55) is
\[ \delta \int_{\mathcal{M}} \psi d\Omega = \oint_{\partial \mathcal{M}} [p_{\alpha}{\delta x}^{\alpha} + z_{A}\delta(D^{A})]\Omega. \]  
(2.56)
The first variation of \( D \) is enclosed in parentheses to avoid confusion with basis vector \( \delta D^{A} \). Energy density per unit reference volume on \( \mathcal{M} \) is of the form
\[ \psi = \psi(F, D, \nabla D, G) = \psi(F_{A}, D_{A}, D_{B}, G_{AB}). \]  
(2.57)
Generalized continuum theories of materials with microstructure [Capriz, 1989], e.g., phase field theories [Clayton and Knap, 2011, 2015a], provide physical impetus for (2.57). Internal state vector \( D \) is viewed as a vector-valued set of order
parameter(s). Thermodynamic forces follow from the first variation of (2.57):
\[ \delta \psi = \frac{\partial \psi}{\partial F_A^a} \delta F_A^a + \frac{\partial \psi}{\partial D^A} \delta (D^A) + \frac{\partial \psi}{\partial D_{[B}^A} \delta D_{[B}^A + \frac{\partial \psi}{\partial G_{AB}} \delta G_{AB} \]
\[ = P_a^A \delta F_A^a + Q_A \delta (D^A) + Z_B^A \delta D_{[B}^A + S^{AB} \delta G_{AB}. \] (2.58)
Spatial coordinate invariance requires
\[ \psi = \psi[C(F, g), D, \nabla D, G] = \psi(C_{AB}, D^A, D_{[B}^A, G_{AB}). \] (2.59)
The first Piola–Kirchhoff stress \( P_a^A \) and Cauchy stress \( \sigma^{ab} \) obey a local angular momentum balance:
\[ P_a^A = 2g_{ab} F_b^b \frac{\partial \psi}{\partial C_{AB}}, \quad \sigma^{ab} = j g^{ac} P_c^A F_A^b = 2j F_a^a F_b^b \frac{\partial \psi}{\partial C_{AB}} = \sigma^{ba}. \] (2.60)
With variation \( \delta(\cdot) \) executed with \( X \) fixed and \( D \) variable,
\[ \delta F_A^a = \delta_A (\delta \varphi^a) + \hat{\varphi}_B \delta_C \varphi^a N_B^a \delta (D^C), \]
\[ \delta D_{[B}^A = [\delta (D^A)]_{[B} - (\hat{\varphi}_C N_B^a - \hat{\varphi}_C K_B^A D^D) \delta (D^C); \]
\[ \delta (d\Omega) = G_{AB} \delta_C G_{AB} \delta (D^C) d\Omega. \] (2.61)
(2.62)
Relations (2.58), (2.61) and (2.62) are substituted into (2.56). The divergence theorem (2.15) and repeated integration by parts then result in an integral/global form of (2.56). Assuming this must hold for admissible variations \( \delta \varphi \) and \( \delta D \), Euler–Lagrange equations in \( \mathcal{M} \) and natural boundary conditions on \( \partial \mathcal{M} \) are obtained (for details see Clayton [2016c]):
\[ \partial_A P_a^A + P_a^B H_{AB} - P_a^C H_{CA} (F_A^b - N_B^a \hat{\varphi}) = (P_a^A C_{BC}^C + \hat{\varphi}_B P_a^A) \partial_A D^B = 0, \]
\[ \partial_A Z_C^A + Z_B^B H_{AB} - Z_B^C H_{AB} + \hat{\varphi}_B Z_C^A \partial_A D^B + Z_B^C (\hat{\varphi}_C N_B^a - \hat{\varphi}_C K_B^A D^D)
\[ + \delta C_E C_{ED}^D) + P_a^A \hat{\varphi}_B \delta_D \partial_A \varphi^a \partial_A D^B - (S^{AB} + \psi G_{AB}) \hat{\varphi}_C G_{AB} = Q_C; \]
\[ p_a = P_a^A N_A, \quad z_A = Z_B^B N_B. \] (2.63)
(2.64)
(2.65)
Equation (2.63) is the local balance of linear momentum; (2.64) is the local balance of director momentum or micro-momentum. Operation (2.63) has been used in (2.63) for covariant differentiation of \( P = P_a^A dx^a \otimes \frac{\partial}{\partial x^a} \). Reductions of balance equations for (pseudo)-Riemannian or (pseudo)-Minkowskian spaces are derived in Clayton [2016c]. In Cartesian spaces–i.e., global metrics \( G_{AB} = \delta_{AB} \) and \( g_{ab} = \delta_{ab} \)–balance laws reduce to
\[ \partial_A P_a^A + \partial_B P_a^A \partial_A D^B = 0, \quad \partial_A Z_C^A + \partial_B Z_C^A \partial_A D^B + P_a^A \partial_B \partial_D \varphi^a \partial_A D^B = Q_C. \] (2.66)
The model becomes complete upon assignment of a few more features. A metric tensor \( G \) is introduced, from which all connection coefficients are derived via differentiation using relations listed in Sec. 2.1.1. Horizontal and vertical connection
coefficients in (2.8) and (2.9) must be chosen, e.g., the Chern–Rund connection or Cartan’s connection. Similar features are assigned for the current configuration, including metric $g$, from which connection coefficients are derived via equations in Sec. 2.1.2. Constitutive equations may be supplied for the solid material must be assigned a more specific form. Depending on the form of this function, constitutive equations for inelastic components of the deformation gradient, $F^D$, and the director motion gradient, $\theta^D$, of Sec. 2.1.4 may also be required. Then with boundary conditions assigned on $\partial \Omega$, (2.63) and (2.64) are six coupled non-linear partial differential equations for six unknown fields $\varphi^a[X, D(X)]$ and $D^A(X)$ with $a, A = 1, 2, 3$.

2.2.1. Multiplicative thermodynamics

Following example problems solved in Clayton [2016b,a,c], and those addressed in phase field theory [Clayton and Knap, 2011, 2015a], $\psi$ of (2.57) is split into a sum of elastic strain energy density $W$ and structure/internal state dependent energy density $f$:

$$\psi(F^a_a, D^A_{[b}, G_{AB]} = W[(F^E)^a_a, D^A_{[b}, \bar{g}_{\alpha\beta}] + f(D^A_{[b}, D^A_{b}], \bar{G}_{AB}).$$  \hspace{1cm} (2.67)

Functional conditions (2.37) and (2.38) are imposed:

$$(F^E)^a_a[F, F^D(D)] = F^a_a[X, D(X)](F^D)^A_A[D(X)].$$  \hspace{1cm} (2.68)

Under these conditions, and invoking (2.47) for the intermediate metric components $\bar{g}_{\alpha\beta}$, thermodynamic forces introduced in (2.58), at fixed $X$, are

$$P^A_a = \frac{\partial \psi}{\partial F^a_A} = \frac{\partial W}{\partial F^a_A} = (F^D)^{A}_a \frac{\partial W}{\partial (F^E)^{a}_A};$$

$$Q^B_A = \frac{\partial \psi}{\partial D^A_{[b],}} = \frac{\partial W}{\partial D^A_{[b],}} + \frac{\partial f}{\partial D^A_{[b],}} - P^B_a (F^E)^a_a \frac{\partial (F^D)^{B}_a}{\partial D^A_{[b],}};$$  \hspace{1cm} (2.69)

Furthermore, $\partial \psi/\partial G_{AB} \rightarrow \partial \psi/\partial \bar{G}_{AB}$ and $\delta \bar{G}_{AB}(X) = 0$, so $S^{AB} \rightarrow 0$ in (2.58) and (2.64). Spatial invariance analogous to (2.59) can be ensured via letting $W$ depend on $C^E$ rather than $F^E$, where

$$(C^E)^{a}_B = (F^E)^{a}_a \bar{g}_{ab}(F^E)^{b}_{B} = (F^D)^{a}_a \bar{C}_{ab}(F^D)^{B}_{B}, \quad \bar{C}_{ab} = F^a_a \bar{g}_{ab} F^B_B.$$  \hspace{1cm} (2.70)

Given functions $F^D$, $W$ and $f$, substitution of thermodynamic forces found via (2.69) into (2.63) and (2.64) and invoking $F^E = (\partial \varphi/\partial X)(F^D)^{-1}$ gives six equations in six unknowns $\varphi^a(X, D)$ and $D^A(X)$. 

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2.2.2. Spherical inelasticity: Balance equations

The particular kinematic model of Sec. 2.1.5 is now applied, recalling that \( \chi \) is the scalar dilatation measure. From (2.53),

\[
(F^D)_{\alpha}^A [D(X)] = \frac{1}{1 - \chi [D(X)]} \bar{g}_{\alpha}^A (D, X),
\]

such that

\[
\frac{\partial (F^D)_{\beta}^A}{\partial D^A} = \frac{-1}{3(1 - \chi)^{4/3}} \frac{\partial \chi}{\partial D^A} g_{\beta}^A + \frac{1}{(1 - \chi)^{1/3}} \partial_A (g_{\beta}^A),
\]

which can subsequently be substituted into the expression for \( Q_A \) in (2.69). For the particular yet inessential choice in (2.47) and (2.54), this reduces to

\[
\frac{\partial (F^D)_{\beta}^A}{\partial D^A} = \frac{-1}{3(1 - \chi)^{4/3}} \frac{\partial \chi}{\partial D^A} \delta_{\beta}^A \Rightarrow \quad Q_A = \frac{\partial W}{\partial D^A} + \frac{\partial f}{\partial D^A} + \frac{1}{3(1 - \chi)^{4/3}} P_{\alpha}^B (F^{E})_{\alpha} \frac{\partial \chi}{\partial D^A} \delta_{\beta}^B.
\]

The convenience of the choice of identical reference and intermediate metrics, one of several proposed in Clayton [2012a, 2014b] and Clayton et al. [2004] in the context of Riemannian geometry, is apparent from (2.73) for pseudo-Finsler geometry. This choice also maintains invariance of components of the elastic deformation measure \( C^E \) in (2.70) under transformations of the spatial coordinate frame(s). Furthermore, for cases in which inelastic deformation does not occur, the kinematic and geometric framework reduces to one similar to non-linear elasticity in the sense that possibly curvilinear intermediate and referential coordinates become coincident. Another possibility, as written in (2.48), imposes identical spatial and intermediate metric tensors. This choice was advocated in Clayton [2012a] for hyperelastic–plastic solids since the classical balance of linear momentum can be expressed completely in terms of quantities referred to the spatial frame. While this advantage may simplify some calculations, physical components of elastic deformation terms become non-standard, and invariance of \( C^E \) is not ensured. The latter point thus requires the strain energy function to be constructed from deformation functions referred to a different basis that is fixed under spatial rotations, or to be constructed from scalar invariants of elastic deformation/strain, e.g., limited to isotropic elasticity.

3. Application: Tensile Cylindrical Fracture of Magnesium

Finsler-geometric continuum theory with multiplicative kinematics is now applied to modeling fracture in metallic crystals. The problems addressed in Sec. 3 involve degradation and failure of Mg deformed in tension. The Finsler metric considers effects of void nucleation and growth on a local volume element of material. In the absence of such voids, the present treatment reduces to a description of perfectly brittle fracture, e.g., perfect cleavage along a failure plane. First, somewhat general
model characteristics and derivations are obtained for quasi-static loading protocols for a cylindrical sample. Then, particular solutions for uniaxial stress extension along the axis of the cylinder are discussed, with material properties corresponding to a single crystal of Mg stretched parallel to its \(c\)-axis ([0001]) of transverse isotropy.

### 3.1. Geometry and deformation

A cylindrical material body of initial external radius \(R_0\) and length \(L_0\) is considered. The material manifold is \(\{M : R \in [0, R_0], \Theta \in (-\pi, \pi], Z \in [0, L_0]\}\), with \(\Theta\) the referential angular coordinate. By construction, the internal structure field associated with fracture along the \(Z\)-axis is axial in direction and varies potentially only with \(X^3 = Z\). This assumption requires that \(D(X) = D^3(X^3) = D^Z(Z)\).

Referential coordinate systems are \(\{R, \Theta, Z\} = \{X^1, X^2, X^3\}\); \(\{D^R, D^\Theta, D^Z\} = \{D^1, D^2, D^3\} = \{0, 0, D\}\), \(D = D(Z)\).

Let \(\bar{G} = \bar{G}(X)\) be the usual metric tensor of Euclidean space in cylindrical coordinates [Clayton, 2014b, 2015b]. The following multiplicatively separable form of the metric tensor \(G(X, D)\), an example of (2.44), is used:

\[
G(X, D) = G(X) \bar{G}(D) = \begin{bmatrix} \bar{G}_{11} & 0 & 0 \\ 0 & \bar{G}_{22}(X) & 0 \\ 0 & 0 & \bar{G}_{33} \end{bmatrix} \begin{bmatrix} \bar{G}_1^1(D) & 0 & 0 \\ 0 & \bar{G}_2^2(D) & 0 \\ 0 & 0 & \bar{G}_3^3(D) \end{bmatrix} = \begin{bmatrix} \bar{G}_1^1(D) & 0 & 0 \\ 0 & \bar{G}_2^2(D) & 0 \\ 0 & 0 & \bar{G}_3^3(D) \end{bmatrix}.
\]

(3.2)

Here, \(B\) is a differentiable scalar function of the internal state. The metric is thus scaled isotropically by the factor \(B\), an example of a conformal transformation or Weyl-type scaling [Clayton, 2016a; Weyl, 1952]. The determinant of the total metric is

\[
G(X, D) = \det[G(X, D)] = R^2 B^3[D(Z)].
\]

(3.3)

Christoffel symbols of the second kind are

\[
\gamma^A_{BC} = G^{AD} \gamma_{BCD} = \bar{G}^{AD} \gamma_{BCD} = \bar{\gamma}^A_{BC}.
\]

(3.4)

Non-zero Christoffel symbols resulting from (3.2) are thus, with \((1, 2, 3) \leftrightarrow (R, \Theta, Z)\),

\[
\gamma^\Theta_R = \gamma^R_\Theta = \gamma^R_\Theta = 1/R, \quad \gamma^R_{\Theta \Theta} = -R.
\]

(3.5)
Since the only non-vanishing component of $D$ is axial $(D_Z)$ and since $\gamma^A_{Z2} = 0$, the spray and canonical non-linear connection coefficients vanish

$$G^A = \frac{1}{2} \gamma^A_{BC} D^B D^C = \frac{1}{2} \gamma^A_{ZZ} D \cdot D = 0, \quad N^A_B = G^A_B = \delta_B^A G^A = 0 \Rightarrow \partial_A(\cdot) = \delta_A(\cdot). \quad (3.6)$$

With $B' = dB/dD$, components of Cartan’s tensor in (2.5) are, with others all vanishing

$$C_{113} = C_{RRZ} = -B'/2, \quad C_{223} = C_{\theta\theta Z} = -R^2 B'/2, \quad C_{333} = C_{ZZ Z} = B'/2, \quad C_{131} = C_{311} = C_{RZR} = C_{ZRR} = B'/2, \quad C_{232} = C_{322} = C_{\phi Z\theta} = C_{Z\phi \theta} = R^2 B'/2. \quad (3.7)$$

The trace in the axial direction of Cartan’s tensor will be used later in the equilibrium equations:

$$C^A_{ZA} = C^A_{31} + C^A_{32} + C^A_{33} = G^{AB} C_{3AB} = 3B'/2B). \quad (3.8)$$

The Chern–Rund connection is used, similarly to prior work [Stumpf and Saczuk, 2000; Clayton, 2016b,c]. Noting that vanishing non-linear connection coefficients arise from (3.6), horizontal coefficients of the Chern–Rund connection are equal to Levi–Civita coefficients derived from $\bar{G}_{AB}$, and vertical coefficients vanish by definition:

$$H^A_{BC} = K^A_{BC} = \Gamma^A_{BC} = \gamma^A_{BC} = \bar{\gamma}^A_{BC}; \quad V^A_{BC} = Y^A_{BC} = 0. \quad (3.9)$$

The analogous geometric description is used for the deformed solid in the spatial representation. The deformed body is a right circular cylinder of length $L$ and external radius $r_0$, and the spatial base manifold is $\{m : r \in [0, r_0], \theta \in (-\pi, \pi), z \in [0, L]\}$. The internal structure field associated with fractures on planes normal to the direction of extension is axial and varies potentially only with $x^3 = z$, so $d(x) = d^3(x^3) = d^3(z) = d(z)$. Spatial analogs of (3.1)–(3.9) are written as follows, with lower-case notation corresponding to variables in the spatial frame that are complementary to those in capitals written for the reference configuration:

$$\{r, \theta, z\} = \{x^1, x^2, x^3\}; \quad \{d^1, d^2, d^3\} = \{d^1, d^2, d^3\} = \{0, 0, d\}; \quad d = d(z); \quad (3.10)$$

$$g(x, d) = \bar{g}(x) \bar{g}(d) = \begin{bmatrix} \bar{g}_{11} & 0 & 0 \\ 0 & \bar{g}_{22}(x) & 0 \\ 0 & 0 & \bar{g}_{33} \end{bmatrix} \begin{bmatrix} \bar{g}_1^1(d) & 0 & 0 \\ 0 & \bar{g}_2^2(d) & 0 \\ 0 & 0 & \bar{g}_{33}(d) \end{bmatrix}$$

\[= \begin{bmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} b(d) & 0 & 0 \\ 0 & b(d) & 0 \\ 0 & 0 & b(d) \end{bmatrix}; \quad (3.11)\]
\[ g(x, d) = \det[g(x, d)] = r^2 b^3 [d(z)]; \quad (3.12) \]

\[ \gamma^a_{bc} = g^{ad} \gamma_{bcd} = g^{ad} \gamma_{bdc} = \tilde{\gamma}^a_{bc}; \quad (3.13) \]

\[ \gamma^0_{r\theta} = \gamma^0_{\theta r} = 1/r, \quad \gamma^r_{\theta \theta} = -r; \quad (3.14) \]

\[ g^a = \frac{1}{2} \gamma^a_{bc} d^b d^c = \frac{1}{2} \gamma^a_{zz} d^z = 0, \quad n^a_b = g^a_b \Rightarrow \partial_b (\cdot) = \delta_a (\cdot); \quad (3.15) \]

\[ C_{113} = C_{rrz} = -b'/2, \quad C_{223} = C_{\theta \theta z} = -r^2 b'/2, \quad C_{333} = C_{zzz} = b'/2, \]

\[ C_{131} = C_{311} = C_{rzr} = C_{zrr} = b'/2, \quad C_{232} = C_{322} = C_{\theta z \theta} = C_{z \theta \theta} = r^2 b'/2; \quad (3.16) \]

\[ C^a_{za} = C^1_{za} + C^2_{za} + C^3_{za} = g^{ab} C_{3ab} = 3b'/(2b); \quad (3.17) \]

\[ H^a_{bc} = K^a_{bc} = \Gamma^a_{bc} = \tilde{\gamma}^a_{bc} = \tilde{\gamma}^a_{bc}; \quad V^a_{bc} = Y^a_{bc} = 0. \quad (3.18) \]

The following assumptions are made regarding deformation kinematics for the class of problems considered in Sec. 3. No twisting occurs, radial deformation is uniform along the length of the cylinder when fracture or rupture does not occur, and axial extension depends on axial position only. Fracture and its associated micromechanisms such as voids may contribute to radial and axial deformations. Motions, deformations, and director/state variable fields first introduced in Sec. 2.1.3 are of the following functional forms:

\[ r = r[R, D(Z)] = \alpha[D(Z)] r(R), \quad \Theta = \Theta, \quad z = z[Z, D(Z)]; \quad d = d[Z, D(Z)]. \quad (3.19) \]

The radial motion is assumed to be a product of two scalar functions \( \alpha \) and \( \tilde{r} \), the first depending on internal state and the second depending on referential radial position. Furthermore, it is understood that \( \alpha(0) = 1 \) such that a perfectly elastic description is recovered in the absence of fracture, i.e., \( D = 0 \Rightarrow r(R, D) = \tilde{r}(R) \).

Referred to the present cylindrical coordinate systems \{ \( R, \Theta, Z \) \} and \{ \( r, \theta, z \) \}, coincident reference and intermediate configuration metric tensor components are used:

\[ g_{\alpha \beta}(X, D) = g_{\alpha \beta}[R, B(D)] = \delta^A_{\alpha} \delta^B_{\beta} G_{AB}[R, B(D)], \quad (3.20) \]

a particular example of (2.47). This in turn implies that identical basis vectors are used to label components of vectors and tensors in referential and intermediate configurations. The choice (2.47) and (3.20), one of several advocated in Clayton [2012a, 2014b], is most efficient in the present case of cylindrical geometry and kinematics, wherein inelastic deformation will later be prescribed as spherical and wherein elastic deformations are described using the usual curvilinear basis vectors referred to spatial and material coordinates. Use of the standard Cartesian frame for the intermediate metric tensor [Clayton et al., 2004; Regueiro et al., 2002] would be
highly impractical since cylindrical coordinates are invoked for material and spatial configurations.

Applying the multiplicative description of (2.37) with spherical inelastic kinematics of Sec. 2.1.5, the inelastic portion contains structural, i.e., $D$-dependent, terms. The total deformation gradient in natural coordinates is

$$F(R, Z; D) = \begin{bmatrix}
\alpha(D)d\vec{r}(R)/dR & 0 & 0 \\
0 & d\theta(\Theta)/d\Theta & 0 \\
0 & 0 & \partial z(Z, D)/\partial Z
\end{bmatrix}$$

$$= F^{E}(R, Z)F^{D}[D(Z)]$$

$$= \begin{bmatrix}
(F^{E})_{r}(R, Z) & 0 & 0 \\
0 & (F^{E})_{\Theta}(Z) & 0 \\
0 & 0 & (F^{E})_{z}(Z)
\end{bmatrix}$$

$$= \begin{bmatrix}
\phi[D(Z)] & 0 & 0 \\
0 & \phi[D(Z)] & 0 \\
0 & 0 & \phi[D(Z)]
\end{bmatrix}.$$  (3.21)

Recalling from (2.53) that $\chi$ is the local porosity, the inelastic term is

$$\phi[D(Z)] = (J^{D}[D(Z)])^{1/3} = \left(1 - \chi[D(Z)]\right)^{-1/3}. \quad (3.22)$$

The elastic deformation gradient is

$$F^{E}(R, Z) = \frac{1}{\phi(Z)} \begin{bmatrix}
\alpha(D)d\vec{r}(R)/dR & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & \partial z(Z, D)/\partial Z
\end{bmatrix}$$

$$= \frac{1}{\phi(Z)} \begin{bmatrix}
r'(R, Z) & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & z'(Z, D)
\end{bmatrix}, \quad (3.23)$$

with the condensed notation $r' = \alpha d\vec{r}/dR$ and $z' = \partial z$. The Jacobian determinant and non-zero mixed-variant symmetric deformation tensor components are computed as

$$J(X; D) = J(R, Z; D)$$

$$= \sqrt{g(x, d)G(X, D)F_{1}^{1}(X, D)F_{3}^{3}(X, D)}$$

$$= r'(R, Z)z'(Z, D)\left\{\frac{g[r(R), d(Z, D)]}{G(R, D)}\right\}^{1/2}$$

$$= r'(R, Z)[r(R, Z)/R]z'(Z, D)\left\{\frac{b(d(Z, D))}{B(D)}\right\}^{1/2}, \quad (3.24)$$

$$C_{1}^{1} = \frac{b}{B}(r')^{2}, \quad C_{2}^{2} = \frac{b}{B}(r/R)^{2}, \quad C_{3}^{3} = \frac{b}{B}(z')^{2}. \quad (3.25)$$

As noted already, the internal state variable $D$ is physically identified with tensile fracture in the direction of the $Z$-axis, on planes normal to this direction.
(e.g., on basal planes in a hexagonal crystal structure). Dilatation due to ductile fracture, i.e., void nucleation and growth complementary to the fracture process, is quantified by the spherical inelastic deformation gradient:

$$\mathbf{F}^D(D) = \phi(D) \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \exp(k\xi/3) \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

(3.26)

$$\mathbf{F}^D_{\alpha} = \phi \delta_{\alpha}^D = \exp[kD/(3l)]\delta_{\alpha}^D = \exp(k\xi/3)\delta_{\alpha}^D.$$  

(3.27)

As introduced in (3.27), \(l\) is a regularization constant with dimensions of length. A normalized order parameter is denoted by \(\xi \in [0, 1]\), with derivative with respect to referential axial coordinate

$$\xi = D/l, \quad \xi' = D'/l.$$  

(3.28)

From (3.6) and (3.28), the horizontal gradient of the internal state vector is

$$D^3_{\alpha} = \partial_{\alpha}D - N^3_{\alpha\beta}D = D^3_{\alpha} = \partial D/\partial Z = D'.$$  

(3.29)

The constant \(l\) will later be identified as the value of state variable \(D\) at which the specimen is locally fully fractured with null tensile strength (i.e., \(\xi = 1\)). The fully elastic and pristine material at \(X\) is represented by \(\xi(X) = 0\). The constant \(k\) depends on the material of interest (e.g., Mg) and is used to scale the contribution of the order parameter to the inelastic component of the deformation gradient. When \(k = 0\), bulk deformation is fully elastic, i.e., \(k \rightarrow 0 \Rightarrow \phi \rightarrow 1 \Rightarrow \mathbf{F} \rightarrow \mathbf{F}^E\) in (2.37).

A more specific form of the Finsler metric in (3.2) is introduced as

$$\hat{G}^A_B(D) = B(D)\delta^A_B = B[\xi(D)]\delta^A_B = \exp(2k\xi/3)\delta^A_B \Rightarrow 3B'/2B = C^A_B = k/l.$$  

(3.30)

The length of a referential line element and the corresponding volume form become

$$|d\mathbf{X}|^2 = \exp(2k\xi/3)(dR \cdot dR + R^2 d\Theta \cdot d\Theta + dZ \cdot dZ),$$

$$d\Omega = \sqrt{G}dR \wedge d\Theta \wedge dZ = \exp(k\xi)RdR \wedge d\Theta \wedge dZ.$$  

(3.31)

Expansion occurs when \(k > 0\) and contraction (i.e., pore collapse) occurs when \(k < 0\), when \(\xi > 0\). A symmetric inelastic deformation tensor referred to material coordinates can be introduced as

$$\mathbf{C}^D = (\mathbf{F}^D)^T \mathbf{F}^D = \begin{bmatrix} [(\mathbf{F}^D)_{R\theta}]^2 & 0 & 0 \\ 0 & [(\mathbf{F}^D)_{\Theta\theta}]^2 & 0 \\ 0 & 0 & [(\mathbf{F}^D)_Z]^2 \end{bmatrix} = \phi^2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$  

(3.32)
Finsler-geometric continuum mechanics

As in prior work [Clayton, 2016b], this tensor and the material metric tensor canonically coincide with respect to structural dependence

\[(C_D)_{AB}(R, D) = [\phi(D)]^2 \hat{G}_{AB}(R) = \exp[2k\xi(D)/3]
\]

\[\hat{G}_{AB}(R) = B(D)\hat{G}_{AB}(R); \quad B = \phi^2. \quad (3.33)\]

Also as in prior work [Clayton, 2016b,c], the spatial and referential state variables are chosen to most simply coincide in (3.10):

\[d[x(X, D), D] = D(X) \Rightarrow d[z(Z, D), D] = D(Z) = l\xi(Z). \quad (3.34)\]

The spatial metric tensor and Jacobian determinant then reduce to

\[\hat{g}^a_b[d(D, Z)] = b[d(D)]\delta^a_b = \exp[(2/3)kd(D)/l]\delta^a_b = \exp(2k\xi/3)\delta^a_b = B(D)\delta^a_b,
\]

\[J = r'(r/R)z' = \sqrt{C_1^1 C_2^2 C_3^3}. \quad (3.35)\]

The porosity or dilatation is related to the order parameter \(\xi \in [0, 1]\) for non-negative \(k\) via

\[\chi = 1 - \exp(-k\xi), \quad k \in [0, \infty) \Rightarrow \chi \in [0, 1). \quad (3.36)\]

Used in the constitutive model for Mg described in forthcoming detail in Sec. 3.2 is an Eulerian elastic strain tensor referred to material coordinates [Clayton, 2013b, 2014a,d]. This tensor is sometimes referred to as a Piola strain tensor and has general representation

\[D^E = \frac{1}{2} \left( I - (F^E)^{-1}(F^E)^{-T} \right), \quad (D^E)_{\alpha \beta} = \frac{1}{2} [\delta^\alpha_\beta - (F^E^{-1})_a^\alpha (F^E^{-1})_b^\beta \hat{g}^{ab} \hat{g}^{\gamma \gamma}]. \quad (3.37)\]

As demonstrated in prior analysis [Clayton, 2014d, 2015a], this strain tensor more accurately represents the non-linear elastic response of ductile solids with a large ratio of effective bulk to shear modulus and/or low yield strength, e.g., many metals (including Mg), than the Green elastic strain used in classical non-linear elastic models [Clayton, 2011]. For the present class of problems with (2.47), (3.20) and (3.23) now invoked, (3.37) gives three potentially non-zero components of elastic strain:

\[(D^E)_R^R = (D^E)_1^1 = \frac{1}{2} \left[ 1 - \left( \frac{\phi R}{r} \right)^2 \right], \quad (D^E)_\Theta^\Theta = (D^E)_2^2 = \frac{1}{2} \left[ 1 - \left( \frac{\phi R}{r} \right)^2 \right], \quad (3.38)\]

\[(D^E)_Z^Z = (D^E)_3^3 = \frac{1}{2} \left[ 1 - \left( \frac{\phi R}{r} \right)^2 \right]. \quad (3.38)\]
3.2. Balance equations

The free energy per unit reference volume $\psi$ in (2.57) is additively separated into elastic strain energy per unit reference volume $W$ and structure dependent energy per unit reference volume $f$, following (2.67). More specifically, a sum of quadratic forms is invoked

$$\psi(F_A^a, D^A, D_{[A]}^A, G_{AB}) = W[(D^E)_\alpha^\beta, D^A] + f(D^A, D_{[A]}^A);$$

(3.39)

$$W = \frac{1}{2} C^{\alpha\gamma}_{\beta\delta} ([D]) (D^E)_\alpha^\beta (D^E)_\delta^\gamma,$$

and

$$f = \frac{1}{2} |D|^2 + \frac{1}{7} |\nabla D|^2.$$

(3.40)

Components of the second-order elasticity tensor $C^{\alpha\gamma}_{\beta\delta}$ may generally depend on the state variable to enable degradation commensurate with fracture. Surface energy associated with crack surfaces, measured per unit reference area, is represented by the intrinsic material constant $\Upsilon$. With kinematic and functional conditions (2.37) and (2.38) applied, along with (3.29) where $D(Z) = t\xi(Z)$, terms affecting the strain energy function reduce to

$$(F^E)_a^\alpha [F, F^D(\xi)] = F_A^a [X, \xi(X)](F^D-1)_a^\alpha [\xi(X)];$$

(3.41)

$$\hat{C}^{\alpha\gamma}_{\beta\delta} = C^{\alpha\gamma}_{\beta\delta}(\xi), \quad f = \Upsilon[|\xi|^2/|I| + (\xi')^2].$$

More specific forms of thermodynamic forces for Finsler continuum mechanics given in (2.69) and (2.73) at a fixed material point $X$ are then derived as follows:

$$P_a^A = \frac{\partial \psi}{\partial F_A^a} = (F^D-1)_a^\alpha \frac{\partial W}{\partial (F^E)_a^\alpha} = (F^D-1)_a^\alpha \frac{\partial W}{\partial (D^E)_\beta} \frac{\partial (D^E)_\gamma}{\partial (F^E)_a^\alpha}$$

$$= (F^E-1)_C^\alpha (F^E-1)_\gamma^\epsilon (F^E-1)_\beta^a \hat{S}_C^\epsilon$$

$$= \frac{1}{\phi} \hat{\delta}_X^\alpha (F^E-1)_C^\alpha (F^E-1)_\gamma^\epsilon (F^E-1)_\beta^a \hat{C}^{\beta\epsilon}_{\gamma\delta}(D^E)_\delta^\gamma;$$

(3.42)

$$Q = Q_1 = Q_Z = \frac{\partial \psi}{\partial D} = \frac{1}{7} \left[ \frac{\partial W}{\partial \xi} - P_a^A (F^E)_a^\alpha \frac{\partial (F^E)_\gamma^\alpha}{\partial \xi} + \frac{\partial f}{\partial \xi} \right]$$

$$= \frac{1}{7} \left[ \frac{1}{2} \frac{\partial \hat{C}^{\alpha\gamma}_{\beta\delta}}{\partial (D^E)_\rho^\gamma (D^E)_\delta^\rho} \frac{\partial (D^E)_\epsilon^\rho}{\partial \xi} - \frac{k\phi}{3} P_a^A (F^E)_a^\alpha \delta_\rho^\alpha + \frac{2}{7} \Upsilon \phi' \right];$$

(3.43)

$$T = Z^2_Z = Z^3_1 = \frac{\partial \psi}{\partial D_{[A]}^a} = \frac{1}{7} \frac{\partial f}{\partial \xi'} = 2 \Upsilon \xi'.$$

(3.44)

In non-linear elastic constitutive relation (3.42), the conjugate stress to the elastic strain measure of (3.37) is

$$\hat{S}_\beta^a = \partial W/\partial (D^E)_\alpha^\beta = \hat{C}^{\alpha\gamma}_{\beta\delta}(D^E)_\gamma^\delta.$$

(3.45)
Further derivations invoke the cylindrical geometry and axisymmetric kinematics of Sec. 3.1. The strain energy in (3.39) and (3.40) becomes, for materials with transverse isotropy,

\[
W = W[(D^E)^1_1, (D^E)^2_2, (D^E)^3_3, \xi]
\]

\[
= 1 \left[ \hat{C}_{RR}(D^E)^R_R + \hat{C}_{\Theta\Theta}(D^E)^\Theta_\Theta + \hat{C}_{ZZ}(D^E)^Z_Z \right] + 2 \left[ \hat{C}_{R\Theta}(D^E)^R_\Theta + \hat{C}_{RZ}(D^E)^R_Z + \hat{C}_{\Theta Z}(D^E)^\Theta_Z \right]
\]

\[
= \frac{1}{2} \left[ \hat{C}_{111}(D^E)^1_1 + \hat{C}_{112}(D^E)^2_2 + \hat{C}_{333}(D^E)^3_3 \right],
\]

(3.46)

Notation for material constants in elastic potential and structure potential \(f\) is the following. Structure-dependent variables \(\hat{C}_{ij} = \hat{C}_{ij}(\xi)\) are the appropriate second-order elastic coefficients; in the absence of fracture, these become equivalent to the elastic constants of the perfect crystal for transversely isotropic symmetry \(C_{ij}\) to be introduced in Sec. 3.3 for Mg. Scalar \(\Upsilon\) is the surface energy per unit reference area as mentioned following (3.40), and regularization length \(l\) has been introduced already in (3.28). The total energy function \(\psi\) contains no explicit dependence on \(\hat{G}(D)\).

Possibly non-zero stress components are obtained from (3.42) and (3.46):

\[
P_1^1 = P_1^R = (1/r') (\phi/r')^2 S^R_R, \quad P_2^2 = P_\Theta^\Theta = (\phi R/r')^2 S^\Theta_\Theta,
\]

\[
P_3^3 = P_z^Z = (1/z') (\phi/z')^2 S^Z_Z.
\]

(3.47)

Restricting attention to tensile deformation, elastic coefficients degrade quadratically with increases in the normalized state variable or order parameter

\[
\hat{C}(\xi) = C(1 - \xi)^2, \quad \frac{\partial \hat{C}_{\gamma\delta}}{\partial \xi} = \frac{-2 \hat{C}_{\gamma\delta}}{1 - \xi}.
\]

(3.48)

For completely destroyed material, locally \(\xi \to 1\) so that \(\hat{C}_{ij}(1 - \xi)^2 \to 0\), leading to \(\hat{C}(1) = 0\). This prescription is fully analogous to the degradation models of phase field theories of (tensile) fracture [Borden et al., 2012; Clayton and Knap, 2014, 2015a]. The conjugate thermodynamic force to \(D = l \xi\) in (3.43) then becomes

\[
Q = -\frac{1}{l} \left[ \frac{1}{1 - \xi} C_{\gamma\delta}^{\alpha\beta}(D^E)^\alpha_{\gamma}(D^E)^\beta_{\delta} + \frac{k}{3} (F^E)^R_R P_1^R + (F^E)^\Theta_\Theta P_\Theta^\Theta + (F^E)^Z_Z P_z^Z \right] - 2 \Upsilon \xi.
\]

(3.49)

3.3. Material characteristics

Deformation and fracture in Mg is evaluated in particular solutions that follow later in Sec. 3.4. Mg is a low density crystalline metal of moderate ductility [Yoo,
Table 1. Physical properties of Mg.

<table>
<thead>
<tr>
<th>Property (Units)</th>
<th>Value</th>
<th>Description</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}$ (GPa)</td>
<td>64</td>
<td>Second-order elastic constant</td>
<td>Clayton and Knap [2011]</td>
</tr>
<tr>
<td>$C_{12}$ (GPa)</td>
<td>26</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_{13}$ (GPa)</td>
<td>22</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_{33}$ (GPa)</td>
<td>67</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_{44}$ (GPa)</td>
<td>18</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$E$ (GPa)</td>
<td>56</td>
<td>Young’s modulus</td>
<td>Eq. (3.53)</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.24</td>
<td>Poisson’s ratio</td>
<td>Eq. (3.53)</td>
</tr>
<tr>
<td>$\mu$ (GPa)</td>
<td>23</td>
<td>Shear modulus</td>
<td>$E/(2 + 2\nu)$</td>
</tr>
<tr>
<td>$c$, $a$ (nm)</td>
<td>0.52, 0.32</td>
<td>Lattice parameters</td>
<td>Clayton and Knap [2011]</td>
</tr>
<tr>
<td>$\Upsilon$ (J/m$^2$)</td>
<td>0.69</td>
<td>Surface energy</td>
<td>Yoo [1981]</td>
</tr>
<tr>
<td>$\exp(k)$</td>
<td>1.0–1.2</td>
<td>Dilatation</td>
<td>Kondori and Benzerga [2014] and Delogu [2004]</td>
</tr>
<tr>
<td>$l$ (nm)</td>
<td>0.83</td>
<td>Regularization length</td>
<td>Eq. (3.51)</td>
</tr>
</tbody>
</table>

1979, 1981], of high interest to automotive and aerospace industries requiring light structural components. The crystal structure of Mg in the ambient solid state is hexagonal. Elastic anisotropy is considered low [Hearmon, 1946]. Representative material parameters with supporting references are listed in Table 1; if no reference is listed, the value is obtained from the source given in the row above. Hexagonal elastic constants correspond to the single crystal; the other elastic constants are determined from the calculation procedure described later in Sec. 3.4. For extension along the $c$-axis (the fiber of transverse isotropy), relevant cylindrical elastic constants in terms of hexagonal elastic constants $C_{ij}$, $(i, j = 1, 2, \ldots, 6)$ in a rectangular crystallographic coordinate system [Clayton, 2011] are

$$C_{RR} = C_{\Theta \Theta} = C_{11}, \quad C_{ZZ} = C_{33}, \quad C_{RZ} = C_{\Theta Z} = C_{13}, \quad C_{R\Theta} = C_{12}. \quad (3.50)$$

Remaining parameters are self-explanatory except for regularization length $l$ and Weyl dilatation factor $k$. The regularization length $l$ is chosen in a physically appropriate manner as the cohesive fracture process zone size over which the stress at a crack tip degrades [Rice, 1968; Clayton, 2016c; Clayton et al., 2012]:

$$l = 4\mu\Upsilon/[(1 - \nu)\pi r^2]. \quad (3.51)$$

Here, $\nu$ is Poisson’s ratio and $\tau \approx \frac{10}{11}$ is the theoretical tensile strength for the crystal [Gilman, 1960].

From (2.53), the ratio of volume after dilatation/contraction in a fully degraded region with null shear modulus [$\xi = 1 \rightarrow \mu(1 - \xi)^2 = 0$] is $\exp(k)$, and the porosity is $\chi = 1 - \exp(-k)$. For Mg polycrystals deformed in uniaxial tension experiments, an overall volume increase of $\approx 4\%$ was reported in conjunction with tensile fracture modes [Kondori and Benzerga, 2014]. For pure Mg, a theoretical treatment relating shear instability to amorphization in the failure zone suggests a volume increase of $\approx 12\%$ [Delogu, 2004]. Therefore, the investigated range of $0 \leq k \leq \text{ln}(1.2)$
seems physically reasonable for this material, with the lower limit corresponding to null dilatation from voids or other defects, i.e., perfect cleavage for $k = 0$. Ductile fracture, on the other hand, is represented by positive values of $k$. A similar range of $k$ was studied for problems of shear localization in [Clayton, 2016c].

### 3.4. Solutions and interpretations

The problem of uniaxial stress elongation along the $c$-axis in a (Mg) single crystal with hexagonal symmetry is now addressed. The same solutions apply for a cylinder of a polycrystalline material with isotropic symmetry upon substitution of the isotropic elastic constants. Lateral surfaces of the cylinder are traction-free, and radial and hoop stresses vanish, i.e., $P^R_r = 0$ and $P^θ_θ = 0$. Symmetry consistent with this assumption necessitates that $r' = r/R$. Therefore, (3.38) and (3.47) can be manipulated to yield the axial stress constitutive equation

$$P = P_z = \frac{\dot{E}}{2} \left( \frac{\phi}{z} \right)^2 (D^E)^Z_2 = \frac{E(1-\xi)^2}{2z'} \left( \frac{z'}{\phi} \right)^4 \left[ \left( \frac{z'}{\phi} \right)^2 - 1 \right].$$

(3.52)

Axial force per unit reference area is simply denoted by $P$. The state dependent Young’s modulus $\dot{E}$ and Poisson’s ratio $\nu$ are

$$\dot{E} = \dot{C}_{33} - 2\nu \dot{C}_{13}, \quad \nu = (\dot{C}_{14} + \dot{C}_{13})/(\dot{C}_{11} + \dot{C}_{13}).$$

(3.53)

Poisson’s ratio is unaffected by damage/fracture according to (3.48). The shear modulus of the perfectly intact solid is $\mu = E/(2 + 2\nu)$. The effective Young’s modulus $\dot{E}$ is, consistent with (3.48),

$$\dot{E}(\xi) = (1 - \xi)^2 E, \quad d\dot{E}(\xi)/d\xi = -2E/(1 - \xi).$$

(3.54)

The elastic potential energy density $W$ and the thermodynamic driving force $Q$ become

$$W = \frac{1}{2} \dot{E}[(D^E)^Z_2] = \frac{P^z'}{2} \left( \frac{z'}{\phi} \right)^2 (D^E)^Z_2,$$

$$Q = 2\frac{\phi}{l^2} \xi - \frac{P^z'}{l} \left[ \frac{(z')^2}{\phi^2(1 - \xi)}(D^E)_Z + \frac{k}{3} \right].$$

(3.55)

The only significant equation in linear momentum balance (2.63) describes the axial direction, i.e., $a = z = 3$. Substituting from (3.8), this becomes

$$\frac{\partial P(Z, D)}{\partial Z} + \frac{\partial P(Z, D)}{\partial D} \frac{\partial D}{\partial Z} + \frac{3B'(D)}{2B(D)} \frac{\partial D}{\partial Z} \frac{dP}{dZ} + P\frac{k}{l} \frac{dD}{dZ} = 0.$$ 

(3.56)

The only significant equation in micro-momentum balance (2.64) becomes

$$\frac{\partial T(Z, D)}{\partial Z} + \frac{\partial T(Z, D)}{\partial D} + \frac{3B'(D)}{2B(D)} T \frac{\partial D}{\partial Z} \frac{dP}{dZ} + P\frac{k}{l} \frac{dD}{dZ} = 0.$$

(3.57)
Substituting from (3.28) and (3.55), and denoting by \( z = \varphi[Z, \xi(D)] \) the axial motion, these balance laws reduce as
\[
\frac{dP}{dZ} = -kP \frac{d\xi}{dZ}.
\]

(3.58)

Relations (3.58) are two coupled non-linear differential equations wherein dependent field variables \( P, (D^E)Z \), \( z' = \partial_Z \varphi \), \( \xi \), \( \phi \), and \( \psi \) all are ultimately functions of independent variable \( Z \) (i.e., position along the cylinder’s length). Immediately solving the first (stress) balance in (3.58),
\[
\frac{dP}{P} = -k\frac{d\xi}{\xi} \Rightarrow P = P_0 \exp(-k\xi),
\]

(3.59)

where \( P_0 \) is a constant axial stress corresponding to \( k = 0 \) and/or \( \xi = 0 \). Solution of the second balance law in (3.58) and determination of \( P_0 \) require specification of boundary conditions on the order parameter and the axial extension or its conjugate traction, as described in two subsequent boundary value problems.

3.4.1. Stress-free state

The first problem considers a stress-free state. In other words, axial stress vanishes: \( P = 0 \forall Z \in [0, L_0] \). Regarding the internal state or order parameter, complete rupture of the cylindrical bar is assigned at \( Z = 0 \), with the opposite end undamaged. Boundary conditions on the order parameter \( \xi(Z) \) are therefore
\[
\xi(0) = D(0)/l = 1, \quad \xi(L_0) = 0.
\]

(3.60)

When stresses vanish, elastic strain \( (D^E)Z \) vanishes at points where \( \xi < 1 \), and therefore strain energy \( W = 0 \) in (3.55). The second of governing equations (3.58), with \( W = 0 \) \( \Rightarrow \psi = f \), becomes the following non-linear second-order ordinary differential equation:
\[
\xi'' - \xi/l^2 + k[\xi']^2 - f/(\Upsilon l) = 0 \Rightarrow \xi'' = (\xi/l^2)(1 + k\xi).
\]

(3.61)

A transformation of variables \( \zeta = \xi' \) is prescribed. Then \( \xi'' = \zeta \cdot d\zeta/d\xi \). Invoking this transformation, (3.61) becomes the non-homogeneous first order differential equation and corresponding general solution
\[
\zeta d\xi = (\xi/l^2)(1 + k\xi)d\zeta \Rightarrow \zeta = \pm(\xi/l)\sqrt{1 + 2k\xi^2/3 + c_1/\xi^2}.
\]

(3.62)

For this particular problem, integration constant \( c_1 = 0 \), and the negative root is valid. The second of (3.62) is integrated to yield an implicit solution for \( \xi(Z) \), which in turn is evaluated via numerical quadrature
\[
d\xi = -(\xi/l)\sqrt{1 + 2k\xi^2/3}dZ \Rightarrow Z(\xi) = \int_1^\xi \frac{-1d\beta}{\sqrt{1 + 2k\beta^2/3}}.
\]

(3.63)
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The null stress or null elastic strain condition requires \( \phi(Z)/z'(Z) = 1 \forall \xi(Z) \neq 1 \), meaning that

\[
z'(Z) = \phi(Z) = \exp[(k/3)\xi(Z)] \forall Z \in (0, L_0]. \tag{3.64}
\]

The total free energy per unit circular cross-section of the bar is the line integral

\[
\Psi(\xi) = \Psi_F = \int_0^{L_0} \Upsilon[(\xi')^2l + \xi^2/l]dZ. \tag{3.65}
\]

The boundary condition on displacement of the undamaged end is assumed to be given: \( \phi(L_0, 0) = \phi_L \). Then the problem kinematics in (3.64) produce the axial deformation function for the cylinder:

\[
\phi(Z, D) = z(Z) = \int_0^Z \exp[(k/3)\xi(\Xi)]d\Xi + C_0. \tag{3.66}
\]

The integration constant \( C_0 = \phi(0, 1) = \phi_0 \) indicates any rigid translation of the bar from its failed end at \( Z = 0 \). This constant can be obtained from solution of the equation \( C_0 = \phi_L - \int_0^{L_0} \exp[(k/3)\xi(\Xi)]d\Xi \).

Profiles of the order parameter and displacement or deformation are shown in Fig. 1. The domain size is chosen as \( L_0 = 10l \), displacement boundary conditions are \( \phi_L = L_0 + l = 1.1L_0 \), and \( k \) is varied systematically over the range listed in Table 1: \( 0 \leq k \leq \ln(1.2) \). Specifically shown in Figs. 1(a) and 1(b) is order parameter \( \xi \) computed using (3.63); Fig. 1(b) is focused on behavior near the fractured end at \( Z = 0 \). Results for which \( k \neq 0 \) correspond to pseudo-Finsler geometry and Finsler kinematics, i.e., unique aspects of the present Finsler-geometric continuum mechanics theory. Results for \( k = 0 \) correspond to Riemannian geometry and classical continuum mechanics, analogous to those of a variational phase field theory in Clayton and Knap [2015a]. The magnitude of \( \xi \) decreases rapidly from its maximum at \( Z = 0 \) with increasing \( Z \), with such trends irrespective of \( k \). Influences of \( k \) on the profiles of \( \xi \) are nearly negligible for this problem. Profiles of axial motion \( \phi \), related to axial displacement \( \phi - Z \), are obtained from (3.66) and are reported in Fig. 1(c). The displacement jump at the failed end is \( (\phi_L - L_0)/L_0 = 0.1 \) for \( k = 0 \). Such a displacement jump at \( Z = 0 \) decreases with increasing \( k \) for other cases in the figure, since greater deformation is accommodated by inelastic deformation associated with void formation and growth. In other words, the contribution from \( \phi = \exp[(k/3)\xi] \) to the integral (3.66) increases with increasing \( k \) for small values of \( Z \).

The total energy per unit cross-sectional area of the cylinder is calculated using (3.65) for two different values of \( l/L_0 \). The results are listed in columns 2 and 3 of Table 2, normalized by intrinsic surface energy \( \Upsilon \). The total energy \( \Psi_F \) increases very slightly with increasing \( k \) in each column. A value of \( \Psi_F = \Upsilon \) corresponds to Griffith’s theory of perfectly brittle mode I fracture. As \( l/L_0 \) decreases, convergence towards the exact Griffith result is evident. Therefore, the present results verify that the Finsler model correctly predicts the fracture surface energy in a domain with a fully ruptured cross-section, regardless of the value of \( k \in [0, \ln(1.2)] \). Other
J. D. Clayton

(a) \( 0 \leq Z \leq L_0 \)

(b) \( 0 \leq Z \leq 0.1L_0 \)

(c) \( 0 \leq Z \leq 0.2L_0 \)

Fig. 1. Tensile rupture, stress-free solutions, \( l/L_0 = 0.1 \)

(a) \( \xi : 0 \leq Z \leq L_0 \)

(b) \( \xi : 0 \leq Z \leq 0.1L_0 \)

(c) \( \varphi : 0 \leq Z \leq 0.2L_0 \)

Table 2. Mg, stress-free solutions for \( l/L_0 = 0.1 \) and \( l/L_0 = 10^{-3} \); normalized total energy \( \Psi_F \) and critical displacement \( u_C \) and axial stress \( P_C \) for energetically favorable transition from homogeneous to localized solutions.

<table>
<thead>
<tr>
<th>Final ( k )</th>
<th>( F )</th>
<th>( F )</th>
<th>( u_C / L_0 \cdot 100 )</th>
<th>( P_C / E \cdot 100 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>ln (1.05)</td>
<td>1.009111</td>
<td>1.000000</td>
<td>6.2</td>
<td>4.6</td>
</tr>
<tr>
<td>ln (1.10)</td>
<td>1.009151</td>
<td>1.000004</td>
<td>6.4</td>
<td>4.5</td>
</tr>
<tr>
<td>ln (1.15)</td>
<td>1.009277</td>
<td>1.000151</td>
<td>6.7</td>
<td>4.3</td>
</tr>
<tr>
<td>ln (1.20)</td>
<td>1.009469</td>
<td>1.000335</td>
<td>6.9</td>
<td>4.2</td>
</tr>
</tbody>
</table>

Calculations prove that total energy does not vary significantly with increases in \( L_0 \) at fixed \( l \), since the order parameter and its gradient tend towards null values for \( Z \gg l \). Similar trends for other problems invoking slightly different theory, materials, and/or boundary conditions (e.g., shear fracture in metals, basal plane fracture in ceramics) have been reported in prior work [Clayton, 2016a,b,c].
3.4.2. Homogeneous deformation

The second boundary value problem is described as follows. The order parameter is prescribed as physically homogeneous over the cylindrical material domain. Physically, this corresponds to emergence of micro-fractures, and possibly voids, distributed uniformly over the length of the bar. For such homogeneous damage, \( \xi(Z) = 0 \forall Z \in [0, L_0] \Rightarrow \xi(0) = \xi(L_0) = \xi_H \). In Sec. 3.4.2, the notation \((-)_H\) is used to denote a quantity that is homogeneous over the domain. Particular boundary conditions on displacement are prescribed:

\[
\phi(0, D) = \phi_0 = 0, \quad \phi(L_0, D) = \phi_L. \tag{3.67}
\]

Denote the longitudinal Eulerian elastic strain, positive in tension, by \( a(Z) = (D^E)\frac{\xi}{Z} \) so that \( (F^E)\frac{\xi}{Z} = \sqrt{1/(1-2a)} \). Since \( \xi = \text{constant} \), linear momentum conservation (3.59) requires that \( a = a_H = \text{constant} \) for this boundary value problem, and that \( P = P_H \) is a constant tensile force per unit reference area. Relations (3.52), (3.58) and (3.59), with elastic modulus (3.53) and (3.54), then yield the following set of equations:

\[
P_H = P_0 \exp(-k\xi_H) = \frac{\dot{E}_H}{\dot{z}_H} \left( \frac{\phi_H}{\phi'} \right)^2 a_H = \text{constant}, \quad \dot{E}_H = E(1 - \xi_H)^2,
\]

\[
\phi_H = \exp \left( \frac{k\xi_H}{3} \right), \quad \dot{z}' = \frac{\phi_H}{\sqrt{1-2a_H}};
\]

\[
P_H \left[ \frac{z_H}{2(1-\xi_H)} \left( \frac{z_H}{\phi_H} \right)^2 a_H \right] - \frac{\gamma}{l} \xi_H = k \left[ \psi(a_H, \xi_H) - \frac{P_H z_H}{6} \right]. \tag{3.69}
\]

The motion is obtained by integrating (3.21) with \( (F^D)\frac{z}{Z} = \phi_H = \exp(k\xi_H/3) \) and \( z = \phi(Z, \xi_H) = \phi(Z) \):

\[
\phi(Z) = \int_0^Z z'(\xi) d\xi = \phi_0 + \frac{\phi_H}{\sqrt{1-2a_H}} Z, \tag{3.70}
\]

where a boundary condition in (3.67) has been applied. The other boundary condition requires \( \phi_L = (\phi_H/\sqrt{1-2a_H})L_0 \). Applying boundary conditions, (3.68) and (3.69) can be solved simultaneously for field \( \xi_H \), axial stress \( P_H \) and axial elastic strain \( a_H \). The total energy of the elastic domain with uniform damage is then calculated as

\[
\Psi(\phi_L, \xi_H) = \Psi_H = \int_0^{L_0} \left( \dot{E}_H a_H^2/2 + \gamma \xi_H^2/l \right) dZ
\]

\[
= [E(1 - \xi_H)^2 a_H^2/2 + \gamma \xi_H^2/l]L_0. \tag{3.71}
\]

An unusual case which is simultaneously both homogeneous and stress free—i.e., if a non-zero elastic modulus \( \dot{E} \) in (3.54) is in effect — requires from (3.67)–(3.70) that \( a_H = 0 \Rightarrow F^E = z_H = \phi_H \Rightarrow \phi_L = \exp(k\xi_H/3)L_0 \). In this situation, deformation accommodation occurs completely from porosity, since elastic strain vanishes. The
maximum allowable accommodation in this situation is $\exp(k/3)$, corresponding to the onset of complete rupture, at which point the any portion of the fully destroyed cylinder can undergo further deformation without consequence on (null) stress.

The order parameter, stress, and total energy are shown in Fig. 2: $\xi = \xi_H$, $P = P_H$, and $\Psi = \Psi_H$ versus applied axial stretch $\varphi_L$. These quantities are respectively obtained from (3.68), (3.69) and (3.71). A domain size of $L_0 = 10^{-3}$ is studied, and physical parameters for fracture of single crystals of Mg from Table 1 are invoked, with extension parallel to the crystallographic $c$-axis, i.e., normal to the basal (0001) plane. Results labeled “elastic” correspond to the non-linear elastic solution with null order parameter and thus no fractures: $\xi = 0 \forall Z \in [0, L_0]$. As expected, stress and energy are larger for the elastic results than for the remainder of those in which damage degrades the tensile modulus. The perfectly elastic results can be obtained by taking $\Upsilon / l \rightarrow \infty$ in the Finsler theory, such that $\xi_H \rightarrow 0$ is the trivial homogeneous hyperelastic solution. Setting the regularization length to zero severely penalizes finite values of $\xi_H$ in the energy functional (3.71) such that the

Fig. 2. Mg, tensile degradation, homogeneous damage, $l/L_0 = 10^{-3}$ (a) order parameter $\xi = D/l$ (b) normalized axial stress (c) normalized total energy.
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Table 3. Maximum stress $P_M$ and corresponding strain $\varepsilon_M$ under tensile loading along $c$-axis in Mg single crystal.

<table>
<thead>
<tr>
<th>Source</th>
<th>$P_M/E \cdot 100$</th>
<th>$\varepsilon_M \cdot 100$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Finsler theory, $k = 0$</td>
<td>5.6</td>
<td>12</td>
</tr>
<tr>
<td>$k = \ln(1.05)$</td>
<td>5.5</td>
<td>13</td>
</tr>
<tr>
<td>$k = \ln(1.10)$</td>
<td>5.4</td>
<td>14</td>
</tr>
<tr>
<td>$k = \ln(1.15)$</td>
<td>5.3</td>
<td>15</td>
</tr>
<tr>
<td>$k = \ln(1.20)$</td>
<td>5.2</td>
<td>16</td>
</tr>
<tr>
<td>MD simulation [Tang et al., 2010]</td>
<td>6.2</td>
<td>5</td>
</tr>
<tr>
<td>HQC simulation [Ponga et al., 2016]</td>
<td>4.3</td>
<td>17</td>
</tr>
<tr>
<td>Spall experiment [Kanel et al., 2014]</td>
<td>2.5</td>
<td>—</td>
</tr>
</tbody>
</table>

only homogeneous solution is the trivial one with $\xi_H = 0$. This in turn eliminates any Finsler contribution to the deformation gradient in (3.21); i.e., $\phi \to 1$ as $\xi \to 0$.

For fixed $k$, $\xi$ increases monotonically with increasing displacement (Fig. 2(a)), axial stress $P$ increases to a maximum and then decreases (Fig. 2(b)), and energy $\Psi$ increases monotonically (Fig. 2(c)). As $k$ increases, the total energy $\Psi_H$ tends to decrease at any given applied displacement $\varphi_L$. Peak (i.e., maximum) axial stress $P_M$ and corresponding axial strain $\varepsilon_C = \varphi_L/L_0 - 1$ are listed in Table 3. Peak axial stress decreases and applied displacement at which peak stress is attained increases with increasing $k$, implying a decrease in strength and stability, but increase in ductility, of the material commensurate with microscopic dilatation represented mathematically by $k > 0$.

From Table 3, predicted maximum stresses from the Finsler model are $P_M \approx \frac{E}{20}$, around half of the theoretical tensile strength $\tau = \frac{E}{10}$ [Gilman, 1960]. These values are of comparable magnitude to those calculated using molecular dynamics (MD) [Tang et al., 2010] and hot quasi-continuum (HQC) simulations [Ponga et al., 2016], also listed in Table 3. Predicted peak strain at maximum load is closer to the latter [Ponga et al., 2016], wherein a decrease in peak stress was observed with increasing void diameter, in qualitative agreement with the present results that demonstrate decreased peak stress with increasing porosity quantified by $\chi_H = 1 - \exp(-k\xi_H)$. The spall strength from shock experiments on Mg single crystals is somewhat smaller than the peak strengths reported from the present study and the atomic models; reasons for discrepancies discussed in Ponga et al. [2016] include the presence of initial flaws or impurities in the material not considered in the models.

Further validation of the present theory is reflected by comparison with trends of atomic simulations of tensile fracture of cubic single crystalline metals [Komanduri et al., 2001]. These simulations report fracture mechanisms of void nucleation, growth, and associated dilatation, resulting in load-displacement curves qualitatively matching Fig. 2(b): a gradual stress drop with increasing axial strain after peak stresses are attained.

Relative stability of homogeneous versus localized stress-free solutions of Sec. 3.4.1 is considered next. A possible transition from a homogeneous deformation and damage state of the sort modeled here in Sec. 3.4.2 to a state with localized
fracture is energetically favorable at an applied deformation \( \varphi_L \geq L_0 + u_C \), with \( u_C \) the applied displacement when \( \Psi_H \) of (3.71) equals or exceeds \( \Psi_F \) of (3.65). This transition occurs when the homogeneous solution becomes relatively unstable. Predicted values of displacement \( u_C \) and commensurate stress \( P_C \) at the onset of instability are given in the rightmost two columns of Table 2. The axial strain \( u_C/L_0 \) is on the order of 7% and stress on the order of 5% of the initial Young’s modulus, the former increasing with \( k \) and the latter decreasing with \( k \). An increase in \( k \) correlates with increased ductility but decreased strength at instability.

The current theoretical framework and problem solutions do not directly consider dislocation-mediated plasticity or twinning; either of these inelastic deformation mechanisms are likely to occur in Mg, depending on sample size and boundary conditions. The present application of the model considers very small volumes of material, comparable in size to those addressed in atomic or nanoscale simulations [Tang et al., 2010; Ponga et al., 2016]. In these cases, dislocations and twin nucleation mechanisms become prominent only at applied displacements around or exceeding the those corresponding to peak stresses. Subsequently, load drops and rupture of the sample occur, similarly to those predicted by the present Finsler theory. Furthermore, localized plastic deformation, though not modeled explicitly here, could be interpreted to occur near voids for cases that describe ductile fracture modes with \( k > 0 \). For a more complete description that may be pursued in subsequent work, kinematics of slip and deformation twinning should be incorporated within the multiplicative deformation gradient decomposition, e.g., following prior theoretical developments for metallic and ceramic crystals [Clayton and McDowell, 2003; Clayton, 2009a]. Function \( \alpha \) in (3.19) and (3.21) is arbitrary for the specific boundary conditions considered in Secs. 3.4.1 and 3.4.2: this function does not explicitly affect any of the governing equilibrium equations or their solutions. Physically, this implies that radial expansion (\( \alpha > 1 \)) or contraction (i.e., necking, \( \alpha < 1 \)) are permissible at location \( Z \) for \( D(Z) > 0 \).

3.4.3. Summary

Key points to be noted from analysis of the present results for tensile fracture of Mg single crystals are as follows:

- The Finsler model of continuum physics is able to replicate the Griffith energy with suitable accuracy for small regularization length \( l \leq 0.1L_0 \), with physically valid values of dilatation parameter \( k \in [0, \ln(1.2)] \) having a nearly negligible effect on total energy;
- For a homogeneously deformed bar with uniform micro-fractures and possible voids, increases in \( k \) result in more ductile fracture behavior: lower maximum stress and higher axial strain at which such peak stress occurs;
- Maximum stresses under tensile loading are predicted to be on the order of half the theoretical tensile strength, consistent with predictions of MD or
quasi-continuum models [Tang et al., 2010; Ponga et al., 2016] of single crystalline Mg with voids. Stresses corresponding to a transition from homogeneous to localized deformation are approximately 80% of the aforementioned maximums, i.e., on the order of 4% of the initial elastic modulus for c-axis extension.

4. Application: Shear Localization and Failure of Boron Carbide

Finsler-geometric continuum mechanics with multiplicative kinematics is now applied to a description of shear localization and mode II fracture in ceramic single crystals. The problem considered in Sec. 4 addresses amorphization and failure of anisotropic boron carbide (B₄C). The Finsler metric accounts for local density increase (i.e., local volume decrease) commensurate with the stress-induced phase transformation from a trigonal crystal to glassy phase [Taylor et al., 2012; Clayton, 2012a, 2013a, 2014c; Taylor, 2015; An and Goddard, 2015; Clayton and Tonge, 2015]. In the absence of this density change, the treatment becomes that for perfect mode II cleavage along a weak plane in the crystal. The boundary value problem involves simple shearing of a non-linear elastic slab. Particular solutions for the anisotropic crystal address shearing on a prismatic plane in a direction of basal slip.

4.1. Geometry and deformation

The material body is an elastic slab of length $L_0$ and infinite width and thickness. In three dimensions, the material manifold is specified as $\{\mathcal{M}: X^1 \in [0, L_0], |X^2| \in \infty, |X^3| \in \infty\}$. Plane strain conditions are imposed for the $X^3$-direction. The internal state vector is chosen as $\{D^A\} \to \{0, D^2, 0\}$. By construction, fields vary only with $X = X^1$ and $D = D^2$, and $D^1$ and $D^3$ are superfluous. A Cartesian coordinate system is used for $\{X\}$, so the metric tensor $G$ contains no explicit dependence on $X$.

The following reductions of definitions and identities of Sec. 2.1 hold, consistent with the above protocols, and where an isotropic metric tensor is prescribed:

$$\{X,Y,Z\} = \{X^1, X^2, X^3\}, \quad D = D^2 = D(X);$$  

$$G(D) = G(D) = B(D)1 = \begin{bmatrix} B(D) & 0 & 0 \\ 0 & B(D) & 0 \\ 0 & 0 & B(D) \end{bmatrix};$$  

$$G_{AB} = B \delta_{AB}; \quad G = \det G = B^3(D);$$  

$$\gamma_{ABC} = \frac{1}{2}(\partial_A G_{BC} + \partial_B G_{AC} - \partial_C G_{AB}) = 0, \quad G^A = \frac{1}{2} \gamma^A_{BC} D^B D^C = 0,$$  

$$N^A_B = \bar{\partial}_B G^A = 0 \Rightarrow \delta_A(\cdot) = \partial_A(\cdot);$$  

$$C_{121} = C_{211} = C_{222} = C_{233} = C_{323} = B'/2, \quad C_{112} = C_{332} = -B'/2.$$  

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Here, $B'(D) = dB(D)/dD$, and all other covariant components $C_{ABC}$ of Cartan’s tensor vanish identically. The Cartesian metric is scaled isotropically by the scalar function $B$, an example of a Weyl-type conformal transformation [Clayton, 2016a,c; Weyl, 1952]. The reference configuration space is locally Minkowskian [Minguzzi, 2014].

The Chern–Rund connection is used. The horizontal covariant derivative of the metric vanishes with respect to this connection [e.g., leading to $(\sqrt{G})_{A} = 0$]; thus, use of Rund’s version of Stokes’ theorem in (2.15) to derive Euler–Lagrange equations is acceptable. Vertical connection coefficients ($V^A_{BC}, V^a_{bc}, Y^A_{BC}$, and $Y^a_{bc}$) vanish by definition, which simplifies calculations. The Chern–Rund connection has also been effectively used in prior work on Finsler-geometric mechanics [Saczuk, 1996; Stumpf and Saczuk, 2000; Clayton, 2016a,b,c]. Considering the vanishing non-linear connection coefficients from (4.3),

$$H^A_{BC} = K^A_{BC} = \Gamma^A_{BC}$$

$$= \frac{1}{2} G^{ABCD} (\delta_{C} G_{BD} + \delta_{B} G_{CD} - \delta_{D} G_{BC}) = 0; \quad V^A_{BC} = Y^A_{BC} = 0. \quad (4.5)$$

For the spatial configuration of the slab, with deformed material manifold $\{m : x^1 \in [0, L], |x^2| \in \infty, |x^3| \in \infty\}$, where $L$ is the deformed length of the domain, the coordinates and metric are of the analogous forms used for the reference state. Following the notation conventions of lower case font for the current configuration, this implies

$$\{x, y, z\} = \{x^1, x^2, x^3\}, \quad d = d^2 = d(x); \quad g_{ab} = g_{\bar{a}\bar{b}}, \quad g(d) = \bar{g}(d) = b(\bar{d})1,$$

$$g_{\bar{a}\bar{b}} = b \delta_{\bar{a}\bar{b}}, \quad g(d) = b^3(d);$$

$$\gamma_{\bar{a}\bar{b}\bar{c}} = \frac{1}{2} (\partial_{\bar{d}} g_{\bar{b}\bar{c}} + \partial_{\bar{d}} g_{\bar{c}\bar{a}} - \partial_{\bar{d}} g_{\bar{a}\bar{b}}) = 0, \quad g^{\bar{a}} = \frac{1}{2} \gamma_{\bar{b}\bar{c}} d^\bar{d} d^\bar{c} = 0,$$

$$n_{\bar{a}} = \partial_{\bar{d}} g^\bar{a} = 0 \Rightarrow \delta_{\bar{a}}(\cdot) = \partial_{\bar{a}}(\cdot);$$

$$C_{121} = C_{211} = C_{222} = C_{233} = C_{323} = b'/2, \quad C_{112} = C_{332} = -b'/2 \quad (4.8)$$

with $b'(d) = db(d)/d\bar{d}$. The spatial configuration space is also locally Minkowskian. Invoking the Chern–Rund connection with vanishing non-linear connection coefficients from (4.7),

$$H^a_{bc} = K^a_{bc} = \Gamma^a_{bc} = \frac{1}{2} g^{\bar{a}d}(\delta_{\bar{d}} g_{\bar{c}\bar{d}} + \delta_{\bar{d}} g_{\bar{d}\bar{c}} - \delta_{\bar{d}} g_{\bar{c}\bar{d}}) = 0; \quad V^a_{bc} = Y^a_{bc} = 0. \quad (4.9)$$

Summarizing, non-linear connection coefficients ($N^a_B$ and $n^a_B$) vanish identically in both configurations in their preferred coordinate systems, as do Chern–Rund coefficients ($\Gamma^a_{BC}$ and $\Gamma^a_{bc}$). Cartan’s coefficients ($C^A_{BC}$ and $C^a_{bc}$) do not necessarily vanish.

Motions, deformations, and director gradients defined in Sec. 2.1.3 reduce as discussed next under simple shear. Let $\varphi = \nu + Y$ and $\gamma$ denote respective deformation
and strain in the shearing ($Y$) direction:

\[ x = X, \quad y = \varphi(X,Y,D) = Y + v(X,D), \]
\[ z = Z; \quad d = \theta(X,D); \quad D = D(X); \tag{4.10} \]

\[
F(X,D) = \begin{bmatrix}
\frac{\partial x(X)}{\partial X} & \frac{\partial x(X)}{\partial Y} & \frac{\partial x(X)}{\partial Z} \\
\frac{\partial \varphi(X,Y,D)}{\partial X} & \frac{\partial \varphi(X,Y,D)}{\partial Y} & \frac{\partial \varphi(X,Y,D)}{\partial Z} \\
\frac{\partial z(Z)}{\partial X} & \frac{\partial z(Z)}{\partial Y} & \frac{\partial z(Z)}{\partial Z}
\end{bmatrix}
\]
\[ = \begin{bmatrix}
1 & 0 & 0 \\
0 & 0 & 1
\end{bmatrix}
\gamma(X,D) = \begin{bmatrix}
1 & 0 \end{bmatrix}; \tag{4.11} \]

\[
J(X,D) = \sqrt{g|d(X,D)|/G(D)F_1^1F_2^2F_3^3}
\]
\[ = [g(d)/G(D)]^{1/2} = [b(d)/B(D)]^{3/2}; \tag{4.12} \]
\[ D_2^2 = \partial_1 D - N_2^2 + K_1^2 D = \partial D/\partial X = D'. \tag{4.13} \]

The director component, i.e., internal state variable $D$, is physically associated with a slip discontinuity or slipped displacement. For general applications to the present loading protocol, $D$ could describe a shear band in a metal or geomaterial [Li et al., 2001; Wright, 2002; Sun and Mota, 2014], a stacking fault in a crystal lattice [Clayton, 2011], a sliding grain boundary in a polycrystal [Fang and Zhang, 2016], or a mode II crack in a brittle solid [Clayton and Knap, 2015a]. Here, the latter situation applies, where loss of shear strength is associated with non-zero values of $D$.

Similarly to the treatment in Sec. 3.1, introduced next are a regularization constant $l$ with dimensions of length and a normalized order parameter $\xi \in [0,1]$: \[ \xi = D/l, \quad \xi' = D'/l. \tag{4.14} \]

The scalar $l$ is identified as the value of shear slip-displacement $D$ at which the slab supports no shear stress, and is assumed to be a material property. Letting $k$ denote a constant depending on the material, a more specific form of the Minkowski metric in (4.2) is now invoked:

\[
G(D) = B(D)1 = \exp[2kD/(3l)]1; \tag{4.15}
\]
\[
G(\xi) = B^3(\xi) = \exp(2k\xi) \Rightarrow 3B'/2B = k/l. \]

For later applications, the second component of the trace of Cartan's tensor of (4.4) is

\[
C_{2A}^A = G^{AB}C_{2AB} = G^{11}C_{211} + G^{22}C_{222} + G^{33}C_{233} = 3B/(2B) = k/l. \tag{4.16} \]

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The length of a referential line element in (2.11) and the corresponding volume form in (2.12) become

\[ |d\mathbf{X}|^2 = \exp[2kD/(3l)](dX \cdot dX + dY \cdot dY + dZ \cdot dZ), \]
\[ d\Omega = \exp(kD/l)dX \wedge dY \wedge dZ. \]

(4.17)

For \( \xi > 0 \), expansion occurs when \( k > 0 \) and contraction when \( k < 0 \). In general applications, physical justifications for this choice of generalized non-homogeneous pseudo-Finsler metric may include

- Shear fractures may result in dilatation due to surface roughness [Curran et al., 1993; Rist, 1997];
- Full and/or partial dislocations commensurate with shear bands or stacking faults may result in local dilatation due to non-linear elastic and core effects [Holder and Granato, 1969];
- Voids may nucleate and open within shear bands in ductile solids [Korbel et al., 1984];
- Point defects induce local volume changes [Eshelby, 1954; Clayton, 2009b, 2010];
- Shear instability may accompany a local disordering of the lattice and amorphization, leading to volumetric expansion [Delogu, 2004] or contraction [Yan et al., 2009].

The latter/final above justification is true for the present application of localization in \( B_4C \).

For simplicity, as also chosen in Sec. 3, the spatial and referential state variables are chosen to coincide in (4.10):

\[ d(X,D) = \theta(X,D) = D(X) = l \xi(X). \]

(4.18)

An analogous form of the spatial metric of (4.15) is

\[ g(d) = b(d)1 = \exp[2kD/(3l)]1; \quad g(\xi) = b^3(\xi) = \exp(2k\xi) \Rightarrow 3b^3/(2b) = k/l. \]

(4.19)

This is a Weyl transformation or Weyl rescaling of the Cartesian metric \( \delta_{ab} \). With these choices of metrics, (4.12) reduces to \( J = 1 \), i.e., volume is conserved upon simple shearing as is the case in classical continuum theory.

Now invoking the multiplicative description of (2.37) with spherical inelastic kinematics of Sec. 2.1.5, the inelastic portion contains structural, i.e., \( D \)-dependent, terms. The total deformation gradient in Cartesian coordinates is

\[ \mathbf{F}(X,D) = \begin{bmatrix} 1 & 0 & 0 \\ \gamma(X,D) & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \mathbf{F}^E(X) \mathbf{F}^D[D(X)] \]
Finsler-geometric continuum mechanics

\[
\begin{bmatrix}
(F_E^X)_X(X) & 0 & 0 \\
(F_E^X)_Y(X) & (F_E^Y)_X(X) & 0 \\
0 & 0 & (F_E^Z)_X(X)
\end{bmatrix}
\times
\begin{bmatrix}
\phi[D(X)] & 0 & 0 \\
0 & \phi[D(X)] & 0 \\
0 & 0 & \phi[D(X)]
\end{bmatrix}.
\] (4.20)

The inelastic term is related to the inelastic volume change:

\[
\phi[D(X)] = \{J^D[D(X)]\}^{1/3}.
\] (4.21)

The elastic deformation gradient and elastic shear strain are respectively

\[
F_E(X) = \frac{1}{\phi(X)} \begin{bmatrix} 1 & 0 & 0 \\ \gamma(X,D) & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (F_E^X)_1 = (F_E^Y)_X = \gamma/\phi.
\] (4.22)

Canonical relations such as those in (3.32) and (3.33) apply here as well, since the inelastic deformation gradient and metric tensor are of the same forms as those invoked in Sec. 3.1. The symmetric elastic Eulerian material strain tensor \(D_E\) is used for the constitutive model of boron carbide single crystals outlined in Sec. 4.2. As noted already in Sec. 3.1, this tensor proves accurate for modeling the high pressure response of many crystalline solids [Clayton, 2013b, 2014d]. In Cartesian coordinate charts,

\[
D_E = \frac{1}{2}[1 - (F_E)^{-1}(F_E)^{-T}], \quad (D_E)_{\alpha\beta} = \frac{1}{2}[\delta_{\alpha\beta} - (F_E^{-1})_{\alpha a}(F_E^{-1})_{a\beta}].
\] (4.23)

For the form of elastic deformation in (4.22), \(D_E\) contains five non-zero terms, only two of which are unequal:

\[
D_{XX}^E = D_{YY}^E = D_{ZZ}^E = \frac{1 - \phi^2}{2}, \quad D_{XY}^E = D_{YX}^E = \frac{\gamma \phi^2}{2}.
\] (4.24)

4.2. Balance equations

The free energy per unit reference volume \(\psi\) in (2.57) is again additively split into an elastic strain energy per unit reference volume \(W\) and a structure or phase dependent energy per unit reference volume \(f\), following (2.67). The following sum of quadratic forms is imposed:

\[
\psi(F_A^a, D^A, D_A^A, G_{AB}) = W[(D_E)^{\alpha\beta} D^A] + f(D^A, D_A^A);
\] (4.25)

\[
W = \frac{1}{2}C_{\alpha\beta\gamma\delta}(D)(D_E)^{\alpha\beta}(D_E)^{\gamma\delta},
\]

\[
f = \frac{\gamma}{l} |D|^2 + \frac{\gamma}{l} |\nabla D|^2.
\] (4.26)
Components of the second-order elasticity tensor \( \hat{C}^{\alpha\beta\gamma\delta} \) depend on the phase of the solid: crystalline or glass, with the glass here having fully degraded moduli when \( \xi = 1 \) [Clayton, 2014b]. The surface energy per unit reference area is the intrinsic material constant \( \Upsilon \). Now considering the kinematic and functional conditions (2.37) and (2.38), in conjunction with (4.13) where \( D(X) = l_\xi(X) \), terms affecting strain energy become

\[
(F^E)_\alpha^\gamma[F, F^D(\xi)] = F^A_\alpha[X, \xi(X)][(F^{D^{-1}})^A_\alpha][\xi(X)];
\]

\[
\hat{C}^{\alpha\beta\gamma\delta} = \hat{C}^{\alpha\beta\gamma\delta}(\xi), \quad f = \Upsilon[\xi^2/f^2 + (\xi')^2].
\]

(4.27)

More specific forms of thermodynamic forces for Finsler continuum mechanics given in (2.69) and (2.73) at a fixed material point \( X \) are then derived as follows:

\[
P_a^A = \frac{\partial \psi}{\partial F^A_a} = (F^{D^{-1}})^A_\alpha \frac{\partial W}{\partial (F^E)_{\alpha}^\gamma} = (F^{D^{-1}})^A_\alpha \frac{\partial W}{\partial (F^E)_{\beta}^\gamma} \frac{\partial (F^E)^{\gamma}_{\beta}}{\partial (F^E)_{\alpha}^\gamma} \frac{\partial (F^E)_{\beta}^\gamma}{\partial (F^E)^{\gamma}_{\beta}} = \frac{1}{\phi} \delta^A_\gamma (F^{E^{-1}})_\gamma^\alpha (F^{E^{-1}})^\gamma_\beta \hat{S}^{\beta\gamma};
\]

(4.28)

\[
Q = Q_2 = Q_Y = \frac{\partial \psi}{\partial D} = \frac{1}{\Upsilon} \left[ \frac{\partial W}{\partial \xi} - P^A_a (F^E)^{\alpha}_a \frac{\partial (F^E)^{\gamma}_{\alpha}}{\partial \xi} + \frac{\partial f}{\partial \xi} \right] = \frac{1}{\Upsilon} \left[ \frac{1}{2} \frac{\partial \hat{C}^{\alpha\beta\gamma\delta}}{\partial \xi} (F^E)_{\alpha\beta} (F^E)_{\gamma\delta} - \frac{k_F}{\phi} P^A_a (F^E)^{\gamma}_{\alpha} \delta^\alpha_{\gamma} + 2 \frac{T}{\Upsilon} \right];
\]

(4.29)

\[
T = Z^X_1 = Z^1 = \frac{\partial \psi}{\partial D^1} = \frac{1}{\Upsilon} \frac{\partial f}{\partial \xi} = 2 \Upsilon \xi'.
\]

(4.30)

In (4.28) the conjugate stress \( \hat{S} = \partial W/\partial D^E \) is analogous to that in (3.45).

For the present problem, now consider the Cartesian geometry and simple shearing kinematics of Sec. 4.1. Boron carbide single crystals have rhombohedral, i.e., trigonal symmetry. The current application assigns the \( XY \)-plane as the basal plane, i.e., \((0001)\) in hexagonal Miller–Bravais indices. For shearing of a prismatic plane in the direction of a basal plane lattice vector, i.e., shearing of type \( \langle 12\overline{1}0 \rangle \{10\overline{1}0 \} \), relevant elastic coefficients in Voigt notation are \( \hat{C}_{11} = \hat{C}_{22} = \hat{C}_{33}, \hat{C}_{12} = \hat{C}_{13} = \hat{C}_{23}, \) and \( \hat{C}_{66} = \frac{1}{2} (\hat{C}_{11} - \hat{C}_{12}) \). More general crystal orientations would require consideration of \( \hat{C}_{14} = -\hat{C}_{24} = \hat{C}_{56} \). The strain energy in (4.25) and (4.26) becomes, for the potentially non-zero elastic strain components in (4.24),

\[
W = W[(D^E)_{XX}, (D^E)_{YY}, (D^E)_{ZZ}, (D^E)_{XY}, \xi] = \frac{1}{2} \left[ \hat{C}_{11}[(D^E)_{XX}]^2 + \hat{C}_{11}[(D^E)_{YY}]^2 + \hat{C}_{33}[(D^E)_{ZZ}]^2 \right] + 2 \hat{C}_{12} (D^E)_{XX} (D^E)_{YY} + \hat{C}_{13} (D^E)_{XX} (D^E)_{ZZ} + \hat{C}_{13} (D^E)_{XY} (D^E)_{ZZ} + 4 \hat{C}_{66} [(D^E)_{XY}]^2.
\]

(4.31)
Structure-dependent variables \( \hat{C}_{ij} = \hat{C}_{ij}(\xi) \) are the appropriate second-order elastic coefficients; in the absence of phase transformation and fracture, these reduce to elastic constants of the perfect crystal \( C_{ij} \) to be defined in Sec. 4.3 for boron carbide. Identically to the theory of Sec. 3.2, the elastic coefficients degrade quadratically with increases in the order parameter, such that (3.48) holds. Thus, when complete strength loss ensues, locally \( \xi \to 1 \) so that \( \hat{C}_{ij}(1-\xi)^2 \to 0 \).

Five possibly non-zero stress components emerge from (4.28) and (4.31):

\[
\begin{align*}
P_1^1 &= P^X_x = \phi^2(\hat{S}^{XX} - \gamma \hat{S}^{XY}), \\
P_2^2 &= P^Y_y = \phi^2(\hat{S}^{YY} + \gamma^2 \hat{S}^{XX} - 2\gamma \hat{S}^{XY}), \\
P_3^3 &= P^Z_z = \phi^2 \hat{S}^{ZZ}, \\
P_2^1 &= P^Y_x = \phi^2(\hat{S}^{XY} - \gamma \hat{S}^{XX}) - \gamma P^X_x. \\
\end{align*}
\]

(4.32)

Components of the symmetric elastic stress tensor \( \hat{S} \) are

\[
\begin{align*}
\hat{S}^{XX} &= \hat{S}^{YY} = \frac{1}{2}(\hat{C}_{11} + \hat{C}_{12} + \hat{C}_{13})(1-\phi^2), \\
\hat{S}^{ZZ} &= \frac{1}{2}(\hat{C}_{33} + 2\hat{C}_{13})(1-\phi^2), \\
\hat{S}^{XY} &= \frac{1}{2}(\hat{C}_{11} - \hat{C}_{12})\phi^2\gamma.
\end{align*}
\]

(4.33)

Let \( P \) and \( p \) denote the shear stress and reference pressure, defined as

\[
\begin{align*}
P &= P_2^1, \\
p &= \frac{1}{3}P^A_a \delta^\alpha_A = -\frac{1}{3}(P_1^1 + P_2^2 + P_3^3).
\end{align*}
\]

(4.34)

Then the conjugate thermodynamic force to \( D = \ell \xi \) in (4.29) is

\[
Q = -\frac{1}{T} \left[ \frac{1}{1-\xi} C^{\alpha\beta\gamma\delta}_{,\gamma}(D^E)_{\alpha\beta}(D^E)_{,\gamma\delta} + \frac{k}{3}(P \gamma - 3p) - 2 \frac{\tau}{T} \xi \right].
\]

(4.35)

### 4.3. Material characteristics

Boron carbide (B\(_4\)C) is the particular material for which the theory of Secs. 4.1 and 4.2 is applied. In its ambient solid state, boron carbide is a low density crystalline ceramic of high hardness and elastic stiffness, and with nominally low ductility. Its crystal structure is rhombohedral, i.e., trigonal. Representative material parameters with supporting references are listed in Table 4; a value is obtained from the source given in the row above if no reference is listed.

Following prior phase field analysis [Clayton, 2014c], the elastic shear modulus \( \mu = \hat{C}_{66} \) degrades completely upon solid-state localization, consistent with (3.48) and [Clayton, 2016b]. The regularization length \( \ell \) and intrinsic surface energy are chosen to have magnitudes corresponding to those for fracture since failure accompanies amorphization in experiments and since widths of amorphous zones observed experimentally are on the order of a nanometer [Yan et al., 2009; Grady, 2011], similar in magnitude to the fracture process zone size. In particular, \( \ell \) is computed via (3.51), where here \( \tau = \mu/(2\pi) \) is the theoretical shear strength [Clayton, 2011]. The ratio of mass density of the crystalline phase to that of the amorphous phase is
Table 4. Physical properties of boron carbide.

<table>
<thead>
<tr>
<th>Property (Units)</th>
<th>Value</th>
<th>Description</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}$ (GPa)</td>
<td>543</td>
<td>Second-order elastic constant</td>
<td>Clayton [2012b]</td>
</tr>
<tr>
<td>$C_{12}$ (GPa)</td>
<td>131</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_{13}$ (GPa)</td>
<td>64</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_{14}$ (GPa)</td>
<td>−18</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_{33}$ (GPa)</td>
<td>535</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_{44}$ (GPa)</td>
<td>165</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\mu$ (GPa)</td>
<td>206</td>
<td>Planar shear modulus</td>
<td>Eq. (4.36)</td>
</tr>
<tr>
<td>$c, a$ (nm)</td>
<td>1.21, 0.56</td>
<td>Lattice parameters</td>
<td>Beaudet et al. [2015]</td>
</tr>
<tr>
<td>$\exp(k)$</td>
<td>0.96</td>
<td>Volume reduction (amorphization)</td>
<td>Clayton [2014c]; An and Goddard [2015] and Yan et al. [2009]</td>
</tr>
<tr>
<td>$l$ (nm)</td>
<td>0.97</td>
<td>Regularization length</td>
<td>Eq. (3.51)</td>
</tr>
</tbody>
</table>

used to quantify $k$; this value depends on the composition and structure of the glass [Fanchini et al., 2006]. As in Clayton [2014c], corresponding to a 4% volume reduction (mass density increase) upon structure collapse commensurate with complete amorphization [Taylor, 2015; An and Goddard, 2015; Yan et al., 2009], prescribed here is $\exp(k) = 0.96$. This value is determined for the Finsler-geometric theory via consideration of (4.17) at $\xi = 1$. In summary, the present application, similarly to the prior one in Sec. 3, does not ask the modeler to define or fit any new parameters, implying that forthcoming outcomes are considered fully predictive.

4.4. Solutions and interpretations

The problem of simple shearing on prismatic planes in a boron carbide single crystal is now addressed. The same solutions would apply for a slab of a polycrystalline material with isotropic symmetry upon substitution of the isotropic elastic constants. Recall from (4.34) that the shearing force per unit reference area is simply denoted by $P$, and that pressure, negative in tension, corresponding to the trace of the first Piola-Kirchhoff stress is denoted by $p$. The state dependent shear modulus $\hat{\mu}$ for the present loading protocol is

$$\hat{\mu} = (1 - \xi)^2 \mu = (1 - \xi)^2 C_{66} = \frac{1}{2} (1 - \xi)^2 (C_{11} - C_{12}). \quad (4.36)$$

The other elastic coefficients degrade with solid-state amorphization in the same fashion. The elastic potential energy density $W$ and the thermodynamic driving force $Q$ are given in (4.31) and (4.35). The only significant equation in linear momentum balance (2.63) describes the shearing direction, i.e., $a = y = 2$. Noting that $\partial Y / \partial y (X) = 0$, and substituting from (4.16), this balance equation becomes

$$\frac{\partial P(X, D)}{\partial X} + \frac{\partial P(X, D)}{\partial D} \frac{\partial D}{\partial X} + \frac{3B'(D)}{2B(D)} P \frac{\partial D}{\partial X} = \frac{dP}{dX} + \frac{P k}{T} \frac{dD}{dX} = 0. \quad (4.37)$$
The other two macroscopic linear momentum balance equations simply require that normal stress components \( P^X \) and \( P^Z \) are constant with respect to \( X \) and \( Z \), respectively, the latter condition consistent with the assumed \( Z \) independence of solution fields. The only significant equation in micro-momentum balance (2.64) becomes

\[
\frac{\partial T(X,D)}{\partial X} + \left[ \frac{\partial T(X,D)}{\partial D} + \frac{3B'(D)}{2B(D)}T + P\frac{\partial^2 y(X,D)}{\partial D^2} \right] \frac{\partial D}{\partial X} - \frac{3B'(D)}{B(D)}\psi(X,D) = Q(X, D).
\]

(4.38)

Substituting from (4.35) and denoting by \( y = Y + v[X, \xi(D)] \) the shearing motion, these balance laws become

\[
\frac{dP}{dX} = -kP \frac{d\xi}{dX} \left[ (1 - \xi)C^{\alpha\beta\gamma\delta}(D^E)_{\alpha\beta}(D^E)_{\gamma\delta} + P\frac{\partial^2 \psi}{\partial \xi^2} \right] + 2\Upsilon l\xi'' - 2\frac{\Upsilon}{l} \xi = 2k \left[ \psi - \Upsilon l(\xi')^2 - \frac{P\gamma - 3p}{6} \right].
\]

(4.39)

Relations (4.39) are two coupled non-linear differential equations wherein dependent field variables \( P, \ (D^E)_{\alpha\beta}, \ v, \ \xi, \) and \( \psi \) all are ultimately functions of independent variable \( X \) (i.e., in-plane position along the slab). The stress balance in (4.39) has the solution

\[
\frac{dP}{dX} = -kP \frac{d\xi}{dX} \Rightarrow P = P_0 \exp(-k\xi),
\]

(4.40)

where \( P_0 \) is a constant shear stress corresponding to \( k = 0 \) and/or \( \xi = 0 \). Solution of the micro-momentum balance in (4.39) and the value of \( P_0 \) depend on boundary conditions for the state variable or order parameter and the shearing deformation or its conjugate traction, as described for two subsequent problems.

4.4.1. Stress-free state

The first problem addresses a stress-free state. Shear stress vanishes: \( P = 0 \forall X \in [0, L_0] \). Other components of stress in (4.32) likewise vanish, as does the strain energy density \( W \). For the internal state or order parameter, complete shear failure of the slab is assigned at \( X = 0 \), with the opposite end at \( X = L_0 \) pristine. Boundary conditions on the order parameter \( \xi(X) \) are

\[
\xi(0) = D(0)/l = 1, \quad \xi(L_0) = 0.
\]

(4.41)

The second of governing equations (4.39), with \( W = 0 \Rightarrow \psi = f \), degenerates to the following non-linear second-order ordinary differential equation:

\[
\xi'' - \xi/l^2 + k[(\xi')^2 - f/(\Upsilon l)] = 0 \Rightarrow \xi'' = (\xi/l^2)(1 + k\xi).
\]

(4.42)

Replacing \( Z \) with \( X \), this is identical in form to the stress-free governing equation studied already in Sec. 3.4.1 for Mg. The solution procedure is identical, meaning
that (3.62) and (3.63) are invoked here as well. The total free energy per cross-section of the slab is the line integral

$$
\Psi(\xi) = \Psi_F = \int_0^{L_0} Y[(\xi')^2 l + \xi^2/l] dX.
$$

The boundary condition on displacement of the undamaged end is assumed to be given: \(v(L_0,0) = v_L\). Then the deformation function for the slab becomes

$$
v(X,D) = y(X,D) - Y = \int_X^0 \gamma(X) d\Xi + C_0.
$$

The integration constant \(C_0 = v(0,1) = v_0\) is rigid shear translation of the slab from its failed end at \(X = 0\). The null stress or null elastic strain condition requires \(\gamma(X) = 0\) for \(X \neq 1\), meaning that the shear displacement \(v = \text{constant} = v_0 = v_L\), i.e., a rigid translation.

Profiles of the order parameter for a domain size of \(L_0 = 10l\) are very similar to those shown in Fig. 1(a) and are not included here. Weyl scaling parameter \(k\) is chosen either as 0 or ln(0.96), the latter case being the physically realistic one for density increase commensurate with amorphization in boron carbide. The magnitude of \(\xi\) decreases rapidly from its maximum at \(X = 0\) with increasing \(X\), again with trends independent of \(k\). Influences of \(k\) on the \(\xi\) field are nearly negligible. The total energy per unit cross-sectional area of the slab in the \(YZ\)-plane is calculated using (4.43) for two different values of \(l/L_0\) and the aforementioned two values of \(k\). Results are listed in columns 2 and 3 of Table 5, normalized by isurface energy \(Y\). Total energy \(\Psi_F\) increases very slightly with decreasing \(k\) in each column. A value of \(\Psi_F = Y\) would be equivalent to a Griffith-type theory of perfectly brittle mode II fracture. As \(l/L_0\) decreases, convergence towards the this value becomes apparent. Thus, the Finsler model correctly predicts the surface energy in a domain with a fully failed cross-section, regardless of the value of \(k \in [\ln(0.96), 0]\). This trend, now with \(k < 0\), is in agreement with results of Sec. 3.4.1 that consider positive values of \(k\).

### 4.4.2. Homogeneous deformation

The second boundary value problem considers a homogeneous order parameter field over the non-linear elastic slab. Physically, this corresponds to emergence
of microscopic slip or shear bands or shear cracks distributed uniformly over the domain. For such homogeneous degradation, \( \xi'(X) = 0 \) if \( X \in [0, L_0] \Rightarrow \xi(0) = \xi(L_0) = \xi_H \). In Sec. 4.4.2, the notation \((\cdot)_H\) is again followed for any quantity that is homogeneous over the material manifold. Particular boundary conditions on shear displacement are

\[
v(0, D) = v_0 = 0, \quad v(L_0, D) = v_L. \tag{4.45}
\]

Denote the total shear strain by \( a(X) = \gamma(X) \) so that \((F^E)_X = a/\phi_H = a \exp(-k \xi_H/3)\). Since \( \xi \) is constant, all components of elastic strain in (4.24) are necessarily constant except the shear strain, which depends on \( a \). However, linear momentum conservation (4.40) requires that \( a = a_H \) as constant as well. Thus, \( P = P_H \) is a constant shearing force per unit reference area, and all other stress components are also constant over the domain. Equations (4.39) and (4.40) reduce to

\[
P_H(a_H, \phi_H) = P_0(a_H, \phi_H) \exp(-k \xi_H) = \text{constant}, \quad \phi_H = \exp\left(\frac{k \xi_H}{3}\right); \tag{4.46}
\]

\[
(1 - \xi_H)C^{\alpha\beta\gamma\delta}(D^H_X)^\alpha\beta(D^H_Y)^\gamma\delta - 2 \frac{\Psi}{\gamma} \xi_H = 2 k \left[ \psi_H - \frac{P_H a_H - 3 \rho_H}{6} \right]. \tag{4.47}
\]

The motion is obtained by integrating (4.20) with \( y(X, \xi_H) - Y = v(X, \xi_H) = v(X) \): \( v(X) = \int_0^X \gamma(\Xi)\Xi \Xi = v_0 + a_H X = a_H X, \tag{4.48} \)

where the first boundary condition in (4.45) is used. The other boundary condition requires \( v_L = a_H L_0 \). Once boundary conditions are applied, (4.46) and (4.47) can be solved simultaneously for field \( \xi_H \), shear stress \( P_H \), and shear strain \( a_H \). The total energy of the elastic domain with uniform damage and homogeneous free energy density \( \psi_H \) is the expression

\[
\Psi(v_L, \xi_H) = \Psi_H = \int_0^{L_0} \left[ W_H(a_H, \xi_H) + \frac{\gamma^2_H}{L} \right] dX = \psi_H(a_H, \xi_H)L_0. \tag{4.49}
\]

The only case which is simultaneously both homogeneous and stress free — if elastic stiffness coefficients are non-zero — requires that \( a_H = 0 \Rightarrow v_L = 0 \), i.e., null imposed shear deformation.

Physical parameters for shear failure of single crystals of B\(_4\)C from Table 4 are used in solutions discussed next. Shearing is parallel to the crystallographic \( a \)-axis, with the plane of shear corresponding to a prismatic plane. In other words, the shearing mode is of type \( \{1210\}\{1010\} \). The resulting order parameter, shear stress, total energy, and pressure are shown in Fig. 3: \( \xi = \xi_H, \quad P = P_H, \quad \Psi = \Psi_H \), and \( p = p_H \) versus applied shear displacement \( v_L \). A domain size of \( L_0 = 10^3 l \) is considered. Stress and energy fields labeled “elastic” correspond to the non-linear elastic solution with null order parameter and thus no structural transformation or softening: \( \xi = 0 \) if \( X \in [0, L_0] \). Shear stress, compressive pressure \( (p_H > 0) \) and total energy are larger for the perfectly elastic results than for those in which damage
Fig. 3. Boron carbide, shear degradation, homogeneous damage, $l/L_0 = 10^{-3}$ (a) order parameter $\xi = D/l$ (b) normalized shear stress (c) normalized total energy (d) normalized reference pressure.

$(\xi > 0)$ degrades the elasticity tensor. As discussed in Sec. 3.4.2, perfectly elastic results can be obtained by taking $T/l \to \infty$ in the Finsler geometric representation.

If $k$ is held constant, $\xi$ increases monotonically with increasing displacement (Fig. 3(a)), shear stress $P$ increases to a maximum and then decreases (Fig. 3(b)), and energy $\Psi$ increases monotonically (Fig. 3(c)). If $k$ is reduced from 0 to $\ln(0.96)$, the total energy $\Psi_H$ is relatively unaffected. Peak (i.e., maximum) shear stress $P_M$ and corresponding shear strain $\gamma_C = v_L/L_0$ are listed in Table 6. Peak shear stress decreases, with applied displacement at which peak stress is attained relatively unaffected, with decreasing $k$. Physically, this result demonstrates a decrease in strength and stability of the ceramic crystal accompanying microscopic volumetric collapse represented mathematically by $k < 0$. As shown in Fig. 3(d), pressure is substantially lower (i.e., more tensile) when $k < 0$ than when $k = 0$ for $v_L/L_0 \lesssim 0.5$.

The density increase due to amorphization results in offsetting elastic expansion, leading to a tensile pressure contribution.
As listed in Table 6, predicted maximum shear stresses from the Finsler model are $P_M \approx \frac{\mu}{15}$, around half of the theoretical shear strength $\tau = \frac{\mu}{2\pi}$. These values are somewhat smaller in magnitude to those calculated using quantum molecular dynamics (QMD) [Taylor et al., 2012] and reactive force field atomic (ReaxFF) simulations [An and Goddard, 2015], with such results also given in Table 6. Predicted shear strain at maximum stress (i.e., ductility) is in reasonable agreement with the QMD results [Taylor et al., 2012], wherein a decrease in peak stress was observed with elastic shear instability linked to the onset of crystal structure collapse. This result is physically consistent with the present solutions that demonstrate decreased peak stress with increasing order parameter associated with amorphization. The dynamic shear strength from shock compression experiments on boron carbide polycrystals [Bourne, 2008; Clayton, 2015d] is significantly smaller than the peak strengths reported from the present study and the atomic models. The lower value of the former may be a result of weak grain boundaries or other initial flaws in the polycrystalline material not considered in the models of Table 6. Reasons for differences in peak stresses among the models include domain size, orientation, and boundary condition effects and possible artifacts of choices of elastic and/or atomic potentials.

Some simulations in An and Goddard [2015] also address deformation twinning which is omitted in the present Finsler results, though orientations are also considered in that work that do not demonstrate twinning. However, simulations reported in [An and Goddard, 2015] depict load-displacement curves qualitatively matching Fig. 3(b): a gradual stress drop with increasing shear strain after peak stresses are attained. Furthermore, pressures become more tensile in amorphous zones in An and Goddard [2015], driving the formation of cavities commensurate with shear fractures. This phenomenon is qualitatively similar to the present result in Fig. 3(d), with tensile pressure promoted by increases in order parameter associated with amorphization for the case $k = \ln(0.96)$. In the less realistic case of $k = 0$, the effect is less pronounced, though the predicted pressure is still more tensile (smaller $p_H$) than that of the perfectly elastic solution.

Relative stability of homogeneous versus localized stress-free solutions of Sec. 4.4.1 is addressed in the rightmost two columns of Table 5. Transition from a homogeneous state of the sort modeled here in Sec. 4.4.2 to a state with localized shear failure is deemed energetically favorable at an applied deformation $\nu_L \geq \nu_C$. 

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Table 6. Maximum stress $P_M$ and corresponding strain $\gamma_M$ for shear loading in B$_4$C crystal(s).

<table>
<thead>
<tr>
<th>Source</th>
<th>$P_M/\mu \cdot 100$</th>
<th>$\gamma_M \cdot 100$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Finsler theory, $k = 0$</td>
<td>5.8</td>
<td>10</td>
</tr>
<tr>
<td>$k = \ln(0.96)$</td>
<td>5.6</td>
<td>10</td>
</tr>
<tr>
<td>QMD simulation [Taylor et al., 2012]</td>
<td>9–15</td>
<td>10–15</td>
</tr>
<tr>
<td>ReaxFF simulation [An and Goddard, 2015]</td>
<td>15–22</td>
<td>40–70</td>
</tr>
<tr>
<td>Shock experiment (polycrystal) [Bourne, 2008; Clayton, 2015d]</td>
<td>1.7</td>
<td>—</td>
</tr>
</tbody>
</table>
The value of $\upsilon_C$ is attained when $\Psi_H$ of (4.49) equals or exceeds $\Psi_F$ of (4.43), marking a transition point whereby the homogeneous solution becomes relatively unstable. Shear stress at the onset of instability is labeled $P_C$. The shear strain $\upsilon_C/L_0$ is on the order of 6% and stress is on the order of 5% of the initial shear modulus $\mu$. The strain at instability is relatively unaffected by $k$, but critical shear stress decreases with decreasing $k$. In other words, use of the more physically realistic value of $k$ correlates with decreased shear strength at instability.

4.4.3. Summary

Key points to be noted from analysis of the present results for shear failure of B$_4$C single crystals are as follows:

- The Finsler model of continuum physics is able to describe the Griffith energy with high accuracy for small regularization length $l \leq 0.1L_0$, with physically valid values (for amorphization) of parameter $k \in [0, \ln(0.96)]$ having a nearly negligible effect on total energy;
- For a homogeneously deformed slab with uniform localization modes, a decrease in $k$ from 0 to its realistic value of $\ln(0.96)$ produces lower maximum shear stress and higher tensile pressure commensurate with amorphization, in agreement with observations from discrete molecular physics simulations [An and Goddard, 2015];
- Maximum shear stresses under simple shear loading are predicted to be on the order of half the theoretical shear strength, in between predictions of quantum mechanics or MD models of perfect single crystals [Taylor et al., 2012; An and Goddard, 2015] and experimental shear strengths under shock compression [Bourne, 2008; Clayton, 2015d]. Stresses corresponding to a transition from homogeneous to localized deformation are on the order of 5% of the initial elastic shear modulus for slippage of prismatic planes.

5. Conclusions

A theory of Finsler-geometric continuum mechanics developed recently by the author has been refined to consider volumetric, i.e., spherical, inelastic deformation. Resulting governing equations have been obtained from differential-geometric arguments and variational principles. The theory has been applied to two problems involving geometrically non-linear micromechanics and fracture of single crystals. The first application considers tensile rupture of Mg, while the second considers amorphization and shear failure of boron carbide. In each case, a conformal transformation of the (pseudo)-Finsler metric is invoked. For Mg, the transformation depicts volume increase associated with void growth and ductile fracture. For boron carbide, the transformation depicts density increase associated with structure collapse and shear band formation. Finsler model solutions to boundary value problems for stress-free states of either material demonstrate convergence to Griffith
failure mechanics as the regularization length is decreased. Finsler model solutions for homogeneous states and for transitions to localized failure modes demonstrate favorable qualitative, and in many instances quantitative, agreement with molecular mechanics simulation results from the literature.

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References


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