# *The Stored Energy of Cold Work, Thermal Annealing, and Other Thermodynamic Issues in Single Crystal Plasticity at Small Length Scales*

# The stored energy of cold work, thermal annealing, and other thermodynamic issues in single crystal plasticity at small length scales

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**Abstract**

This paper develops a thermodynamically consistent gradient theory of single-crystal plasticity using the principle of virtual power as a paradigm to develop appropriate balance laws for forces and energy. The resulting theory leads to a system of microscopic force balances, one balance for each slip system, and to an energy balance that accounts for power expended during plastic flow via microscopic forces acting in concert with slip-rates and slip-rate gradients. Central to the theory are an internal energy and entropy, plastic in nature, dependent on densities that account for the accumulation of glide dislocations as well as geometrically necessary dislocations — and that, consequently, represent quantities associated with cold work. Our theory allows us to discuss — within the framework of a gradient theory — the fraction of plastic stress-power that goes into heating, as well as the reduction of the dislocation density in a cold-worked material upon subsequent (or concurrent) thermal annealing.

*Keywords:* A. Crystal plasticity; B. Geometrically necessary dislocations; C. Gradient theory; D. Dislocation densities; E. Cold work

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# 1 Introduction

SCintrostuff

The plastic deformation of metals when conducted at temperatures less than $\approx 0.35\,\vartheta_m$, where $\vartheta_m$ is the melting temperature of the material in degrees Kelvin, is called *cold-working*.[1] In this temperature range the underlying mechanism of plastic deformation of metal single crystals is the glide of *dislocations*, which are crystalline line-defects, on certain crystallographic slip systems in the material. This process of plastic deformation is usually accompanied by a rapid multiplication (and eventual saturation) in the number of dislocations. However, the dislocations so produced are seldom homogeneously distributed in the material; instead they form a heterogeneous "cell"-structure, with cell-walls made of clusters of dislocations and with cell-interiors which are relatively free of dislocations. The increased dislocation density and resulting dislocation cell-structure leads to an increased resistance to subsequent plastic flow. This increase in the resistance to plastic flow is called *strain-hardening*.

When a metal is cold-worked, most of the plastic work done is converted into heat, but a certain portion is stored in the material. In nominally pure metals, the dominant contribution to the stored energy is the energy associated with the evolving dislocation density and sub-structure of the material. The dislocations — being line defects in the crystalline lattice — cause distortion of the lattice and therby store a certain amount elastic energy, which is called the *stored energy of cold-work*.

The microscale dislocation substructure in a ductile metal that has been cold-worked and unloaded, is generally unstable. Upon subsequent heating to a temperature in the range $\approx 0.35$ through $\approx 0.5\,\vartheta_m$ it undergoes a restoration process called *recovery* or *annealing*, during which the dislocation configurations in the cell-walls annihilate, the cell-walls sharpen, and the stored energy is released.[2]

The extensive literature on the experimental and theoretical developments concerning the stored energy of cold work has been reviewed by Bever, Holt & Titchener (1973). The reported values of the ratio of the stored energy to that expended plastically ranges from near zero to approximately 15 percent (cf., e.g., Farren & Taylor, 1925; Taylor & Quinney, 1934, 1937). A discussion of the notion of stored energy of cold work and its ramifications, within a one-dimensional conventional (non-gradient) theoretical framework, is the focus of an important study of Rosakis, Rosakis, Ravichandran & Hodowany (2000). For a recent two-dimensional, discrete-dislocation-plasticity-based numerical study regarding the stored energy of cold work, see Benzerga, Bréchet, Needleman & van der Giessen (2005).

From a fundamental theoretical standpoint, mechanical and thermal effects should be coupled within a consistent thermodynamical framework. Accodingly, the purpose of this paper is to formulate a *thermo-mechanically coupled gradient theory of single-crystal plasticity* at low homologous temperatures, $\vartheta \lessapprox 0.35\,\vartheta_m$. In this temperature range plastic flow of metals is only weakly dependent on the strain-rate; accordingly we limit our considerations to a *rate-independent theory*. Central to our continuum-mechanical theory are an internal energy and entropy, plastic in nature, dependent on dislocation densities that account for the accumulation of statistically-stored as well as geometrically-necessary dislocations — and that, consequently, represent quantities associated with cold work. Our theory allows us to meaningfully discuss — within the framework of a gradient crystal plasticity theory — the fraction of plastic stress-power

[1]Plastic deformation in the temperature range $\approx 0.35$ through $\approx 0.5\,\vartheta_m$ is called *warm-working*, while *hot-working* refers to the plastic deformation of metals into desired shapes at temperatures in the range of $\approx 0.5$ through $\approx 0.9\,\vartheta_m$.

[2]Heavily cold-worked metals when heated to a sufficiently high temperature, $\vartheta \gtrapprox 0.5\,\vartheta_m$, may also undergo a restoration process called recrystallization. We do not consider recrystallization processes in this paper.

that goes into heating, as well as the reduction of the dislocation density in a cold-worked material upon subsequent thermal annealing.

# 2 Basic equations

basics

## 2.1 Kinematics

kinematics

We begin with the requirement that the displacement gradient admit a decomposition

$$\nabla\mathbf{u} = \mathbf{H}^e + \mathbf{H}^p \qquad \Big(u_{i,j} = H^e_{ij} + H^p_{ij}\Big) \tag{2.1}$$

Dlittlek1

in which $\mathbf{H}^e$, the *elastic distortion*, represents stretch and rotation of the underlying microscopic structure, here a lattice, and $\mathbf{H}^p$, the *plastic distortion*, represents the local deformation of material due to the formation and motion of dislocations through that structure. We define *elastic* and *plastic strains* $\mathbf{E}^e$ and $\mathbf{E}^p$ as the symmetric parts of $\mathbf{H}^e$ and $\mathbf{H}^p$, so that the (total) strain $\mathbf{E}$ — which is the symmetric part,

$$\mathbf{E} = \tfrac{1}{2}\big(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\top}\big), \tag{2.2}$$

Enabu

of the displacement gradient $\nabla\mathbf{u}$ — is the sum

$$\mathbf{E} = \mathbf{E}^e + \mathbf{E}^p. \tag{2.3}$$

Delplstrainsrots2

Single-crystal plasticity is based on the physical assumption that the motion of dislocations takes place on prescribed *slip systems* $\alpha = 1, 2, \dots, N$. And the presumption that plastic flow take place through slip manifests itself in the requirement that the plastic distortion $\mathbf{H}^p$ be governed by *slips* $\gamma^\alpha$ on the individual slip systems via the relation

$$\mathbf{H}^p = \sum_\alpha \gamma^\alpha\, \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \qquad \Big(H^p_{ij} = \sum_\alpha \gamma^\alpha s^\alpha_i m^\alpha_j\Big), \tag{2.4}$$

D2.4

where for each $\alpha$ the *slip direction* $\mathbf{s}^\alpha$ and the associated *slip-plane normal* $\mathbf{m}^\alpha$ are *constant* orthonormal lattice vectors; viz.

$$\mathbf{s}^\alpha \cdot \mathbf{m}^\alpha = 0, \qquad |\mathbf{s}^\alpha| = |\mathbf{m}^\alpha| = 1. \tag{2.5}$$

Dsmrelts

Here and in what follows: lower case Greek superscripts $\alpha, \beta, \dots$ denote slip-system labels and as such range over the integers $1, 2, \dots, N$; we do not use the summation convention for Greek superscripts; we use the shorthand

$$\sum_\alpha = \sum_{\alpha=1}^{N}.$$

A consequence of (2.1) and (2.4) is that

$$\nabla\dot{\mathbf{u}} = \dot{\mathbf{H}}^e + \sum_\alpha \dot{\gamma}^\alpha \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \qquad \Big(\dot{u}_{i,j} = \dot{H}^e_{ij} + \sum_\alpha \dot{\gamma}^\alpha s^\alpha_i m^\alpha_j\Big), \tag{2.6}$$

kinematicconstraint

a relation that represents a fundamental *kinematical constraint* on the fields $\mathbf{u}$, $\mathbf{H}^e$, and $\gamma^\alpha$.

The tensor

$$\mathbb{S}^\alpha = \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha$$

is generally referred to as the *Schmid tensor*. Important to what follows is the *symmetric Schmid tensor* defined by

$$\mathbb{S}^{\alpha}_{\rm sym} = \tfrac{1}{2}\big(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}+\mathbf{m}^{\alpha}\otimes\mathbf{s}^{\alpha}\big); \tag{2.7}$$ symschmid

this tensor allows us to write the plastic strain — which is the symmetric part of $\mathbf{H}^p$ — in the form

$$\mathbf{E}^p = \sum_{\alpha}\gamma^{\alpha}\mathbb{S}^{\alpha}_{\rm sym}. \tag{2.8}$$ Epslips

Some notation is useful. For any slip system $\alpha$, $\Pi^{\alpha}$ denotes the $\alpha$th *slip plane*; $\Pi^{\alpha}$ is oriented by the unit normal $\mathbf{m}^{\alpha}$; $\mathbf{s}^{\alpha}$ is tangent to $\Pi^{\alpha}$. The lattice vector

$$\mathbf{l}^{\alpha} \stackrel{\rm def}{=} \mathbf{m}^{\alpha}\times\mathbf{s}^{\alpha} \tag{2.9}$$ introlms

is important to what follows. Indeed, since for any slip-system $\alpha$, $\mathbf{l}^{\alpha}$ is a unit vector on $\Pi^{\alpha}$ orthogonal to $\mathbf{s}^{\alpha}$,

$$\{\mathbf{s}^{\alpha},\mathbf{l}^{\alpha}\}\ \text{represents a right-handed orthonormal basis for the slip plane}\ \Pi^{\alpha}. \tag{2.10}$$ Piabasis

Given any vector $\mathbf{w}$,

$$\mathbf{w}^{\alpha}_{\rm tan} = \mathbf{w} - (\mathbf{m}^{\alpha}\cdot\mathbf{w})\mathbf{m}^{\alpha} = (\mathbf{s}^{\alpha}\cdot\mathbf{w})\mathbf{s}^{\alpha}+(\mathbf{l}^{\alpha}\cdot\mathbf{w})\mathbf{l}^{\alpha} \tag{2.11}$$ bbP2

is the vector component of $\mathbf{w}$ *tangent* to $\Pi^{\alpha}$. We write $\nabla^{\alpha}_{\rm tan}$ for the *tangential gradient* on $\Pi^{\alpha}$, so that, for any scalar field $\phi$,

$$\nabla^{\alpha}_{\rm tan}\phi = (\mathbf{s}^{\alpha}\cdot\nabla\phi)\,\mathbf{s}^{\alpha}+(\mathbf{l}^{\alpha}\cdot\nabla\phi)\,\mathbf{l}^{\alpha} \tag{2.12}$$ tander1

$$= \nabla\phi - (\mathbf{m}^{\alpha}\cdot\nabla\phi)\,\mathbf{m}^{\alpha} \tag{2.13}$$ tander2

and

$$\mathbf{m}^{\alpha}\times\nabla\phi = \mathbf{m}^{\alpha}\times\nabla^{\alpha}_{\rm tan}\phi. \tag{2.14}$$ matimes

Then, for $\mathbf{t}$ tangent to $\Pi^{\alpha}$

$$\mathbf{t}\cdot\nabla\phi = \mathbf{t}\cdot\nabla^{\alpha}_{\rm tan}\phi. \tag{2.15}$$ nablanabaa

## 2.2 Geometrically necessary dislocations

dislocations

Dislocations are *microscopic* defects in a crystal lattice. In a *continuum* theory there can be no dislocations, as such, but *slip gradients* on the individual slip systems result in quantities that *mimic* the behavior of microscopic dislocations; we refer to such *macroscopic* quantities as *geometrically necessary dislocations* (GNDs).[3]

As Arsenlis & Parks (1999) have shown, physically meaningful candidates for edge and screw GND densities are given by

$$\rho^{\alpha}_{\vdash} = -\mathbf{s}^{\alpha}\cdot\nabla\gamma^{\alpha} = -\mathbf{s}^{\alpha}\cdot\nabla^{\alpha}_{\rm tan}\gamma^{\alpha} \qquad\text{and}\qquad \rho^{\alpha}_{\odot} = \mathbf{l}^{\alpha}\cdot\nabla\gamma^{\alpha} = \mathbf{l}^{\alpha}\cdot\nabla^{\alpha}_{\rm tan}\gamma^{\alpha}, \tag{2.16}$$ sceddensities

where $\mathbf{l}^{\alpha}$ is given by (2.9) and, like $\mathbf{s}^{\alpha}$, is tangent to $\Pi^{\alpha}$. Thus,

$$\dot\rho^{\alpha}_{\vdash} = -\mathbf{s}^{\alpha}\cdot\nabla^{\alpha}_{\rm tan}\dot\gamma^{\alpha} \qquad\text{and}\qquad \dot\rho^{\alpha}_{\odot} = \mathbf{l}^{\alpha}\cdot\nabla^{\alpha}_{\rm tan}\dot\gamma^{\alpha}. \tag{2.17}$$ Ddisflowrate0a

As noted by Gurtin & Ohno (2011), a vectorial measure of the flow rate of edge and screw GNDs on slip system $\alpha$ is given by the flow-rate vector

$$\nabla^{\alpha}_{\rm tan}\dot\gamma^{\alpha} = -\dot\rho^{\alpha}_{\vdash}\mathbf{s}^{\alpha}+\dot\rho^{\alpha}_{\odot}\mathbf{l}^{\alpha}, \tag{2.18}$$ Ddisflowrate0

[3]Cf., e. g., Ashby (1970), Fleck, Muller, Ashby & Hutchinson (1994), Arsenlis and Parks (1999).

Note that

$$|\nabla^{\alpha}_{\tan}\dot{\gamma}^{\alpha}| = \sqrt{|\dot{\rho}^{\alpha}_{\vdash}|^2 + |\dot{\rho}^{\alpha}_{\odot}|^2}, \tag{2.19}$$ accum1

clearly represents an accumulation rate of GNDs on $\alpha$.[4]

**Remark** The geometrically necessary dislocation densities $\rho^{\alpha}_{\vdash}$ and $\rho^{\alpha}_{\odot}$ defined in (2.16) are "continuum-mechanical densities." In materials science, dislocation densities are measured in terms of the dislocation line length per unit volume, and hence carry the dimension $length^{-2}$. The continuum-mechanical densities $\rho^{\alpha}_{\vdash}$ and $\rho^{\alpha}_{\odot}$ may be converted to corresponding "materials-science densities," by multiplying each of these densities by $b^{-1}$, where $b$ is the magnitude of the Burgers vector — which is the vector that represents the closure failure of a Burgers circuit around a *single* dislocation in a crystal lattice. The densities $\rho^{\alpha}$, without the subscripts $\vdash$ and $\odot$, defined in the next sub-section — and used in the remaining body of the paper — will be materials science densities, and hence will carry the dimension $length^{-2}$. terminology

## 2.3 Dislocation densities that account for thermal effects

hardvariables

To this point we have limited our discussion to edge and screw GNDs. This was done only to motivate our view of $|\nabla^{\alpha}_{\tan}\dot{\gamma}^{\alpha}|$ as a measure of the accumulation rate of GNDs on slip-system $\alpha$. On the other hand, our goal is a dislocation density that accounts for a *mixture* of glide dislocations and GNDs. With this in mind, we view

$$\dot{\Gamma}^{\alpha}_{\rm acc} \stackrel{\rm def}{=} \sqrt{|\dot{\gamma}^{\alpha}|^2 + \ell^2|\nabla^{\alpha}_{\tan}\dot{\gamma}^{\alpha}|^2} \tag{2.20}$$ netaccrate

as a *generalized scalar slip-rate* or, equivalently, as an *accumulation rate*; here $\alpha$ is the underlying slip system, while $\ell > 0$ is a strictly positive constant whose units are length.[5]

Specifically, we consider **dislocation densities** $\rho^{\alpha} \geq 0$ for the individual slip systems, with each density viewed as a mean-field representation of the distribution of glide dislocations and GNDs.[6] The following notation is useful:

$$\vec{\rho} \stackrel{\rm def}{=} \big(\rho^1\,, \rho^2\,, \ldots\,, \rho^N\big), \qquad \vec{\mathbf{0}} \stackrel{\rm def}{=} \big(\mathbf{0}\,, \mathbf{0}\,, \ldots\,, \mathbf{0}\big). \tag{2.21}$$ netdislist

We assume that the densites $\rho^{\alpha}$ evolve according to constitutive relations of the form

$$\dot{\rho}^{\alpha} = A^{\alpha}(\vartheta, \vec{\rho})\,\dot{\Gamma}^{\alpha}_{\rm acc} - R^{\alpha}(\vartheta, \vec{\rho}) \quad \text{with} \quad \rho^{\alpha}|_{t=0} = \rho^{\alpha}_0. \tag{2.22}$$ accden

In (2.22):

- The first term (on the right) characterizes changes in dislocation density due to plastic flow. We refer to $A^{\alpha}(\vartheta, \vec{\rho})$ as the *dislocation-accumulation modulus* and assume that

$$A^{\alpha}(\vartheta, \vec{\rho}) \geq 0. \tag{2.23}$$ Age0

- The second term (with the minus sign) characterizes decreases in density due to thermal annealing. We refer to $R^{\alpha}(\vartheta, \vec{\rho})$ as the *recovery rate* for $\rho^{\alpha}$, and assume that

$$R^{\alpha}(\vartheta, \vec{\rho}) \geq 0, \qquad \frac{\partial R^{\alpha}(\vartheta, \vec{\rho})}{\partial \vartheta} \geq 0, \tag{2.24}$$ staticpos

  so that the recovery rate increases with temperature.

We refer to (2.22) as **defect-flow equations**.

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[4]Cf. Ohno, Okumura & Shibata (2008).

[5]Cf. Gurtin, Anand & Lele (2007), who refer to $\dot{\Gamma}^{\alpha}_{\rm acc}$ as an *effective flow rate*.

[6]What we refer to as *glide dislocations* here, are usually called *statistically-stored dislocations* in the literature; but we eschew the latter terminology. Also, bear in mind that in actual metal single crystals the dislocations are seldom uniformly distributed; instead they often form cell-structures.

## 2.4 Macroscopic and microscopic force balances derived via the principle of virtual power

Dmacmicbalances

Following Gurtin (2002) we formulate these laws based on a nonstandard version of the principle of virtual power,[7] but here we restrict attention to quasi-static behavior.

We identify the body B with the *closed* region of space it occupies and let P denote an arbitrary *subbody* (subregion) of B. The virtual-power principle is based on a fundamental *power balance* between the *internal power* $\mathcal{W}_{\rm int}({\rm P})$ expended **within** P and the *external power* $\mathcal{W}_{\rm ext}({\rm P})$ expended **on** P. Regarding the internal power we allow for power expended *internally* by a stress $\mathbf{T}$ power-conjugate to $\dot{\mathbf{H}}^e$ and, for each slip-system $\alpha$, a scalar *internal microscopic stress* $\pi^\alpha$ power-conjugate to $\dot\gamma^\alpha$ and a vector *microscopic stress* $\boldsymbol{\xi}^\alpha$ power-conjugate to $\nabla^\alpha_{\tan}\dot\gamma^\alpha$.[8] Because $\nabla^\alpha_{\tan}\dot\gamma^\alpha$ is tangent to $\Pi^\alpha$, we may without loss in generality assume that

$$\boldsymbol{\xi}^\alpha \text{ is tangent to } \Pi^\alpha; \tag{2.25}$$ nonor

then, by (2.15) and (2.25),

$$\boldsymbol{\xi}^\alpha\cdot\nabla^\alpha_{\tan}\dot\gamma^\alpha = \boldsymbol{\xi}^\alpha\cdot\nabla\dot\gamma^\alpha, \tag{2.26}$$ dtfoot

and, by virtue of the divergence theorem, this leads to an identity,

$$\int\limits_{\rm P}\boldsymbol{\xi}^\alpha\cdot\nabla^\alpha_{\tan}\dot\gamma^\alpha\,dv = \int\limits_{\partial{\rm P}}(\boldsymbol{\xi}^\alpha\cdot\mathbf{n})\dot\gamma^\alpha\,da - \int\limits_{\rm P}\dot\gamma^\alpha{\rm div}\,\boldsymbol{\xi}^\alpha\,dv, \tag{2.27}$$ GSCalphoweid2

basic to what follows.

Regarding the external power, we supplement the standard expenditures $\mathbf{t}(\mathbf{n})\cdot\dot{\mathbf{u}}$ and $\mathbf{b}\cdot\dot{\mathbf{u}}$ by tractions and body forces with an additional expenditure $\Xi^\alpha(\mathbf{n})\,\dot\gamma^\alpha$ associated with microscopic tractions power-conjugate to slip rates.[9] We therefore begin with the power balance[10]

$$\underbrace{\int\limits_{\partial{\rm P}}\mathbf{t}(\mathbf{n})\cdot\dot{\mathbf{u}}\,da + \int\limits_{\rm P}\mathbf{b}\cdot\dot{\mathbf{u}}\,dv + \sum_\alpha\int\limits_{\partial{\rm P}}\Xi^\alpha(\mathbf{n})\,\dot\gamma^\alpha\,da}_{\mathcal{W}_{\rm ext}({\rm P})}$$

$$= \underbrace{\int\limits_{\rm P}\mathbf{T}:\dot{\mathbf{H}}^e\,dv + \sum_\alpha\int\limits_{\rm P}(\pi^\alpha\dot\gamma^\alpha + \boldsymbol{\xi}^\alpha\cdot\nabla^\alpha_{\tan}\dot\gamma^\alpha)\,dv}_{\mathcal{W}_{\rm int}({\rm P})}. \tag{2.28}$$ DPVP

Important to what follows is the *resolved shear* defined by

$$\tau^\alpha = \mathbf{s}^\alpha\cdot\mathbf{T}\mathbf{m}^\alpha \tag{2.29}$$ Dresolvedshear

for each slip-system $\alpha$.

The balance equations and traction conditions of the theory — presumed not known in advance — are derived using the principle of virtual power, a principle based on a

[7] Cf. Germain (1973), who developed such a principle for materials whose internal power expenditures involve first and second gradients of the velocity $\dot{\mathbf{u}}$. The kinematics associated with Germain's virtual-power principle bears no relation to that of single-crystal plasticity.

[8] Here, we use the tangential slip-rate gradient $\nabla^\alpha_{\tan}\dot\gamma^\alpha$ rather than $\nabla\dot\gamma^\alpha$ because the underlying power expenditure $\boldsymbol{\xi}^\alpha\cdot\nabla^\alpha_{\tan}\dot\gamma^\alpha$ is meant to characterize power expenditures associated with the flow of GNDs on the $\alpha$th slip-plane $\Pi^\alpha$; by (2.18) this flow is characterized by the *flow-rate vector* $\nabla^\alpha_{\tan}\dot\gamma^\alpha$.

[9] The tractions are defined for all unit vectors $\mathbf{n}$ — with $\mathbf{n}$ in (2.28) the outward unit normal to $\partial$P. We do not assume a priori that the stress $\mathbf{T}$ is symmetric.

[10] Gurtin (2002).

view of the velocity $\dot{\mathbf{u}}$, the elastic distortion-rate $\dot{\mathbf{H}}^e$, and the slip rates $\dot{\gamma}^1, \dot{\gamma}^2, \ldots, \dot{\gamma}^N$ as *virtual velocities* to be specified independently in a manner consistent with (2.6). That is, denoting the virtual velocities by $\tilde{\mathbf{u}}$, $\tilde{\mathbf{H}}^e$, and $\tilde{\gamma}^1, \tilde{\gamma}^2, \ldots, \tilde{\gamma}^N$, we require that

$$\nabla\tilde{\mathbf{u}} = \tilde{\mathbf{H}}^e + \sum_\alpha \tilde{\gamma}^\alpha \mathbb{S}^\alpha, \tag{2.30}$$

scgenvirvel

define a (generalized) *virtual velocity* to be a list

$$\mathcal{V} = (\tilde{\mathbf{u}}, \tilde{\mathbf{H}}^e, \tilde{\gamma}^1, \tilde{\gamma}^2, \ldots, \tilde{\gamma}^N) \tag{2.31}$$

vvlist

consistent with the constraint (2.30), and rewrite (2.28) as a *virtual power balance*

$$\underbrace{\int\limits_{\partial\mathrm{P}} \mathbf{t}(\mathbf{n})\cdot\tilde{\mathbf{u}}\,da + \int\limits_{\mathrm{P}} \mathbf{b}\cdot\tilde{\mathbf{u}}\,dv + \sum_\alpha \int\limits_{\partial\mathrm{P}} \Xi^\alpha(\mathbf{n})\,\tilde{\gamma}^\alpha\,da}_{\mathcal{W}_{\mathrm{ext}}(\mathrm{P},\mathcal{V})}$$

$$= \underbrace{\int\limits_{\mathrm{P}} \mathbf{T}\colon\tilde{\mathbf{H}}^e\,dv + \sum_\alpha \int\limits_{\mathrm{P}} (\pi^\alpha\tilde{\gamma}^\alpha + \boldsymbol{\xi}^\alpha\cdot\nabla^\alpha_{\mathrm{tan}}\tilde{\gamma}^\alpha)\,dv}_{\mathcal{W}_{\mathrm{int}}(\mathrm{P},\mathcal{V})}. \tag{2.32}$$

DGSCvirbalPVP

Further, we say $\mathcal{V}$ is *macroscopic* if the associated virtual slip rates all vanish; *rigid* if

$$\tilde{\mathbf{u}}(\mathbf{x}) = \boldsymbol{\omega}\times\mathbf{x}$$

with $\boldsymbol{\omega}$ a vector constant. The precise statement of the *principle of virtual power* within the present framework then consists of two basic requirements for *any choice* of the subbody P:[11]

(i) the virtual power-balance (2.32) be satisfied for all virtual velocity fields consistent with the kinematic constraint (2.30);

(ii) the internal power vanish whenever the virtual velocity field is macroscopic and rigid.

The virtual-power principle has the following consequences:

(a) The *macroscopic stress* $\mathbf{T}$ is symmetric and consistent with the *macroscopic force balance* and *macroscopic traction condition*

$$\mathrm{div}\,\mathbf{T} + \mathbf{b} = \mathbf{0} \qquad \text{and} \qquad \mathbf{t}(\mathbf{n}) = \mathbf{T}\mathbf{n}. \tag{2.33}$$

DSCPVPmacfb1

(b) The *microscopic stresses* $\pi^\alpha$ and $\boldsymbol{\xi}^\alpha$ are consistent with the *microscopic force balance*[12]

$$\tau^\alpha = \pi^\alpha - \mathrm{div}\,\boldsymbol{\xi}^\alpha \tag{2.34}$$

Dmfb

and the *microtraction condition*

$$\Xi^\alpha(\mathbf{n}) = \boldsymbol{\xi}^\alpha\cdot\mathbf{n} \tag{2.35}$$

Dmfbtraccon

for each slip-system $\alpha$.

[11] Here we follow Germain (1973) in requiring that the principle hold for *all* subbodies P, not just for P = B; this requirement is basic to what follows.
[12] Gurtin (2000, 2002).

(c) The *macroscopic* and *microscopic virtual-power relations*

$$\int\limits_{\partial \mathrm{P}} \mathbf{t}(\mathbf{n}) \cdot \tilde{\mathbf{u}}\, da + \int\limits_{\mathrm{P}} \mathbf{b} \cdot \tilde{\mathbf{u}}\, dv = \int\limits_{\mathrm{P}} \mathbf{T} \colon \tilde{\mathbf{E}}\, dv \tag{2.36}$$

macvprelation

and

$$\sum_{\alpha} \int\limits_{\partial \mathrm{P}} (\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n}) \tilde{\gamma}^{\alpha}\, da = \sum_{\alpha} \int\limits_{\mathrm{P}} \Big( (\pi^{\alpha} - \tau^{\alpha}) \tilde{\gamma}^{\alpha} + \boldsymbol{\xi}^{\alpha} \cdot \nabla^{\alpha}_{\mathrm{tan}} \tilde{\gamma}^{\alpha} \Big)\, dv \tag{2.37}$$

smallGSCmicrovirpower

are satisfied. The microscopic relations are useful in developing a weak form of the microscopic force balance.

A consequence of the symmetry of $\mathbf{T}$, (2.7), and (2.29) is that

$$\tau^{\alpha} = \mathbf{T} \colon \mathbb{S}^{\alpha}_{\mathrm{sym}}. \tag{2.38}$$

tauT

Next, since the symmetric part of $\mathbf{H}^e$ is $\mathbf{E}^e$, we may conclude from the symmetry of $\mathbf{T}$ that

$$\mathbf{T} \colon \dot{\mathbf{H}}^{e} = \mathbf{T} \colon \dot{\mathbf{E}}^{e}, \tag{2.39}$$

TH=TEp

and we may rewrite the internal power — as described by the right side of (2.28) — in the form

$$\mathcal{W}_{\mathrm{int}}(\mathrm{P}) = \int\limits_{\mathrm{P}} \mathbf{T} \colon \dot{\mathbf{E}}^{e}\, dv + \sum_{\alpha} \int\limits_{\mathrm{P}} (\pi^{\alpha} \dot{\gamma}^{\alpha} + \boldsymbol{\xi}^{\alpha} \cdot \nabla^{\alpha}_{\mathrm{tan}} \dot{\gamma}^{\alpha})\, dv. \tag{2.40}$$

intrnalpowerwithconstp

Finally, when discussing plastic flow an important quantity is the *conventional plastic stress-power* defined by

$$\mathbf{T} \colon \dot{\mathbf{E}}^{p} = \mathbf{T} \colon \dot{\mathbf{H}}^{p} = \mathbf{T} \colon \Big( \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha} \Big) = \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{s}^{\alpha} \cdot \mathbf{T} \mathbf{m}^{\alpha} = \sum_{\alpha} \tau^{\alpha} \dot{\gamma}^{\alpha}, \tag{2.41}$$

pasticstresspower

where we have used (2.4), (2.29), and the counterpart of (2.39) for $\mathbf{H}^p$ and $\mathbf{E}^p$. The plastic stress-power is therefore the net power expended by the resolved shears acting in concert with the slip rates.

noproblem **Remark** Our derivation of the microscopic force balances (2.34) followed a procedure, common in mathematical physics, in which the underlying fields are assumed to be smooth enough to render the underlying differential operations meaningful. However, as noted by Gurtin and Reddy (2014), to characterize the relevant physics within the present framework the theory should be capable of coping with situations in which the slip-rate gradients $\nabla^{\alpha}_{\mathrm{tan}} \dot{\gamma}^{\alpha}$ and the microscopic stresses $\boldsymbol{\xi}^{\alpha}$ suffer *jump discontinuities*.

# 3 Thermodynamics

thermodynamics

The first two laws of thermodynamics for a continuum consist of balance of energy and an entropy imbalance generally referred to as the Clausius-Duhem inequality; given any subregion P, these laws have the respective forms[13]

$$\begin{aligned} \overline{\int\limits_{\mathrm{P}} \varepsilon\, dv}^{\boldsymbol{\cdot}} &= \mathcal{W}_{\mathrm{ext}}(\mathrm{P}) - \int\limits_{\partial \mathrm{P}} \mathbf{q} \cdot \mathbf{n}\, da + \int\limits_{\mathrm{P}} q\, dv \\ \overline{\int\limits_{\mathrm{P}} \eta\, dv}^{\boldsymbol{\cdot}} &\geq - \int\limits_{\partial \mathrm{P}} \frac{\mathbf{q}}{\vartheta} \cdot \mathbf{n}\, da + \int\limits_{\mathrm{P}} \frac{q}{\vartheta}\, dv, \end{aligned} \tag{3.1}$$

2L

[13] Cf., e.g., Truesdell and Noll (1965, §79). The use of a virtual-power principle to generate an appropriate form of the external power expenditure in thermodynamic relations is due to Gurtin (2002, §6).

where $\varepsilon$ and $\eta$ represent the internal energy and entropy, $\mathbf{q}$ is the heat flux, $q$ is the heat supply, and $\vartheta > 0$ is the absolute temperature, and where $\mathcal{W}_{\text{ext}}(\mathrm{P})$ is the external power expended on the subregion P. Applying the power balance (2.28) in conjunction with (2.40) we can rewrite balance of energy in the form

$$\overline{\int_{\mathrm{P}} \varepsilon \, dv}^{\,\cdot} = \int_{\mathrm{P}} \mathbf{T} \colon \dot{\mathbf{E}}^e \, dv + \sum_\alpha \int_{\mathrm{P}} (\pi^\alpha \dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha \cdot \nabla^\alpha_{\tan} \dot{\gamma}^\alpha) \, dv - \int_{\partial \mathrm{P}} \mathbf{q} \cdot \mathbf{n} \, da + \int_{\mathrm{P}} q \, dv; \qquad (3.2)$$

enbal2

thus using the divergence theorem and the arbitrary nature of the subregion P we arrive at the local form of the first two laws:

$$\begin{aligned} \dot{\varepsilon} &= \mathbf{T} \colon \dot{\mathbf{E}}^e + \sum_\alpha (\pi^\alpha \dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha \cdot \nabla^\alpha_{\tan} \dot{\gamma}^\alpha) - \mathrm{div}\, \mathbf{q} + q, \\ \dot{\eta} &\geq -\mathrm{div} \left( \frac{\mathbf{q}}{\vartheta} \right) + \frac{q}{\vartheta}. \end{aligned} \qquad (3.3)$$

locthermlaws

If we introduce the *free energy* defined by

$$\psi = \varepsilon - \vartheta \eta, \qquad (3.4)$$

freeenergy

and multiply $(3.3)_2$ by $\vartheta$ and subtract it from $(3.3)_1$, we arrive at the *free-energy imbalance*

$$\dot{\psi} + \eta \dot{\vartheta} + \frac{1}{\vartheta} \mathbf{q} \cdot \nabla \vartheta - \mathbf{T} \colon \dot{\mathbf{E}}^e - \sum_\alpha (\pi^\alpha \dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha \cdot \nabla^\alpha_{\tan} \dot{\gamma}^\alpha) \leq 0. \qquad (3.5)$$

thermfei

The left side of $(3.3)_2$ minus the right side,

$$\mathcal{N} \stackrel{\text{def}}{=} \dot{\eta} + \mathrm{div} \left( \frac{\mathbf{q}}{\vartheta} \right) - \frac{q}{\vartheta} \geq 0, \qquad (3.6)$$

entropyprod

represents the *entropy production* per unit volume. On the other hand, the quantity $\vartheta \mathcal{N}$, which turns out to be the negative of the left side of (3.5), represents the *dissipation* per unit volume.[14]

# 4 Boundary and initial conditions

bcsandICs

## 4.1 Macroscopic boundary conditions

macBC

We consider more or less conventional boundary conditions for the macroscopic fields:

(i) We assume that the displacement $\mathbf{u}$ and traction $\mathbf{t} = \mathbf{T}\mathbf{n}$ are prescribed on *complementary subsurfaces* $\partial \mathrm{B}_{\text{disp}}$ and $\partial \mathrm{B}_{\text{trac}}$ of $\partial \mathrm{B}$. These conditions take the form

$$\mathbf{u} = \mathbf{u}^* \;\text{ on }\; \partial \mathrm{B}_{\text{disp}}, \qquad \mathbf{T}\mathbf{n} = \mathbf{t}^* \;\text{ on }\; \partial \mathrm{B}_{\text{trac}}, \qquad (4.1)$$

mechBC

with $\mathbf{u}^*$ and $\mathbf{t}^*$ prescribed vector fields.

(ii) As thermal boundary conditions we assume that the temperature $\vartheta$ and the normal component $\mathbf{q} \cdot \mathbf{n}$ of the heat flux are specified on *complementary subsurfaces* $\partial \mathrm{B}_{\text{temp}}$ and $\partial \mathrm{B}_{\text{flux}}$ of $\partial \mathrm{B}$. These conditions take the form

$$\vartheta = \vartheta^* \;\text{ on }\; \partial \mathrm{B}_{\text{temp}}, \qquad \mathbf{q} \cdot \mathbf{n} = q^*_n \;\text{ on }\; \partial \mathrm{B}_{\text{flux}}, \qquad (4.2)$$

thermBC

with $\vartheta^*$ and $q^*_n$ prescribed fields.

[14] Cf. e. g. Truesdell and Noll(1965), Gurtin, Fried and Anand (2010).

## 4.2 Microscopic boundary conditions

The microscopic boundary conditions are nonconventional and for that reason their prescription is a bit more delicate.[15] We assume that the body B is the union

$$\mathrm{B} = \mathrm{B}^p(t) \cup \mathrm{B}^e(t) \tag{4.3}$$

BCelasticregiondef

of a *plastic region* $\mathrm{B}^p(t)$ and an *elastic region* $\mathrm{B}^e(t)$ — each assumed closed — that intersect along an *elastic-plastic interface* $\mathcal{I}(t)$ (which need not be connected). Note that the set

$$\mathcal{S}^p(t) \overset{\text{def}}{=} \partial\mathrm{B}^p(t) \cap \partial\mathrm{B} \tag{4.4}$$

BCextplasbdry

— which we refer to as the *external plastic boundary* — represents that portion of $\partial\mathrm{B}^p(t)$ which lies on the external boundary $\partial\mathrm{B}$.

Let $\partial\mathrm{B}^{\mathrm{env}}_{\mathrm{hard}}$ and $\partial\mathrm{B}^{\mathrm{env}}_{\mathrm{free}}$ denote *time-independent* complementary subsurfaces of $\partial\mathrm{B}$, so that

$$\partial\mathrm{B} = \partial\mathrm{B}^{\mathrm{env}}_{\mathrm{hard}} \cup \partial\mathrm{B}^{\mathrm{env}}_{\mathrm{free}}, \tag{4.5}$$

BCdBpartition

with the subsurfaces $\partial\mathrm{B}^{\mathrm{env}}_{\mathrm{hard}}$ and $\partial\mathrm{B}^{\mathrm{env}}_{\mathrm{free}}$ presumed to characterize physical characteristics of the body's environment. Here we limit our discussion to:

(i) *microscopically hard subsurfaces* $\partial\mathrm{B}^{\mathrm{env}}_{\mathrm{hard}}$ that form a *barrier* to flows of glide dislocations;[16]

(ii) *microscopically free subsurfaces* $\partial\mathrm{B}^{\mathrm{env}}_{\mathrm{free}}$ that form *no obstacle* to flows of glide dislocations.

BCmmm

The subsurfaces $\partial\mathrm{B}^{\mathrm{env}}_{\mathrm{hard}}$ and $\partial\mathrm{B}^{\mathrm{env}}_{\mathrm{free}}$ *are related to plastic flow via their intersections with the external plastic boundary* $\mathcal{S}^p(t)$; these are given by

$$\mathcal{S}^p_{\mathrm{hard}}(t) = \partial\mathrm{B}^{\mathrm{env}}_{\mathrm{hard}} \cap \mathcal{S}^p(t) \qquad \text{and} \qquad \mathcal{S}^p_{\mathrm{free}}(t) = \partial\mathrm{B}^{\mathrm{env}}_{\mathrm{free}} \cap \mathcal{S}^p(t), \tag{4.6}$$

BChardfreesub

respectively, and satisfy

$$\mathcal{S}^p(t) = \mathcal{S}^p_{\mathrm{hard}}(t) \cup \mathcal{S}^p_{\mathrm{free}}(t). \tag{4.7}$$

BCSpadecomp

In contrast, the subsurfaces of $\partial\mathrm{B}^{\mathrm{env}}_{\mathrm{hard}}$ and $\partial\mathrm{B}^{\mathrm{env}}_{\mathrm{free}}$ that are *exterior* to $\mathcal{S}^p(t)$ do not affect plastic flow.

Based on the foregoing discussion, we consider boundary conditions which require that, at each time,

$$\begin{aligned} \dot{\gamma}^\alpha(\mathbf{x},t) = 0 \quad &\text{on} \quad \mathcal{S}^p_{\mathrm{hard}}(t), \\ \boldsymbol{\xi}^\alpha(\mathbf{x},t)\cdot\mathbf{n}(\mathbf{x}) = 0 \quad &\text{on} \quad \mathcal{S}^p_{\mathrm{free}}(t). \end{aligned} \tag{4.8}$$

BCDhardbcgold

We refer to $(4.8)_1$ and $(4.8)_2$, respectively, as the *microscopically hard* and *microscopically free boundary conditions* for $\mathcal{S}^p(t)$.

**Remarks**

1. The boundary conditions

$$\begin{gathered} \dot{\gamma}^\alpha = 0 \quad \text{on} \quad \mathcal{S}_{\mathrm{hard}} \quad \text{and} \quad \boldsymbol{\xi}^\alpha\cdot\mathbf{n} = 0 \quad \text{on} \quad \mathcal{S}_{\mathrm{free}}, \\ \mathcal{S}_{\mathrm{hard}} \cup \mathcal{S}_{\mathrm{free}} = \partial\mathrm{B}, \end{gathered} \tag{4.9}$$

GurBC

introduced by Gurtin (2000) and used by him and others[17] are *conceptually incorrect* because they are independent of time and hence incapable of characterizing conditions on the external plastic boundary $\mathcal{S}^p(t)$. Moreover, in (4.9) the role of $\mathcal{S}^p(t)$ is incorrectly played by $\partial\mathrm{B}$.

[15] Cf. Gurtin and Reddy (2014).
[16] For example, a portion of a crystal surface in contact with a hard anvil.
[17] Cf. e.g. Kuroda & Tvergaard (2008a, p.1596).

2. It has been argued by Reddy (2011), and in greater detail by Gurtin and Reddy (2014), that from the point of view of constructing a well-posed problem there is no need to posit "boundary" conditions along the elastic-plastic interface $\mathcal{I}$. Further, Gurtin and Reddy (2014) elaborate on the continuity or otherwise of microscopic quantities across $\mathcal{I}$, and derive from the microscopic virtual-power relation jump conditions for normal components of microscopic stress across $\mathcal{I}$.

### 4.3 Initial conditions

With regard to macroscopic quantities we prescribe the initial displacement and temperature by setting

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x})\,, \qquad \vartheta(\mathbf{x},0) = \vartheta_0(\mathbf{x}) \ \text{ on } \partial\mathrm{B}\,, \tag{4.10}$$

icsmacro

for given functions $\mathbf{u}_0$ and $\vartheta_0$. In addition, it is necessary to specify initial conditions for the slips $\gamma^\alpha$ and the dislocation densities $\rho^\alpha$: we assume these to be given by[18]

$$\gamma^\alpha(\mathbf{x},0) = 0\,, \qquad \rho^\alpha(\mathbf{x},0) = \rho_0^\alpha \ \text{ on } \partial\mathrm{B}\,, \tag{4.11}$$

icsmicro

for a given function $\rho_0^\alpha$.

## 5 The plasticity spaces $\mathcal{H}^\alpha$

plasticityspace

Given a slip-system $\alpha$, we let

$$\mathcal{H}^\alpha = \text{the set of all pairs } \mathfrak{v} = (a, \mathbf{b}) \text{ such that}$$
$$a \text{ is a scalar and } \mathbf{b} \text{ is a vector } \textbf{tangent} \text{ to } \Pi^\alpha, \tag{5.1}$$

Ha

and we endow $\mathcal{H}^\alpha$ with the (natural) **inner product**

$$\mathfrak{a} \bullet \bar{\mathfrak{a}} = a\bar{a} + \mathbf{b}\cdot\bar{\mathbf{b}}, \tag{5.2}$$

circ

so that the norm on $\mathcal{H}^\alpha$ is given by[19]

$$|\mathfrak{v}| = \sqrt{|a|^2 + |\mathbf{b}|^2}. \tag{5.3}$$

Hnorm

We refer to $\mathcal{H}^\alpha$ as to the **plasticity space** for system $\alpha$; and to $a$ and $\mathbf{b}$ as the **scalar** and **vector components** of an element $\mathfrak{v} = (a, \mathbf{b}) \in \mathcal{H}^\alpha$. Note that $\mathcal{H}^\alpha$ is a vector space of dimension 3.

## 6 Generalized slip-rate. Generalized stress

ce

We refer to

$$\dot{\mathbf{\Gamma}}^\alpha \stackrel{\text{def}}{=} (\dot{\gamma}^\alpha, \ell\nabla^\alpha_{\text{tan}}\dot{\gamma}^\alpha) \tag{6.1}$$

Gamma

as the *generalized slip-rate* on $\alpha$; clearly $\dot{\mathbf{\Gamma}}^\alpha \in \mathcal{H}^\alpha$.

Note that — by (5.2), (5.3), and (6.1) — the *generalized scalar slip-rate*, (2.20), takes the simple forms

$$\begin{aligned} \dot{\Gamma}^\alpha_{\text{acc}} &= |\dot{\mathbf{\Gamma}}^\alpha| \\ &= \frac{\dot{\mathbf{\Gamma}}^\alpha}{|\dot{\mathbf{\Gamma}}^\alpha|} \bullet \dot{\mathbf{\Gamma}}^\alpha. \end{aligned} \tag{6.2}$$

dotrhoa

[18] Cf. $(2.22)_2$

[19] We use the symbol $|\cdot|$ for the norm on $\mathcal{H}^\alpha$ and also for the magnitude of a scalar or a vector; it should be clear from the content which is meant.

As a complement to the generalized slip-rate we introduce a *generalized stress*

$$\boldsymbol{\Sigma}^\alpha = (\pi^\alpha, \ell^{-1}\boldsymbol{\xi}^\alpha). \tag{6.3}$$ Sigma

Then, by (5.2), the plastic stress-power takes a form,

$$\boldsymbol{\Sigma}^\alpha \bullet \dot{\boldsymbol{\Gamma}}^\alpha = \pi^\alpha\dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha\cdot\nabla^\alpha_{\rm tan}\dot{\gamma}^\alpha, \tag{6.4}$$ plasstresspow

that allows us to rewrite the free-energy imbalance (3.5) as follows:

$$\dot{\psi} + \eta\dot{\vartheta} + \frac{1}{\vartheta}\mathbf{q}\cdot\nabla\vartheta - \mathbf{T}:\dot{\mathbf{E}}^e - \sum_\alpha \boldsymbol{\Sigma}^\alpha\bullet\dot{\boldsymbol{\Gamma}}^\alpha \le 0. \tag{6.5}$$ thermfei2

# 7 Constitutive theory

ce

## 7.1 Some preliminary constitutive assumptions. Coleman–Noll procedure

prelimce

We seek constitutive relations for the fields $\psi$, $\eta$, $\mathbf{T}$, $\mathbf{q}$, $\boldsymbol{\xi}^\alpha$, and $\pi^\alpha$ compatible with the free-energy imbalance (6.5). We begin by assuming that the free energy, the entropy, the Cauchy stress, and the heat flux are given by the constitutive relations

$$\psi = \hat{\psi}(\mathbf{E}^e,\vartheta,\vec{\rho}), \quad \eta = \hat{\eta}(\mathbf{E}^e,\vartheta,\vec{\rho}), \quad \mathbf{T} = \hat{\mathbf{T}}(\mathbf{E}^e,\vartheta,\vec{\rho}), \quad \mathbf{q} = \hat{\mathbf{q}}(\vartheta,\nabla\vartheta); \tag{7.1}$$ psietaT

and that the free energy is the sum

$$\hat{\psi}(\mathbf{E}^e,\vartheta,\vec{\rho}) = \hat{\psi}^e(\mathbf{E}^e,\vartheta) + \hat{\psi}^p(\vartheta,\vec{\rho}) \tag{7.2}$$ psissep1

of elastic and plastic free energies $\hat{\psi}^e$ and $\hat{\psi}^p$. Our first step is to determine those constitutive restrictions implied by the free-energy imbalance (6.5).[20] We begin by noting, as a consequence of (7.1) and (7.2), that

$$\dot{\psi} = \frac{\partial\hat{\psi}^e(\mathbf{E}^e,\vartheta)}{\partial\mathbf{E}^e}:\dot{\mathbf{E}}^e + \frac{\partial\hat{\psi}(\mathbf{E}^e,\vartheta,\vec{\rho})}{\partial\vartheta}\dot{\vartheta} + \sum_\alpha\frac{\partial\hat{\psi}^p(\vartheta,\vec{\rho})}{\partial\rho^\alpha}\dot{\rho}^\alpha. \tag{7.3}$$ dotpsi

We introduce *thermodynamic forces*

$$F^\alpha_{\rm CW}(\vartheta,\vec{\rho}) \stackrel{\rm def}{=} \frac{\partial\hat{\psi}^p(\vartheta,\vec{\rho})}{\partial\rho^\alpha}, \tag{7.4}$$ Fpsip

and assume these to satisfy

$$F^\alpha_{\rm CW}(\vartheta,\vec{\rho}) > 0. \tag{7.5}$$ Fpsip2

We then find, with the aid of the evolution equation (2.22) for $\rho^\alpha$ and (6.2), that

$$\begin{aligned}\sum_\alpha\frac{\partial\hat{\psi}^p(\vartheta,\vec{\rho})}{\partial\rho^\alpha}\dot{\rho}^\alpha &= \sum_\alpha F^\alpha_{\rm CW}(\vartheta,\vec{\rho})\Big(A^\alpha(\vartheta,\vec{\rho})\dot{\Gamma}^\alpha - R^\alpha(\vartheta,\vec{\rho})\Big) & (7.6)\\ &= \sum_\alpha \underbrace{F^\alpha_{\rm CW}(\vartheta,\vec{\rho})A^\alpha(\vartheta,\vec{\rho})\frac{\dot{\boldsymbol{\Gamma}}^\alpha}{|\dot{\boldsymbol{\Gamma}}^\alpha|}}_{\boldsymbol{\Sigma}^\alpha_{\rm NR}}\bullet\dot{\boldsymbol{\Gamma}}^\alpha - \sum_\alpha F^\alpha_{\rm CW}(\vartheta,\vec{\rho})\,R^\alpha(\vartheta,\vec{\rho}). & (7.7)\end{aligned}$$ newlastterm

[20]Here we use a version of the Coleman–Noll procedure appropriate to single-crystal plasticity.

The under-braced term in (7.7) suggests that we introduce **energetic nonrecoverable generalized stresses** $\boldsymbol{\Sigma}^\alpha_{\rm NR}$ defined by the constitutive relations

$$\boldsymbol{\Sigma}^\alpha_{\rm NR} = F^\alpha_{\rm CW}(\vartheta,\vec{\rho})A^\alpha(\vartheta,\vec{\rho})\,\frac{\dot{\boldsymbol{\Gamma}}^\alpha}{|\dot{\boldsymbol{\Gamma}}^\alpha|}, \tag{7.8}$$ genstressce

for then

$$\boldsymbol{\Sigma}^\alpha_{\rm NR}\bullet\dot{\boldsymbol{\Gamma}}^\alpha$$

has the form of an elastic stress-power. Thus using (7.7) we may write (7.3) as folows;

$$\dot{\psi} = \frac{\partial\hat{\psi}^e(\mathbf{E}^e,\vartheta)}{\partial\mathbf{E}^e}:\dot{\mathbf{E}}^e + \frac{\partial\hat{\psi}(\mathbf{E}^e,\vartheta,\vec{\rho})}{\partial\vartheta}\dot{\vartheta} + \sum_\alpha \boldsymbol{\Sigma}^\alpha_{\rm NR}\bullet\dot{\boldsymbol{\Gamma}}^\alpha - \sum_\alpha F^\alpha_{\rm CW}(\vartheta,\vec{\rho})\,R^\alpha(\vartheta,\vec{\rho}). \tag{7.9}$$ dotpsi2

Finally, by an analog of (6.3)

$$\boldsymbol{\Sigma}^\alpha_{\rm NR} = (\pi^\alpha_{\rm NR},\ell^{-1}\boldsymbol{\xi}^\alpha_{\rm NR}) \tag{7.10}$$ Sigmaen

and (7.8) has the component form

$$\pi^\alpha_{\rm NR} = F^\alpha_{\rm CW}(\vartheta,\vec{\rho})A^\alpha(\vartheta,\vec{\rho})\,\frac{\dot{\gamma}^\alpha}{|\dot{\boldsymbol{\Gamma}}^\alpha|}, \qquad \boldsymbol{\xi}^\alpha_{\rm NR} = \ell^2 F^\alpha_{\rm CW}(\vartheta,\vec{\rho})A^\alpha(\vartheta,\vec{\rho})\,\frac{\nabla^\alpha_{\rm tan}\dot{\gamma}^\alpha}{|\dot{\boldsymbol{\Gamma}}^\alpha|}. \tag{7.11}$$ Sigmaencpts

The quantity $\boldsymbol{\Sigma}^\alpha_{\rm NR}$ represents a generalized energetic stress associated with plastic flow; hence we may define generalized dissipative stresses via the relations

$$\boldsymbol{\Sigma}^\alpha_{\rm dis} = \boldsymbol{\Sigma}^\alpha - \boldsymbol{\Sigma}^\alpha_{\rm NR} \qquad \text{and} \qquad \boldsymbol{\Sigma}^\alpha_{\rm dis} = (\pi^\alpha_{\rm dis},\ell^{-1}\boldsymbol{\xi}^\alpha_{\rm dis}). \tag{7.12}$$ Sigmadis

By (6.1) and $(7.12)_2$

$$\boldsymbol{\Sigma}^\alpha_{\rm dis}\bullet\dot{\boldsymbol{\Gamma}}^\alpha = \pi^\alpha_{\rm dis}\dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha_{\rm dis}\cdot\nabla^\alpha_{\rm tan}\dot{\gamma}^\alpha. \tag{7.13}$$ MHdis0

Next, a consequence of (7.9) and $(7.12)_1$ is that the free-energy imbalance (6.5) becomes

$$\Big(\frac{\partial\hat{\psi}^e(\mathbf{E}^e,\vartheta)}{\partial\mathbf{E}^e} - \hat{\mathbf{T}}(\mathbf{E}^e,\vartheta,\vec{\rho})\Big):\dot{\mathbf{E}}^e + \Big(\frac{\partial\hat{\psi}(\mathbf{E}^e,\vartheta,\vec{\rho})}{\partial\vartheta} + \hat{\eta}(\mathbf{E}^e,\vartheta,\vec{\rho})\Big)\dot{\vartheta}$$
$$- \sum_\alpha \boldsymbol{\Sigma}^\alpha_{\rm dis}\bullet\dot{\boldsymbol{\Gamma}}^\alpha - \sum_\alpha F^\alpha_{\rm CW}(\vartheta,\vec{\rho})\,R^\alpha(\vartheta,\vec{\rho}) + \frac{1}{\vartheta}\hat{\mathbf{q}}(\vartheta,\nabla\vartheta)\cdot\nabla\vartheta \le 0. \tag{7.14}$$ CN1

We assume that — constitutively — the stresses $\boldsymbol{\Sigma}^\alpha_{\rm dis}$ are independent of $\dot{\mathbf{E}}^e$ and $\dot{\vartheta}$; thus, since these rates appear *linearly* in the inequality (7.14), this inequality can hold for all values of $\dot{\mathbf{E}}^e$ and $\dot{\vartheta}$ only if the Cauchy stress and the entropy are given by the constitutive relations

$$\mathbf{T} = \hat{\mathbf{T}}(\mathbf{E}^e,\vartheta) = \frac{\partial\hat{\psi}^e(\mathbf{E}^e,\vartheta)}{\partial\mathbf{E}^e}, \qquad \eta = \hat{\eta}(\mathbf{E}^e,\vartheta,\vec{\rho}) = -\frac{\partial\hat{\psi}(\mathbf{E}^e,\vartheta,\vec{\rho})}{\partial\vartheta}, \tag{7.15}$$ ceTeta

and the free-energy imbalance reduces to a *dissipation inequality*

$$\sum_\alpha \boldsymbol{\Sigma}^\alpha_{\rm dis}\bullet\dot{\boldsymbol{\Gamma}}^\alpha + \sum_\alpha F^\alpha_{\rm CW}(\vartheta,\vec{\rho})\,R^\alpha(\vartheta,\vec{\rho}) - \frac{1}{\vartheta}\hat{\mathbf{q}}(\vartheta,\nabla\vartheta)\cdot\nabla\vartheta \ge 0.$$

Further, assuming that the stresses $\boldsymbol{\Sigma}^\alpha_{\rm dis}$ are independent of $\nabla\vartheta$, we arrive at the *heat-conduction* and *mechanical dissipation inequalities*

$$\hat{\mathbf{q}}(\vartheta,\nabla\vartheta)\cdot\nabla\vartheta \le 0 \qquad \text{and} \qquad \sum_\alpha \boldsymbol{\Sigma}^\alpha_{\rm dis}\bullet\dot{\boldsymbol{\Gamma}}^\alpha + \sum_\alpha F^\alpha_{\rm CW}(\vartheta,\vec{\rho})\,R^\alpha(\vartheta,\vec{\rho}) \ge 0. \tag{7.16}$$ inequalities

By (2.24) and (7.5)

$$F^{\alpha}_{\rm CW}(\vartheta,\vec{\rho})\,R^{\alpha}(\vartheta,\vec{\rho}) \geq 0, \tag{7.17}$$ FRge0

a result central to what follows. Further, we assume that the material is *strongly dissipative* in the sense that

$$\boldsymbol{\Sigma}^{\alpha}_{\rm dis} \bullet \dot{\boldsymbol{\Gamma}}^{\alpha} \geq 0 \tag{7.18}$$ inequalities3

*for each* $\alpha$.

Dissipation is therefore characterized by the three inequalities,

$$\hat{\mathbf{q}}(\vartheta,\nabla\vartheta)\cdot\nabla\vartheta \leq 0, \quad \boldsymbol{\Sigma}^{\alpha}_{\rm dis} \bullet \dot{\boldsymbol{\Gamma}}^{\alpha} \geq 0, \quad F^{\alpha}_{\rm CW}(\vartheta,\vec{\rho})\,R^{\alpha}(\vartheta,\rho^{\alpha}) \geq 0, \tag{7.19}$$ inequalities

with the second and third of these required to hold for all slip-systems $\alpha$. These inequalities are of three distinct types, but only two have a more or less standard structure: the first, $-\vartheta\,\mathbf{q}\cdot\nabla\vartheta$, represents dissipation associated with the flow of heat; the second $\boldsymbol{\Sigma}^{\alpha}_{\rm dis}\bullet\dot{\boldsymbol{\Gamma}}^{\alpha}$, represents stress-power. But the third type, $F^{\alpha}_{\rm CW}R^{\alpha}$, being *atypical of quantities that characterize dissipation*, requires some discussion. First of all,[21]

$$F^{\alpha}_{\rm CW} = \frac{\partial\psi^{p}}{\partial\rho^{\alpha}}$$

represents a thermodynamic *force* associated with the presence of glide dislocations and GNDs on system $\alpha$. Secondly, a consequence of the bulleted remark containing (2.24) is that $-R^{\alpha}$ represents a *recovery rate* for such dislocations; that is, a decrease-rate in dislocation density due to heating. Thus the product $F^{\alpha}_{\rm CW}R^{\alpha}$ represents a *force-power*. But what is most important, consistent with our use of the term *dissipation inequality* for $F^{\alpha}_{\rm CW}R^{\alpha} \geq 0$, and a consequence of the requirement that[22] $F^{\alpha}_{\rm CW} > 0$ and $R^{\alpha} \geq 0$ is that

$$R^{\alpha} > 0 \quad\Longrightarrow\quad F^{\alpha}_{\rm CW}R^{\alpha} > 0, \tag{7.20}$$ diswithrecovery

and hence that

recdis • *recovery represents a dissipative process.*

**Remark** It is important to note that the expression (7.8) is valid only when $\dot{\boldsymbol{\Gamma}}^{\alpha} \neq \mathbf{0}$. Reddy (2011) has proposed a formulation for energetic microstresses of this nature that circumvents complications arising when the generalized slip rate is zero. This is achieved by extending the definition to include the case in which $\dot{\boldsymbol{\Gamma}}^{\alpha} = \mathbf{0}$. The microstress is then defined by

$$\boldsymbol{\Sigma}^{\alpha}_{\rm NR} = F^{\alpha}_{\rm CW}A^{\alpha}\frac{\dot{\boldsymbol{\Gamma}}^{\alpha}}{|\dot{\boldsymbol{\Gamma}}^{\alpha}|} \qquad \text{if } \dot{\boldsymbol{\Gamma}}^{\alpha} \neq \mathbf{0}\,, \tag{7.21a}$$

$$\boldsymbol{\Sigma}^{\alpha}_{\rm NR} \bullet \tilde{\boldsymbol{\Gamma}}^{\alpha} \leq F^{\alpha}_{\rm CW}A^{\alpha}|\tilde{\boldsymbol{\Gamma}}^{\alpha}| \qquad \text{if } \dot{\boldsymbol{\Gamma}}^{\alpha} = \mathbf{0} \text{ for all } \tilde{\boldsymbol{\Gamma}}^{\alpha} \in \mathcal{H}^{\alpha}. \tag{7.21b}$$

Sigmaalt *Equivalently*, we define the function $\phi$ by

$$\phi(\vartheta,\vec{\rho},\dot{\boldsymbol{\Gamma}}^{\alpha}) = F^{\alpha}_{\rm CW}(\vartheta,\vec{\rho})A^{\alpha}(\vartheta,\vec{\rho})|\dot{\boldsymbol{\Gamma}}^{\alpha}|\,; \tag{7.22}$$ phiSigma

then the relations (7.21) are equivalent to the inequality

$$\phi(\tilde{\boldsymbol{\Gamma}}^{\alpha}) \geq \phi(\dot{\boldsymbol{\Gamma}}^{\alpha}) + \boldsymbol{\Sigma}^{\alpha}_{\rm NR} \bullet (\tilde{\boldsymbol{\Gamma}}^{\alpha} - \dot{\boldsymbol{\Gamma}}^{\alpha})\,, \tag{7.23}$$ phiineq

[21] Cf. (7.4).
[22] Cf. $(2.24)_1$, (7.5).

in which $\tilde{\boldsymbol{\Gamma}}^\alpha$ is an arbitrary generalized slip-rate. Here, for convenience we have written $\phi(\vartheta, \vec{\rho}, \dot{\boldsymbol{\Gamma}}^\alpha) \equiv \phi(\dot{\boldsymbol{\Gamma}}^\alpha)$. Note that the function $\phi$ is convex, positively homogeneous, and differentiable except at $\dot{\boldsymbol{\Gamma}}^\alpha = \mathbf{0}$. For $\dot{\boldsymbol{\Gamma}}^\alpha \neq \mathbf{0}$ one can show that (7.23) becomes

$$\boldsymbol{\Sigma}^\alpha_{\rm NR} = \frac{\partial \phi}{\partial \dot{\boldsymbol{\Gamma}}^\alpha},$$

which is equivalent to (7.21a). The advantage of the formulation (7.23) is that it accommodates all values of $\dot{\boldsymbol{\Gamma}}^\alpha$ in a single expression.

## 7.2 Further consequences of thermodynamics

Further, (7.9) and (7.15) imply that

$$\dot{\psi} = \mathbf{T} : \dot{\mathbf{E}}^e - \eta\dot{\vartheta} + \sum_\alpha \boldsymbol{\Sigma}^\alpha_{\rm NR} \bullet \dot{\boldsymbol{\Gamma}}^\alpha - \sum_\alpha F^\alpha_{\rm CW}\, R^\alpha, \qquad (7.24)$$ ndotpsi3

where, for brevity, we have introduced the notation

$$F^\alpha_{\rm CW} = F^\alpha_{\rm CW}(\vartheta, \vec{\rho}), \qquad \text{and} \qquad R^\alpha = R^\alpha(\vartheta, \vec{\rho}). \qquad (7.25)$$ shorthand1

Hence temporal changes in the free energy as described by (7.24) may be viewed as the sum of

a *net stress power*

$$\underbrace{\mathbf{T} : \dot{\mathbf{E}}^e}_{\substack{\text{elastic}\\ \text{stress power}}} + \underbrace{\sum_\alpha \boldsymbol{\Sigma}^\alpha_{\rm NR} \bullet \dot{\boldsymbol{\Gamma}}^\alpha}_{\substack{\text{plastic energetic}\\ \text{stress power}}}, \qquad (7.26)$$ npsidot

an *entropic free-energy change* $-\eta\dot{\vartheta}$,

and a *decrease*

$$-\sum_\alpha F^\alpha_{\rm CW}\, R^\alpha$$

mmm in free-energy.

Further, from (7.24) and (3.4)

$$\dot{\varepsilon} = \vartheta\dot{\eta} + \mathbf{T} : \dot{\mathbf{E}}^e + \sum_\alpha \boldsymbol{\Sigma}^\alpha_{\rm NR} \bullet \dot{\boldsymbol{\Gamma}}^\alpha - \sum_\alpha F^\alpha_{\rm CW}\, R^\alpha, \qquad (7.27)$$ gr525

using which, balance of energy $(3.3)_1$ may be written as

$$\vartheta\dot{\eta} = -\mathrm{div}\,\mathbf{q} + q + \sum_\alpha \boldsymbol{\Sigma}^\alpha_{\rm dis} \bullet \dot{\boldsymbol{\Gamma}}^\alpha + \sum_\alpha F^\alpha_{\rm CW}\, R^\alpha\,. \qquad (7.28)$$ etabal

Granted the thermodynamically restricted constitutive relations (7.15), this entropy relation is equivalent to balance of energy.

Next, the expression (3.4) for the free energy together with $(7.1)_{1,2}$ yield a subsidiary relation

$$\varepsilon = \hat{\varepsilon}(\mathbf{E}^e, \vartheta, \vec{\rho}) = \hat{\psi}(\mathbf{E}^e, \vartheta, \vec{\rho}) + \vartheta\hat{\eta}(\mathbf{E}^e, \vartheta, \vec{\rho}) \qquad (7.29)$$ nepsub

for the internal energy, and an important consequence of this relation and $(7.15)_2$ is that

$$\frac{\partial \hat{\varepsilon}(\mathbf{E}^e, \vartheta, \vec{\rho})}{\partial \vartheta} = \vartheta \frac{\partial \hat{\eta}(\mathbf{E}^e, \vartheta, \vec{\rho})}{\partial \vartheta}. \qquad (7.30)$$ npardsep=thetpardset

In addition, differentiating the expression (7.2) with respect to $\vartheta$ we find, upon using $(7.15)_2$, a decomposition

$$\hat{\eta}(\mathbf{E}^e, \vartheta, \vec{\rho}) = \hat{\eta}^e(\mathbf{E}^e, \vartheta) + \hat{\eta}^p(\vartheta, \vec{\rho}) \tag{7.31}$$

npsissep

of the entropy into elastic and plastic entropies

$$\hat{\eta}^e(\mathbf{E}^e, \vartheta) = -\frac{\partial \hat{\psi}^e(\mathbf{E}^e, \vartheta)}{\partial \vartheta}, \qquad \hat{\eta}^p(\vartheta, \vec{\rho}) = -\frac{\partial \hat{\psi}^p(\vartheta, \vec{\rho})}{\partial \vartheta}. \tag{7.32}$$

netaep

Next, as is standard, the *heat capacity* is defined by

$$c = c(\mathbf{E}^e, \vartheta, \vec{\rho}) \stackrel{\text{def}}{=} \frac{\partial \hat{\varepsilon}(\mathbf{E}^e, \vartheta, \vec{\rho})}{\partial \vartheta}, \tag{7.33}$$

spheat1a

and assumed to be strictly positive. Using (7.30) through (7.32), the heat capacity is alternatively given by

$$c(\mathbf{E}^e, \vartheta, \vec{\rho}) = -\vartheta\Big(\frac{\partial^2 \hat{\psi}^e(\mathbf{E}^e, \vartheta)}{\partial \vartheta^2} + \frac{\partial^2 \hat{\psi}^p(\vartheta, \vec{\rho})}{\partial \vartheta^2}\Big). \tag{7.34}$$

spheat3a

Thus, from (7.31), (7.32), and (7.34)

$$\vartheta\,\dot{\eta} = -\vartheta\,\frac{\partial^2 \hat{\psi}^e(\mathbf{E}^e, \vartheta)}{\partial \vartheta\,\partial \mathbf{E}^e} : \dot{\mathbf{E}}^e - \vartheta \sum_\alpha \frac{\partial^2 \hat{\psi}^p(\vartheta, \vec{\rho})}{\partial \vartheta\,\partial \rho}\,\dot{\rho}^\alpha + c(\mathbf{E}^e, \vartheta, \vec{\rho})\,\dot{\vartheta}\,. \tag{7.35}$$

heat1

The use of (7.35) in (7.28) gives the following partial differential equation

$$\begin{aligned} c(\mathbf{E}^e, \vartheta, \vec{\rho})\dot{\vartheta} = -\mathrm{div}\mathbf{q} + q + \sum_\alpha \mathbf{\Sigma}^\alpha_{\mathrm{dis}} \bullet \dot{\mathbf{\Gamma}}^\alpha + \sum_\alpha F^\alpha_{\mathrm{CW}}\, R^\alpha \\ + \vartheta\,\frac{\partial^2 \hat{\psi}^e(\mathbf{E}^e, \vartheta)}{\partial \vartheta\,\partial \mathbf{E}^e} : \dot{\mathbf{E}}^e + \sum_\alpha \vartheta\,\frac{\partial^2 \hat{\psi}^p(\vartheta, \vec{\rho})}{\partial \vartheta\,\partial \rho}\,\dot{\rho}^\alpha \end{aligned}$$

for the temperature. By $(7.15)_1$ and (7.4), the last equation can be written in the form

$$\begin{aligned} c(\mathbf{E}^e, \vartheta, \vec{\rho})\dot{\vartheta} = -\mathrm{div}\mathbf{q} + q + \sum_\alpha \mathbf{\Sigma}^\alpha_{\mathrm{dis}} \bullet \dot{\mathbf{\Gamma}}^\alpha + \sum_\alpha F^\alpha_{\mathrm{CW}}\, R^\alpha \\ + \vartheta\Big(\frac{\partial \hat{\mathbf{T}}(\mathbf{E}^e, \vartheta)}{\partial \vartheta}\Big) : \dot{\mathbf{E}}^e + \sum_\alpha \vartheta\,\frac{\partial F^\alpha_{\mathrm{CW}}}{\partial \vartheta}\,\dot{\rho}^\alpha\,, \end{aligned} \tag{7.36}$$

etabal3c

so that with

$$\mathbf{M} = \mathbf{M}(\mathbf{E}^e, \vartheta) \stackrel{\text{def}}{=} \vartheta\,\frac{\partial \hat{\mathbf{T}}(\mathbf{E}^e, \vartheta)}{\partial \vartheta} \tag{7.37}$$

etabal3d

defining a *stress-temperature modulus*, and noting from (7.12), (6.4), and (7.8) that

$$\sum_\alpha \mathbf{\Sigma}^\alpha_{\mathrm{dis}} \bullet \dot{\mathbf{\Gamma}}^\alpha + \sum_\alpha F^\alpha_{\mathrm{CW}}\, R^\alpha = \sum_\alpha \pi^\alpha \dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha \cdot \nabla^\alpha_{\tan} \dot{\gamma}^\alpha - \sum_\alpha F^\alpha_{\mathrm{CW}} \dot{\rho}^\alpha,$$

we may rewrite (7.36) as

$$\begin{aligned} c(\mathbf{E}^e, \vartheta, \vec{\rho})\dot{\vartheta} = -\mathrm{div}\mathbf{q} + q + \sum_\alpha \pi^\alpha \dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha \cdot \nabla^\alpha_{\tan} \dot{\gamma}^\alpha \\ + \mathbf{M} : \dot{\mathbf{E}}^e - \sum_\alpha \Big(F^\alpha_{\mathrm{CW}} - \vartheta\,\frac{\partial F^\alpha_{\mathrm{CW}}}{\partial \vartheta}\Big)\,\dot{\rho}^\alpha\,. \end{aligned} \tag{7.38}$$

etabal3e

Next, multiplying the microscopic force balance (2.34) by $\dot{\gamma}^\alpha$ we obtain

$$\sum_\alpha \tau^\alpha \dot{\gamma}^\alpha = \sum_\alpha \big(\pi^\alpha \dot{\gamma}^\alpha - \dot{\gamma}^\alpha \mathrm{div}\, \boldsymbol{\xi}^\alpha\big), \tag{7.39}$$

Dmfbet

use of which in (7.38) gives

$$c(\mathbf{E}^e, \vartheta, \vec{\rho})\dot{\vartheta} + \mathrm{div}\mathbf{q} - q = \sum_\alpha \tau^\alpha \dot{\gamma}^\alpha - \sum_\alpha \Big(F^\alpha_{\rm CW} - \vartheta\,\frac{\partial F^\alpha_{\rm CW}}{\partial \vartheta}\Big)\,\dot{\rho}^\alpha + \mathbf{M}\colon\dot{\mathbf{E}}^e + \sum_\alpha \mathrm{div}\,(\dot{\gamma}^\alpha \boldsymbol{\xi}^\alpha)\,. \tag{7.40}$$

etabal3f

This form of the energy balance is the main result of this section.

## 7.3 The Mises–Hill framework

MHframe

This section is based on an alternative framework for gradient single-crystal plasticity — due to Reddy (2011) — that generalizes the conventional *rate-independent* Mises–Hill theory.[23]

We introduce, for each slip-system $\alpha$,

(i) a *yield function*

$$\mathcal{F}^\alpha(\boldsymbol{\Sigma}^\alpha_{\rm dis}, \vec{\rho}, \vartheta) = |\boldsymbol{\Sigma}^\alpha_{\rm dis}| - Y^\alpha(\vec{\rho}, \vartheta) \tag{7.41}$$

yieldfunction

with *slip resistance* $Y^\alpha(\vec{\rho}, \vartheta)$ consistent with

$$Y^\alpha(\vec{\rho}, \vartheta) > 0 \qquad \text{and} \qquad Y^\alpha(\vec{\rho}_0, \vartheta_0) > 0, \tag{7.42}$$

Halpha

where $Y^\alpha(\vec{\rho}_0, \vartheta_0)$ and $Y^\alpha(\vec{\rho}, \vartheta)$ represent the *initial and current values* of the plastic flow resistance, while $\vec{\rho}_0$ and $\vartheta_0$ represent the initial values of the dislocation densities $\vec{\rho}$ and temperature $\vartheta$.[24]

(ii) a *normality relation*[25]

$$\dot{\boldsymbol{\Gamma}}^\alpha = \lambda^\alpha \frac{\boldsymbol{\Sigma}^\alpha_{\rm dis}}{|\boldsymbol{\Sigma}^\alpha_{\rm dis}|} \quad \text{for } \boldsymbol{\Sigma}^\alpha_{\rm dis} \neq \mathbf{0}, \tag{7.43}$$

norel

with $\lambda^\alpha$ a scalar multiplier, together with *complementarity conditions*

$$\mathcal{F}^\alpha(\boldsymbol{\Sigma}^\alpha_{\rm dis}, \vec{\rho}, \vartheta) \le 0, \qquad \lambda^\alpha \ge 0, \qquad \lambda^\alpha \mathcal{F}^\alpha(\boldsymbol{\Sigma}^\alpha_{\rm dis}, \vec{\rho}, \vartheta) = 0. \tag{7.44}$$

comps

By (6.1) and $(7.12)_2$ the normality relation (7.43) may be written in the "component form"

$$\left.\begin{aligned} \dot{\gamma}^\alpha &= \lambda^\alpha \frac{\pi^\alpha_{\rm dis}}{\sqrt{|\pi^\alpha_{\rm dis}|^2 + \ell^{-2}|\boldsymbol{\xi}^\alpha_{\rm dis}|^2}} \\ \nabla^\alpha_{\rm tan}\dot{\gamma}^\alpha &= \lambda^\alpha \frac{\ell^{-2}\boldsymbol{\xi}^\alpha_{\rm dis}}{\sqrt{|\pi^\alpha_{\rm dis}|^2 + \ell^{-2}|\boldsymbol{\xi}^\alpha_{\rm dis}|^2}} \end{aligned}\right\} \quad \text{for} \quad \boldsymbol{\Sigma}^\alpha_{\rm dis} \neq \mathbf{0}. \tag{7.45}$$

floweqt

In addition, (7.43) implies that

$$\lambda^\alpha = |\dot{\boldsymbol{\Gamma}}^\alpha| \quad \text{for} \quad \boldsymbol{\Sigma}^\alpha_{\rm dis} \neq \mathbf{0}, \tag{7.46}$$

lamsig

[23] Cf., e. g., Simo and Hughes (1998), Han and Reddy (2013).

[24] Initial value here means the value at the onset of plastic flow.

[25] Or equivalently $\dot{\boldsymbol{\Gamma}}^\alpha = \lambda^\alpha\, \partial\mathcal{F}^\alpha/\partial\boldsymbol{\Sigma}^\alpha_{\rm dis}$.

and yields the *codirectionality relation*

$$\frac{\dot{\mathbf{\Gamma}}^\alpha}{|\dot{\mathbf{\Gamma}}^\alpha|} = \frac{\mathbf{\Sigma}^\alpha_{\rm dis}}{|\mathbf{\Sigma}^\alpha_{\rm dis}|}. \tag{7.47}$$
codir

Important physical consequences of the normality relation and the complementarity conditions are the *plastic-flow conditions*

$$\left.\begin{aligned} |\mathbf{\Sigma}^\alpha_{\rm dis}| \le Y^\alpha(\vec{\rho},\vartheta), \\ \dot{\mathbf{\Gamma}}^\alpha \ne \mathbf{0} \quad \Rightarrow \quad |\mathbf{\Sigma}^\alpha_{\rm dis}| = Y^\alpha(\vec{\rho},\vartheta), \\ |\mathbf{\Sigma}^\alpha_{\rm dis}| < Y^\alpha(\vec{\rho},\vartheta) \quad \Rightarrow \quad \dot{\mathbf{\Gamma}}^\alpha = \mathbf{0}. \end{aligned}\right\} \tag{7.48}$$
plasticflowconditions

The first of (7.48), a consequence of $(7.44)_1$, defines the *elastic range*. The second defines the *yield condition*

$$|\mathbf{\Sigma}^\alpha_{\rm dis}| = Y^\alpha(\vec{\rho},\vartheta).$$

The third, which we refer to as the *no-flow condition*, asserts that there be no flow interior to the elastic range.

Conversely, granted the normality relation, so that (7.46) is satisfied, the plastic-flow conditions imply that $\lambda^\alpha = |\dot{\mathbf{\Gamma}}^\alpha|$ for $\dot{\mathbf{\Gamma}}^\alpha \ne \mathbf{0}$ and that the complementarity conditions (7.44) are satisfied. Thus, granted the normality relation, we may replace the complementarity conditions by the *reduced complementarity conditions*

$$\mathcal{F}^\alpha(\mathbf{\Sigma}^\alpha_{\rm dis},\vec{\rho},\vartheta) \le 0, \qquad \dot{\mathbf{\Gamma}}^\alpha \mathcal{F}^\alpha(\mathbf{\Sigma}^\alpha_{\rm dis},\vec{\rho},\vartheta) = \mathbf{0}. \tag{7.49}$$
reducedcomps

Next, using (7.41), $(7.48)_2$, and (7.47) we can invert the normality relation (7.43) and arrive at an equation — called the *flow rule* — that does not involve the multiplier $\lambda^\alpha$:

$$\mathbf{\Sigma}^\alpha_{\rm dis} = Y^\alpha(\vec{\rho},\vartheta)\frac{\dot{\mathbf{\Gamma}}^\alpha}{|\dot{\mathbf{\Gamma}}^\alpha|} \quad \text{for } \dot{\mathbf{\Gamma}}^\alpha \ne \mathbf{0}. \tag{7.50}$$
invertednorel

By (6.1) and (7.12) we can express the flow rule (7.50) in terms of the stresses $\pi^\alpha_{\rm dis}$ and $\boldsymbol{\xi}^\alpha_{\rm dis}$:

$$\left.\begin{aligned} \pi^\alpha_{\rm dis} &= Y^\alpha(\vec{\rho},\vartheta)\frac{\dot{\gamma}^\alpha}{\sqrt{|\dot{\gamma}^\alpha|^2 + \ell^2|\nabla^\alpha_{\rm tan}\dot{\gamma}^\alpha|^2}} \\ \boldsymbol{\xi}^\alpha_{\rm dis} &= Y^\alpha(\vec{\rho},\vartheta)\frac{\ell^2\nabla^\alpha_{\rm tan}\dot{\gamma}^\alpha}{\sqrt{|\dot{\gamma}^\alpha|^2 + \ell^2|\nabla^\alpha_{\rm tan}\dot{\gamma}^\alpha|^2}} \end{aligned}\right\} \quad \text{for } \dot{\mathbf{\Gamma}}^\alpha \ne \mathbf{0}. \tag{7.51}$$
cptinvertednorel

Note that by (7.50), the mechanical dissipation inequalities (7.18) become

$$Y^\alpha(\vec{\rho},\vartheta)\dot{\Gamma}^\alpha_{\rm acc} \ge 0 \qquad \text{for each } \alpha, \tag{7.52}$$
mechdissip

and by $(7.42)_1$ are satisfied.

completecondts **Remark** The elastic-range inequality $(7.48)_1$ and the flow rule (7.50) together imply the remaining plastic-flow conditions $(7.48)_{2,3}$ and hence may be viewed as representing (a complete set of) *constitutive relations for plastic flow*. We associate the flow rule (7.50) with the reduced complementarity conditions (7.49), which also do not involve $\lambda^\alpha$.

**Remark** A consequence of the flow rule (7.50) is that the mechanical *dissipation* $(7.18)_1$ is given by a function of the form

$$D^\alpha(\dot{\mathbf{\Gamma}}^\alpha,\vec{\rho},\vartheta) = Y^\alpha(\vec{\rho},\vartheta)|\dot{\mathbf{\Gamma}}^\alpha|\,. \tag{7.53}$$
deltafn

Then the flow relation (7.43) together with (7.44) can be shown to be *equivalent* to the inequality

$$D(\tilde{\mathbf{\Gamma}}^{\alpha}, \vec{\rho}, \vartheta) \geq D(\dot{\mathbf{\Gamma}}^{\alpha}, \vec{\rho}, \vartheta) + \mathbf{\Sigma}^{\alpha}_{\text{dis}} \bullet (\tilde{\mathbf{\Gamma}}^{\alpha} - \dot{\mathbf{\Gamma}}^{\alpha}) \tag{7.54}$$

ineqD

for arbitrary $\tilde{\mathbf{\Gamma}}^{\alpha} = (\tilde{\gamma}^{\alpha}, \ell\nabla^{\alpha}_{\text{tan}}\tilde{\gamma}^{\alpha})$.

The equivalence may be seen as follows[26]: first, for $\dot{\mathbf{\Gamma}}^{\alpha} = \mathbf{0}$ (7.54) with (7.53) reduces to

$$Y^{\alpha}(\vec{\rho}, \vartheta)|\tilde{\mathbf{\Gamma}}^{\alpha}| \geq \mathbf{\Sigma}^{\alpha}_{\text{dis}} \bullet \tilde{\mathbf{\Gamma}}^{\alpha}$$

which holds if and only if

$$|\mathbf{\Sigma}^{\alpha}_{\text{dis}}| \leq Y^{\alpha};$$

that is, the dissipative generalized stress must lie in the elastic range. On the other hand, for $\dot{\mathbf{\Gamma}}^{\alpha} \neq \mathbf{0}$ the relation (7.54) becomes

$$Y^{\alpha}(|\tilde{\mathbf{\Gamma}}^{\alpha}| - |\dot{\mathbf{\Gamma}}^{\alpha}|) - \mathbf{\Sigma}^{\alpha}_{\text{dis}} \bullet (\tilde{\mathbf{\Gamma}}^{\alpha} - \dot{\mathbf{\Gamma}}^{\alpha}) \geq 0\,,$$

which can be shown to be equivalent to

$$\mathbf{\Sigma}^{\alpha}_{\text{dis}} = \frac{\partial}{\partial \dot{\mathbf{\Gamma}}^{\alpha}} \Big( Y^{\alpha}(|\dot{\mathbf{\Gamma}}^{\alpha}|\Big)\,;$$

this is precisely (7.50).

# 8 Plastic free energy

interactions

The constitutive relation $\psi^{p} = \hat{\psi}^{p}(\vartheta, \vec{\rho})$ for the plastic free energy is capable of accounting for interactions between slip systems via dependencies on the dislocation densities $\rho^{\alpha}$ on different slip systems. However, at this point in time the physical mechanisms and reasons for such interactions are not clear, and because an accounting for such interactions is beyond the scope of this study,

- *we henceforth neglect slip-system interactions in the plastic free-energy.*

Consistent with this we assume that the constitutive relation for the plastic free-energy has the form

$$\psi^{p} = \hat{\psi}^{p}(\vartheta, \vec{\rho}) = \sum_{\alpha} \bar{\psi}^{p}(\vartheta, \rho^{\alpha}), \tag{8.1}$$

aanointce

where — importantly — given any choice of $\vartheta$ we use the *same function* $\bar{\psi}^{p}(\vartheta, \cdot)$ for all slip systems, leaving it up to the *argument* $\rho^{\alpha}$ of $\bar{\psi}^{p}(\vartheta, \rho^{\alpha})$ to indicate the slip-system $\alpha$ in question. As a consequence the constitutive relation (8.1) does not involve interactions between slip systems. Similarly, using (7.32) we are led to a corresponding relation for the plastic entropy; viz.

$$\eta^{p} = \hat{\eta}^{p}(\vartheta, \vec{\rho}) = \sum_{\alpha} \bar{\eta}^{p}(\vartheta, \rho^{\alpha}). \tag{8.2}$$

anointetace

[26]see Gurtin & Reddy (2014), Section 5.2 for a similar argument in the purely mechanical setting.

## 9 The internal energy and entropy of cold work

Important to the determination of the internal energy and entropy of cold work is the *heat capacity* defined by (7.33), in which the heat capacity is possibly dependent on the dislocation densities $\vec{\rho}$. As reviewed by Bever, Holt & Titchener (1973, §1.3.4), a number of researchers have previously recognized the possibility that the dislocations produced by cold working may alter the heat capacity of a material by changing the modes of atomic vibrations of the metal, and to investigate such a possibility these researchers compared the measured heat capacities of both annealed and heavily cold worked metals, that is metals with low and high dislocation densities, respectively. The differences in the measured heat capacities for a given metal with low and high dislocation densities were seldom found to be more than a fraction of one percent. Accordingly, following Lubliner (1972) and Rosakis, Rosakis, Ravichandran and Hodowany (2000), to generate our candidates for the internal energy and entropy of cold work, we assume here that

- the heat capacity is independent of the dislocation densities $\vec{\rho}$; viz.

$$c = c(\mathbf{E}^e, \vartheta). \tag{9.1}$$ cforn

Granted this, (7.34) and (8.1) imply that

$$\frac{\partial}{\partial \rho^\alpha}\left(\frac{\partial^2 \bar{\psi}^p(\vartheta, \rho^\alpha)}{\partial \vartheta^2}\right) = \frac{\partial^2}{\partial \vartheta^2}\left(\frac{\partial \bar{\psi}^p(\vartheta, \rho^\alpha)}{\partial \rho^\alpha}\right) = 0 \tag{9.2}$$ consequence

for each slip system $\alpha$. Thus we choose a slip-system $\alpha$, write

$$\varrho = \rho^\alpha,$$

and find as a consequence of (9.2) that $\partial \bar{\psi}^p(\vartheta, \varrho)/\partial \varrho$ is linear in $\vartheta$,

$$\frac{\partial \bar{\psi}^p(\vartheta, \varrho)}{\partial \varrho} = a(\varrho) + \vartheta b(\varrho). \tag{9.3}$$ midCW

Assuming that $\bar{\psi}^p(\vartheta, 0) = 0$, and noting that

free energy = internal energy - (temperature)entropy

represents the generic structure of a free energy, we find, upon integrating (9.3) from $\varrho = 0$ to an arbitrary value $\varrho = \rho^\alpha$, a relation of the form

$$\bar{\psi}^p(\vartheta, \rho^\alpha) = E_{\rm CW}(\rho^\alpha) - \vartheta N_{\rm CW}(\rho^\alpha) \tag{9.4}$$ CWs

with $E_{\rm CW}(0) = N_{\rm CW}(0) = 0$. The constitutive relation (8.1) for the plastic free-energy therefore takes the form

$$\begin{gathered} \hat{\psi}^p(\vartheta, \vec{\rho}) = \hat{\varepsilon}^p_{\rm CW}(\vec{\rho}) - \vartheta \hat{\eta}^p_{\rm CW}(\vec{\rho}), \\ \hat{\varepsilon}^p_{\rm CW}(\vec{\rho}) = \sum_\alpha E_{\rm CW}(\rho^\alpha), \qquad \hat{\eta}^p_{\rm CW}(\vec{\rho}) = \sum_\alpha N_{\rm CW}(\rho^\alpha), \end{gathered} \tag{9.5}$$ CW

or, equivalently,

$$\hat{\psi}^p(\vartheta, \vec{\rho}) = \sum_\alpha \bar{\psi}^p(\vartheta, \rho^\alpha). \tag{9.6}$$ psipCW

We refer to

$$\varepsilon^p_{\rm CW} = \hat{\varepsilon}^p_{\rm CW}(\vec{\rho}) \qquad \text{and} \qquad \eta^p_{\rm CW} = \hat{\eta}^p_{\rm CW}(\vec{\rho}) \tag{9.7}$$ CWvallues

as the *internal energy* and *entropy of cold work*. A consequence of $(9.5)_{2,3}$ is that this energy and entropy do not involve interactions between slip systems.

Next, by $(9.5)_1$

$$\hat{\eta}_{\rm CW}(\vec{\rho}) = -\frac{\partial \hat{\psi}^p(\vartheta, \vec{\rho})}{\partial \vartheta}, \tag{9.8}$$

justetCW

as might be expected. Moreover, $(7.15)_2$, (7.2), and (9.8) imply that

$$\eta = -\frac{\partial \hat{\psi}^e(\mathbf{E}^e, \vartheta)}{\partial \vartheta} + \hat{\eta}_{\rm CW}(\vec{\rho}),$$

and hence defining

$$\eta^e = \hat{\eta}^e(\mathbf{E}^e, \vartheta) = -\frac{\partial \hat{\psi}^e(\mathbf{E}^e, \vartheta)}{\partial \vartheta}, \tag{9.9}$$

ceetae

we see that $\eta$ is the sum

$$\eta = \hat{\eta}^e(\mathbf{E}^e, \vartheta) + \hat{\eta}^p_{\rm CW}(\vec{\rho}) \tag{9.10}$$

etasum

of elastic and plastic entropies. Finally, (7.34) and (9.10) imply that

$$c(\mathbf{E}^e, \vartheta) = \vartheta \frac{\partial \hat{\eta}^e(\mathbf{E}^e, \vartheta)}{\partial \vartheta}. \tag{9.11}$$

cfinal

We let

$$f^\alpha_{\rm CW}(\vec{\rho}) = \frac{\partial \hat{\varepsilon}^p_{\rm CW}(\vec{\rho})}{\partial \rho^\alpha} \qquad \text{and} \qquad g^\alpha_{\rm CW}(\vec{\rho}) = \frac{\partial \hat{\eta}^p_{\rm CW}(\vec{\rho})}{\partial \rho^\alpha} \tag{9.12}$$

thermenforces2

denote *thermodynamic forces* associated with the internal energy and entropy of cold work and note that, by $(9.5)_{2,3}$,

$$\begin{aligned} f^\alpha_{\rm CW}(\vec{\rho}) &= E'_{\rm CW}(\rho^\alpha) \stackrel{\rm def}{=} f_{\rm CW}(\rho^\alpha) \\ g^\alpha_{\rm CW}(\vec{\rho}) &= N'_{\rm CW}(\rho^\alpha) \stackrel{\rm def}{=} g_{\rm CW}(\rho^\alpha), \end{aligned} \tag{9.13}$$

simpfstherm

where a prime is used to denote the derivative of a function of a single scalar variable. We refer to $f_{\rm CW}(\rho^\alpha)$ and $g_{\rm CW}(\rho^\alpha)$ as the *internal-energetic* and *entropic forces* for slip-system $\alpha$.

We assume that

$$f_{\rm CW}(\rho^\alpha) > 0 \qquad \text{and} \qquad g_{\rm CW}(\rho^\alpha) > 0. \tag{9.14}$$

f>0

Then (6.2), (9.7), (9.12), and (9.13) imply that

$$\begin{aligned} \dot{\varepsilon}^p_{\rm CW} &= \sum_\alpha f_{\rm CW}(\rho^\alpha)\dot{\rho}^\alpha \\ \dot{\eta}^p_{\rm CW} &= \sum_\alpha g_{\rm CW}(\rho^\alpha)\dot{\rho}^\alpha. \end{aligned} \tag{9.15}$$

secw

disorderremark **Remark** The requirement that the entropic force satisfy

$$g_{\rm CW}(\rho^\alpha) = \frac{\partial \hat{\eta}_{\rm CW}(\vec{\rho})}{\partial \rho^\alpha} > 0$$

seems consistent with the expectation that an increase in the value of the dislocation density $\rho^\alpha$ results in a concomitant increase in the degree of disorder in the system.

Next, by $(9.5)_1$ and (9.13) the thermodynamic forces (7.4) associated with the plastic free-energy are given by

$$F^\alpha_{\rm CW}(\vartheta,\vec{\rho}) = f_{\rm CW}(\rho^\alpha) - \vartheta g_{\rm CW}(\rho^\alpha) \stackrel{\rm def}{=} F_{\rm CW}(\vartheta,\rho^\alpha), \tag{9.16}$$

feforce2

and hence the energetic stresses (7.8) take the form

$$\boldsymbol{\Sigma}^\alpha_{\rm NR} = F^\alpha_{\rm CW}(\vartheta,\rho^\alpha)\, A^\alpha(\vartheta,\vec{\rho})\frac{\dot{\boldsymbol{\Gamma}}^\alpha}{|\dot{\boldsymbol{\Gamma}}^\alpha|}. \tag{9.17}$$

Sigmaen2

Further, on account of the assumption (7.5)

$$F_{\rm CW}(\vartheta,\rho^\alpha) > 0; \tag{9.18}$$

FCW>0

hence (9.16) implies that

$$f_{\rm CW}(\rho^\alpha) > \vartheta g_{\rm CW}(\rho^\alpha).$$

Then, by (7.4), (9.6), and (9.16),

psipden
- *the plastic free-energy* $\bar{\psi}^p(\vartheta,\rho^\alpha)$ *is a strictly increasing function of the dislocation density* $\rho^\alpha$.

Next, (9.16), (9.17) and (9.18) imply that the stress power associated with the stress $\boldsymbol{\Sigma}^\alpha_{\rm NR}$ has the form

$$\boldsymbol{\Sigma}^\alpha_{\rm NR}\bullet\dot{\boldsymbol{\Gamma}}^\alpha = \underbrace{f_{\rm CW}(\rho^\alpha)A^\alpha(\vartheta,\vec{\rho})\,\dot{\Gamma}^\alpha_{\rm acc}}_{\substack{\text{internal-energetic}\\ \text{power}}} - \underbrace{\vartheta g_{\rm CW}(\rho^\alpha)A^\alpha(\vartheta,\vec{\rho})\,\dot{\Gamma}^\alpha_{\rm acc}}_{\substack{\text{entropic}\\ \text{power}}} \geq 0. \tag{9.19}$$

xianpowerge0

Thus, interestingly, provided $A^\alpha(\vartheta,\vec{\rho}) > 0$, the stresses $\boldsymbol{\Sigma}^\alpha_{\rm NR}$ mimic dissipative behavior, even though they derive from an energy.[27]

**Remark** As noted by Bever, Holt & Titchener (1973), the entropy of dislocations has been estimated by Cottrell (1953) to be quite small, and that, at ordinary and low temperatures, the temperature-entropy product

$$\vartheta\sum_\alpha N_{\rm CW}(\rho^\alpha)$$

may be *neglected* relative to the energetic contribution $\sum_\alpha E_{\rm CW}(\rho^\alpha)$ to the plastic energy $\hat{\psi}^p(\vartheta,\vec{\rho})$.

# 10 Balance of energy revisited

enagain

Next, we revisit the energy balance (7.40). Using (9.16) and $(9.15)_1$

$$\sum_\alpha\Big(F^\alpha_{\rm CW} - \vartheta\,\frac{\partial F^\alpha_{\rm CW}}{\partial\vartheta}\Big)\,\dot{\rho}^\alpha = \sum_\alpha f_{\rm CW}(\rho^\alpha)\dot{\rho}^\alpha = \dot{\varepsilon}^p_{\rm CW}. \tag{10.1}$$

revisit1

Use of (10.1) and (9.1) in the energy balance expression (7.40) gives

$$c\,\dot{\vartheta} + {\rm div}\mathbf{q} - q = \sum_\alpha \tau^\alpha\dot{\gamma}^\alpha - \dot{\varepsilon}^p_{\rm CW} + \mathbf{M}\colon\dot{\mathbf{E}}^e + \sum_\alpha {\rm div}\,(\dot{\gamma}^\alpha\boldsymbol{\xi}^\alpha)\,. \tag{10.2}$$

etabal3g

[27] Cf. Gurtin & Reddy (2009, p. 242), Gurtin & Ohno (2011, p. 333).

If we integrate (10.2) over the body B we are led to the *global energy balance*

$$\int_{\mathrm{B}} c\dot{\vartheta}\,dv = \sum_{\alpha}\int_{\mathrm{B}} \tau^{\alpha}\dot{\gamma}^{\alpha}\,dv - \int_{\mathrm{B}} \dot{\varepsilon}^{p}_{\mathrm{CW}}\,dv + \int_{\mathrm{B}} \mathbf{M}\colon\dot{\mathbf{E}}^{e}\,dv + \sum_{\alpha}\int_{\partial\mathrm{B}} \dot{\gamma}^{\alpha}\boldsymbol{\xi}^{\alpha}\cdot\mathbf{n}\,da - \int_{\partial\mathrm{B}} \mathbf{q}\cdot\mathbf{n}\,da + \int_{\mathrm{B}} q\,dv. \tag{10.3}$$

enbaltherm5

Note that if

$$\mathbf{M}\colon\dot{\mathbf{E}}^{e} \approx 0 \tag{10.4}$$

Maprox

— a standard assumption equivalent to neglecting thermal expansion — and if the body is *insulated and microscopically noninteractive* in the sense that

$$\mathbf{q}\cdot\mathbf{n} = 0 \quad \text{and} \quad \dot{\gamma}^{\alpha}\boldsymbol{\xi}^{\alpha}\cdot\mathbf{n} = 0 \quad \text{for all} \quad \alpha \text{ on } \partial\mathrm{B}, \tag{10.5}$$

dBnoint

and $q = 0$ on B, then (10.3), when rearranged, represents a partition

$$\sum_{\alpha}\int_{\mathrm{B}} \tau^{\alpha}\dot{\gamma}^{\alpha}\,dv = \int_{\mathrm{B}} c\dot{\vartheta}\,dv + \int_{\mathrm{B}} \dot{\varepsilon}^{p}_{\mathrm{CW}}\,dv \tag{10.6}$$

enbaltherm10

of the plastic stress-power into terms involving temporal changes in temperature and energy storage due to cold work.

## 11 The fraction $\beta$ of plastic stress-power that goes into heating

fraction

Ever since the classical experimental work of G. I. Taylor and co-workers (cf., e.g., Farren & Taylor, 1925; Taylor & Quinney, 1934, 1937), an important notion in thermodynamic considerations of plastic deformation is the *fraction*

$$\beta = \frac{\text{heating}}{\text{plastic stress-power}} \tag{11.1}$$

gh7

*of the plastic stress-power that goes into heating.* "Heating" is best described by the term $c\dot{\theta}$ because it involves the temperature an experimenter would measure at a point *within the body*. Accordingly, in the context of the present gradient single crystal plasticity theory, the fraction of the plastic stress-power that goes into heating is given by

$$\beta = \frac{c\dot{\vartheta}}{\mathbf{T}\colon\dot{\mathbf{E}}^{p}} \tag{11.2}$$

betgrad1

$$= \frac{c\dot{\vartheta}}{\sum_{\alpha}\tau^{\alpha}\dot{\gamma}^{\alpha}}, \tag{11.3}$$

betgrad2

where we have used (2.41). Use of the energy balance (10.2) in the definition (11.3) gives

$$\beta = \frac{c\dot{\vartheta}}{\sum_{\alpha}\tau^{\alpha}\dot{\gamma}^{\alpha}} = \frac{c\dot{\vartheta}}{c\dot{\vartheta} + \dot{\varepsilon}^{p}_{\mathrm{CW}} - \sum_{\alpha}\mathrm{div}\,(\dot{\gamma}^{\alpha}\boldsymbol{\xi}^{\alpha}) + \mathrm{div}\,\mathbf{q} - q - \mathbf{M}\colon\dot{\mathbf{E}}^{e}}. \tag{11.4}$$

betadef1

In traditional considerations (cf., e.g. Rosakis, Rosakis, Ravichandran and Hodowany, 2000) of the fraction of stress power that goes into heating, gradient effects are neglected ($\sum_{\alpha}\mathrm{div}\,(\dot{\gamma}^{\alpha}\boldsymbol{\xi}^{\alpha}) = 0$), the body is presumed to be thermally insulated ($q = 0$), heat conduction is neglected ($\mathbf{q} = \mathbf{0}$), as is the small thermo-elastic coupling term ($\mathbf{M}\colon\dot{\mathbf{E}}^{e} = 0$). Under these approximations,

$$\beta \approx \frac{c\dot{\vartheta}}{c\dot{\vartheta} + \dot{\varepsilon}^{p}_{\mathrm{CW}}}, \tag{11.5}$$

betadef

from which it is clear that in general $\beta$ is a history-dependent quantity and *is not expected to be a constant*.[28] The parameter $\beta$ deviates from unity, and as to how much it deviates depends on the rate of change of the stored energy of cold work $\dot{\varepsilon}^p_{\mathrm{CW}}$.

The fraction (11.3) is local; a fraction $\beta$ that includes higher-order contributions begins with the definitions

$$\text{heating} = \int_{\mathrm{B}} c\dot{\vartheta}\, dv + \int_{\partial\mathrm{B}} \mathbf{q}\cdot\mathbf{n}\, da - \int_{\mathrm{B}} q\, dv$$

$$\text{plastic stress-power} = \sum_{\alpha} \left( \int_{\mathrm{B}} \tau^{\alpha}\dot{\gamma}^{\alpha}\, dv + \int_{\partial\mathrm{B}} \dot{\gamma}^{\alpha}\boldsymbol{\xi}^{\alpha}\cdot\mathbf{n}\, da \right)$$

and results in the *global fraction*

$$\beta_{\mathrm{B}} = \frac{\int_{\mathrm{B}} c\dot{\vartheta}\, dv + \int_{\partial\mathrm{B}} \mathbf{q}\cdot\mathbf{n}\, da - \int_{\mathrm{B}} q\, dv}{\sum_{\alpha} \left( \int_{\mathrm{B}} \tau^{\alpha}\dot{\gamma}^{\alpha}\, dv + \int_{\partial\mathrm{B}} \dot{\gamma}^{\alpha}\boldsymbol{\xi}^{\alpha}\cdot\mathbf{n}\, da \right)}. \tag{11.6}$$

globnalbetagradth

The term $\sum_{\alpha}\int_{\partial\mathrm{B}} \dot{\gamma}^{\alpha}\boldsymbol{\xi}^{\alpha}\cdot\mathbf{n}\, da$ represents energy flow out of B across $\partial$B associated with the *flow of glide-dislocations*, so that the denominater of (11.6) represents the net plastic stress-power associated with this flow. If the body is insulated and microscopically noninteractive in the sense of (10.5), then

$$\beta_{\mathrm{B}} = \frac{\int_{\mathrm{B}} c\dot{\vartheta}\, dv}{\sum_{\alpha}\int_{\mathrm{B}} \tau^{\alpha}\dot{\gamma}^{\alpha}\, dv} \tag{11.7}$$

globnalbetagradthinint

or equivalently, by (10.6) granted $\mathbf{M} \approx \mathbf{0}$,

$$\beta_{\mathrm{B}} = \frac{\int_{\mathrm{B}} c\dot{\vartheta}\, dv}{\int\limits_{\mathrm{B}} c\dot{\vartheta}\, dv + \int\limits_{\mathrm{B}} \dot{\varepsilon}^p_{\mathrm{CW}}\, dv}, \tag{11.8}$$

globnalbetagradthinint

which shows that $\beta_{\mathrm{B}}$ deviates from unity because of the term

$$\int\limits_{\mathrm{B}} \dot{\varepsilon}^p_{\mathrm{CW}}\, dv,$$

which represents the rate of change of stored energy in B.[29]

# 12 Temperature changes during to thermal annealing in the absence of mechanical deformation

In the absence of mechanical deformation — that is, assuming that $\mathbf{u} \equiv \mathbf{0}$ and $\gamma^{\alpha} \equiv 0$ — the energy balance equation (10.2) reduces to

$$c\,\dot{\vartheta} + \mathrm{div}\mathbf{q} - q = -\dot{\varepsilon}^p_{\mathrm{CW}}. \tag{12.1}$$

recov1

Recall (9.15), viz.

$$\dot{\varepsilon}^p_{\mathrm{CW}} = \sum_{\alpha} f_{\mathrm{CW}}(\rho^{\alpha})\dot{\rho}^{\alpha} \quad \text{with} \quad f_{\mathrm{CW}}(\rho^{\alpha}) \geq 0, \tag{12.2}$$

recov2

[28] As noted by Rosakis, Rosakis, Ravichandran and Hodowany (2000) and shown by Hodowany, Ravichandran, Rosakis and Rosakis (2000): "forcing $\beta$ to be a constant is an assumption of an approximate nature that is not supported by experimental evidence."

[29] Dividing the numerator and denominator of (11.6), (11.7) and (11.8) by the volume of B leads us to expressions for $\beta_{\mathrm{B}}$ in terms of averages.

and from (2.22) that in the absence of mechanical deformation

$$\dot{\rho}^\alpha = -R^\alpha(\vartheta, \vec{\rho}) \quad \text{with} \quad R^\alpha(\vartheta, \vec{\rho}) \geq 0. \tag{12.3}$$

recov3

Using (12.2) and (12.3) in (12.1) gives

$$c\,\dot{\vartheta} + \mathrm{div}\mathbf{q} - q = \sum_\alpha f_{\rm CW}(\rho^\alpha) R^\alpha(\vartheta, \vec{\rho}), \tag{12.4}$$

recov4

and integrating this relation over the body B gives

$$\int_{\rm B} c\dot{\vartheta}\, dv + \int_{\partial\rm B} \mathbf{q}\cdot\mathbf{n}\, da - \int_{\rm B} q\, dv = \sum_\alpha \int_{\rm B} f_{\rm CW}(\rho^\alpha) R^\alpha(\vartheta, \vec{\rho})\, dv. \tag{12.5}$$

calorimetry

Equation (12.5) provides guidance for interpreting results from calorometric experiments typically used for measuring the stored energy of cold-work by comparing the thermal behavior of a cold-worked specimen against that of a standard specimen; cf. §2.2 of Bever, Holt and Titchener (1973).

## 13 Summary of governing equations

summary

We present here for convenience a summary of the governing equations for the problem:

macroscopic equilibrium:

$$\mathrm{div}\,\mathbf{T} + \mathbf{b} = \mathbf{0}; \tag{13.1}$$

DSCPVPmacfb1a

microscopic force balance:

$$\tau^\alpha = \pi^\alpha - \mathrm{div}\,\boldsymbol{\xi}^\alpha; \tag{13.2}$$

Dmfba

energy balance:

$$c\dot{\vartheta} + \mathrm{div}\mathbf{q} - q = \sum_\alpha \tau^\alpha \dot{\gamma}^\alpha - \sum_\alpha \left( F^\alpha_{\rm CW} - \vartheta \frac{\partial F^\alpha_{\rm CW}}{\partial\vartheta} \right) \dot{\rho}^\alpha + \sum_\alpha \mathrm{div}\,(\dot{\gamma}^\alpha \boldsymbol{\xi}^\alpha)\,. \tag{13.3}$$

etabal3fa

In stating the last equation we have made use of (9.1) and have invoked the assumption (10.4).

For a complete formulation these three equations must be supplemented by

(i) expressions for the heat capacity $c(\mathbf{E}^e, \vartheta)$, thermodynamic force $F^\alpha_{\rm CW}(\vartheta, \vec{\rho})$, as well as the evolution equations for the dislocation densities $\rho^\alpha$; and

(ii) constitutive relations for the stress $\mathbf{T}$, the heat flux $\mathbf{q}$, and the generalized stress $\boldsymbol{\Sigma} = (\pi^\alpha, \ell^{-1}\boldsymbol{\xi}^\alpha)$.

From (7.2) and (9.4) the free energy $\psi$ is given by

$$\psi(\mathbf{E}^e, \vartheta, \vec{\rho}) = \hat{\psi}^e(\mathbf{E}^e, \vartheta) + \underbrace{\sum_\alpha E_{\rm CW}(\rho^\alpha) - \vartheta N_{\rm CW}(\rho^\alpha)}_{\hat{\psi}^p(\vartheta, \vec{\rho})} \tag{13.4}$$

psitot

with $E_{\rm CW}(0) = N_{\rm CW}(0) = 0$. Thus from (7.34), (9.1), and (7.4) respectively, the heat capacity $c(\mathbf{E}^e, \vartheta)$ and thermodynamic force $F^\alpha_{\rm CW}(\vartheta, \rho^\alpha)$ are found from

$$c(\mathbf{E}^e, \vartheta) = -\vartheta \frac{\partial^2 \hat{\psi}^e(\mathbf{E}^e, \vartheta)}{\partial\vartheta^2} \tag{13.5}$$

heatcap2

and

$$F^\alpha_{\mathrm{CW}}(\vartheta, \vec{\rho}) = F^\alpha_{\mathrm{CW}}(\vartheta, \rho^\alpha) = \frac{\partial \hat{\psi}^p}{\partial \rho^\alpha}\,. \tag{13.6}$$ Fpsip22

The evolution equation for $\rho^\alpha$ is

$$\dot{\rho}^\alpha = A^\alpha(\vartheta, \vec{\rho})\,\dot{\Gamma}^\alpha_{\mathrm{acc}} - R^\alpha(\vartheta, \vec{\rho}). \tag{13.7}$$ accdena

The equations for the stress, resolved shear stress and heat flux are given by

$$\mathbf{T} = \hat{\mathbf{T}}(\mathbf{u}, \vec{\gamma}, \vartheta) = \frac{\partial \psi^e(\mathbf{E}^e, \vartheta)}{\partial \mathbf{E}^e}, \tag{13.8}$$ stressa

$$\tau^\alpha = \tau^\alpha(\mathbf{u}, \vec{\gamma}, \vartheta) = \mathbf{s}^\alpha \cdot \hat{\mathbf{T}}(\mathbf{u}, \vec{\gamma}, \vartheta)\mathbf{m}^\alpha, \tag{13.9}$$ ressheara

$$\mathbf{q} = \hat{\mathbf{q}}(\vartheta, \nabla\vartheta). \tag{13.10}$$ heatfluxa

The equation for the generalized stress is

$$\begin{aligned}\boldsymbol{\Sigma}^\alpha &= (\pi^\alpha, \ell^{-1}\boldsymbol{\xi}^\alpha) = \boldsymbol{\Sigma}^\alpha_{\mathrm{NR}} + \boldsymbol{\Sigma}^\alpha_{\mathrm{dis}} \\ &= \left(F^\alpha_{\mathrm{CW}}(\vartheta, \vec{\rho})A^\alpha(\vartheta, \vec{\rho}) + Y^\alpha(\vec{\rho}, \vartheta)\right)\frac{\dot{\boldsymbol{\Gamma}}^\alpha}{\dot{\Gamma}^\alpha_{\mathrm{acc}}} \qquad \text{for } \dot{\boldsymbol{\Gamma}}^\alpha \neq \mathbf{0},\end{aligned} \tag{13.11}$$ genstressa

where $\dot{\boldsymbol{\Gamma}}^\alpha = (\dot{\gamma}^\alpha, \ell\nabla^\alpha_{\tan}\dot{\gamma}^\alpha)$ and $\dot{\Gamma}^\alpha_{\mathrm{acc}} = \sqrt{(\dot{\gamma}^\alpha)^2 + \ell^2|\nabla^\alpha_{\tan}\dot{\gamma}^\alpha|^2}$. Plastic flow is determined by the complementarity conditions

$$\mathcal{F}^\alpha \leq 0, \qquad |\dot{\boldsymbol{\Gamma}}^\alpha| \geq 0, \qquad \mathcal{F}^\alpha\,|\dot{\boldsymbol{\Gamma}}^\alpha| = 0 \tag{13.12}$$ compa

with the yield function $\mathcal{F}^\alpha$ given by

$$\mathcal{F}^\alpha(\boldsymbol{\Sigma}^\alpha_{\mathrm{dis}}, \vec{\rho}, \vartheta) = |\boldsymbol{\Sigma}^\alpha_{\mathrm{dis}}| - Y^\alpha(\vec{\rho}, \vartheta). \tag{13.13}$$ yieldfunctiona

Alternatively, the generalized stresses are given by

$$D(\tilde{\boldsymbol{\Gamma}}^\alpha, \vec{\rho}, \vartheta) \geq D(\dot{\boldsymbol{\Gamma}}^\alpha, \vec{\rho}, \vartheta) + \boldsymbol{\Sigma}^\alpha_{\mathrm{dis}} \bullet (\tilde{\boldsymbol{\Gamma}}^\alpha - \dot{\boldsymbol{\Gamma}}^\alpha)\,, \tag{13.14a}$$ ineqSigmaa

$$\phi(\tilde{\boldsymbol{\Gamma}}^\alpha) \geq \phi(\dot{\boldsymbol{\Gamma}}^\alpha) + \boldsymbol{\Sigma}^\alpha_{\mathrm{NR}} \bullet (\tilde{\boldsymbol{\Gamma}}^\alpha - \dot{\boldsymbol{\Gamma}}^\alpha)\,, \tag{13.14b}$$ ineqSigmab

with $\phi$ and $D$ defined by (7.22) and (7.53) respectively.

The equations or inequalities in this section are required to hold in the domain B for all times $t > 0$, and to be solved for the displacement $\mathbf{u}$, temperature $\vartheta$, and slips $\gamma^\alpha$ $(\alpha = 1, \ldots, N)$. For the problem to be properly posed the governing equations must be supplemented by a set of boundary and initial conditions; cf. §4.

## 14 Variational formulation of the problem

reformulation

Gurtin & Reddy (2014) have derived a weak or variational formulation of the purely mechanical problem. The flow relations take the form of a global variational inequality, which incorporates the macroscopic balance equation, and which is supplemented by a weak formulation of the microscopic balance equation. In this section that variational theory is extended to the problem considered in this work.

**Step 1: The flow relation, microscopic force balance, and energetic microstress.** For convenience in what follows we write

$$D^\alpha(\dot{\mathbf{\Gamma}}^\alpha) \equiv D^\alpha(\dot{\mathbf{\Gamma}}^\alpha, \vec{\rho}, \vartheta).$$

Virtual fields $\tilde{\mathbf{u}}$ and $\vec{\tilde{\mathbf{\Gamma}}}$ consistent with $(4.1)_1$ and $(4.8)_1$ are referred to as *kinematically admissible*.

The flow relation is given by the inequality (13.14a), which is local. It has an important global counterpart which follows upon integrating (13.14a) over B:

$$\int\limits_{\mathrm{B}} \Big( D^\alpha(\tilde{\mathbf{\Gamma}}^\alpha) - D^\alpha(\dot{\mathbf{\Gamma}}^\alpha) - \mathbf{\Sigma}^\alpha_{\mathrm{dis}} \bullet (\tilde{\mathbf{\Gamma}}^\alpha - \dot{\mathbf{\Gamma}}^\alpha)\Big)\, dv \geq 0. \tag{14.1}$$

intcvxdelta

We view (14.1) as an inequality to be satisfied for all kinematically admissible virtual fields $\tilde{\mathbf{\Gamma}}^\alpha$ on B.

Next, we turn to the microscopic balance equation (13.2): multiplying both sides of this equation once by $\tilde{\gamma}^\alpha$ and another time by $\dot{\gamma}^\alpha$, integrating over B, and then integrating by parts the term involving $\operatorname{div} \boldsymbol{\xi}^\alpha$, and finally subtracting the two equations we obtain

$$\int\limits_{\mathrm{B}} \pi^\alpha(\tilde{\gamma}^\alpha - \dot{\gamma}^\alpha) + \boldsymbol{\xi}^\alpha \cdot \nabla(\tilde{\gamma}^\alpha - \dot{\gamma}^\alpha)\, dv = \int\limits_{\mathrm{B}} \tau^\alpha(\tilde{\gamma}^\alpha - \dot{\gamma}^\alpha)\, dv. \tag{14.2}$$

weakmfb1

Here the boundary conditions (4.8) have been invoked. From the definitions (6.3) and (6.1) of $\mathbf{\Sigma}^\alpha$ and $\dot{\mathbf{\Gamma}}^\alpha$, with similar definitions for the virtual counterparts, and by expressing the stress $\mathbf{\Sigma}^\alpha$ in terms of its nonrecoverable energetic and dissipative components using (7.12), equation (14.2) becomes

$$\int\limits_{\mathrm{B}} (\mathbf{\Sigma}^\alpha_{\mathrm{dis}} + \mathbf{\Sigma}^\alpha_{\mathrm{NR}}) \bullet \big(\tilde{\mathbf{\Gamma}}^\alpha - \dot{\mathbf{\Gamma}}^\alpha\big)\, dv - \int\limits_{\mathrm{B}} \tau^\alpha(\tilde{\gamma}^\alpha - \dot{\gamma}^\alpha)\, dv = 0\,. \tag{14.3}$$

Dvirpowerformsucc1

By adding (14.3) and (14.1) we eliminate $\mathbf{\Sigma}^\alpha_{\mathrm{dis}}$ from (14.1) to arrive at the inequality

$$\int\limits_{\mathrm{B}} D^\alpha(\tilde{\mathbf{\Gamma}}^\alpha)\, dv - \int\limits_{\mathrm{B}} D^\alpha(\dot{\mathbf{\Gamma}}^\alpha)\, dv + \int\limits_{\mathrm{B}} \mathbf{\Sigma}^\alpha_{\mathrm{NR}} \bullet \big(\tilde{\mathbf{\Gamma}}^\alpha - \dot{\mathbf{\Gamma}}^\alpha\big)\, dv - \int\limits_{\mathrm{B}} \tau^\alpha(\tilde{\gamma}^\alpha - \dot{\gamma}^\alpha)\, dv \geq 0. \tag{14.4}$$

mfb1

Next, integration of (13.14b) over the domain B gives the global inequality

$$\int\limits_{\mathrm{B}} \phi(\tilde{\mathbf{\Gamma}}^\alpha)\, dv - \int\limits_{\mathrm{B}} \phi(\dot{\mathbf{\Gamma}}^\alpha)\, dv - \int\limits_{\mathrm{B}} \mathbf{\Sigma}^\alpha_{\mathrm{NR}} \bullet \big(\tilde{\mathbf{\Gamma}}^\alpha - \dot{\mathbf{\Gamma}}^\alpha\big)\, dv \geq 0. \tag{14.5}$$

enineq

By adding (14.5) and (14.4) and using the identity (2.38) we obtain the inequality

$$\int\limits_{\mathrm{B}} (D^\alpha(\tilde{\mathbf{\Gamma}}^\alpha) + \phi(\tilde{\mathbf{\Gamma}}^\alpha))\, dv - \int\limits_{\mathrm{B}} (D^\alpha(\dot{\mathbf{\Gamma}}^\alpha) + \phi(\dot{\mathbf{\Gamma}}^\alpha))\, dv - \int\limits_{\mathrm{B}} \mathbf{T} : \mathbb{S}^\alpha_{\mathrm{sym}}(\tilde{\gamma}^\alpha - \dot{\gamma}^\alpha)\, dv \geq 0. \tag{14.6}$$

basicVIa

When summed over all slip systems this inequality takes the form

$$\sum_\alpha \int\limits_{\mathrm{B}} (D^\alpha(\tilde{\mathbf{\Gamma}}^\alpha) + \phi(\tilde{\mathbf{\Gamma}}^\alpha))\, dv - \sum_\alpha \int\limits_{\mathrm{B}} (D^\alpha(\dot{\mathbf{\Gamma}}^\alpha) + \phi(\dot{\mathbf{\Gamma}}^\alpha))\, dv - \sum_\alpha \int\limits_{\mathrm{B}} \mathbf{T} : \mathbb{S}^\alpha_{\mathrm{sym}}(\tilde{\gamma}^\alpha - \dot{\gamma}^\alpha)\, dv \geq 0. \tag{14.7}$$

mfb2

**Step 2: Macroscopic force balance.** Consider the macroscopic virtual-power relation (2.36) with P replaced by B and $\tilde{\mathbf{u}}$ replaced by $\tilde{\mathbf{u}} - \dot{\mathbf{u}}$, and with $\tilde{\mathbf{u}}$ and $\dot{\mathbf{u}}$ consistent with the boundary conditions $(4.1)_1$; the result — which we require to hold for all kinematically admissible virtual velocity fields $\tilde{\mathbf{u}}$ on B — is

$$\int\limits_{\mathrm{B}} \mathbf{T}\colon \big(\mathbf{E}(\tilde{\mathbf{u}}) - \mathbf{E}(\dot{\mathbf{u}})\big)\, dv - \int\limits_{\partial \mathrm{B}_{\mathrm{trac}}} \mathbf{t}^{*}\cdot (\tilde{\mathbf{u}} - \dot{\mathbf{u}})\, da - \int\limits_{\mathrm{B}} \mathbf{b}\cdot(\tilde{\mathbf{u}} - \dot{\mathbf{u}})\, dv = 0. \tag{14.8}$$

macvprelation2

**Step 3: Combined flow relations and force balances.** We now add (14.8) to (14.7); the result is

$$\begin{aligned}\sum_{\alpha}\int\limits_{\mathrm{B}} \big(D^{\alpha}(\tilde{\mathbf{\Gamma}}^{\alpha}) + \phi(\tilde{\mathbf{\Gamma}}^{\alpha})\big)\, dv &- \sum_{\alpha}\int\limits_{\mathrm{B}} \big(D^{\alpha}(\dot{\mathbf{\Gamma}}^{\alpha}) + \phi(\dot{\mathbf{\Gamma}}^{\alpha})\big)\, dv \\ &+ \int\limits_{\mathrm{B}} \mathbf{T}\colon \Big(\mathbf{E}(\tilde{\mathbf{u}}) - \mathbf{E}(\dot{\mathbf{u}}) - \sum_{\alpha}\mathbb{S}^{\alpha}_{\mathrm{sym}}(\tilde{\gamma}^{\alpha} - \dot{\gamma}^{\alpha})\Big)\, dv \\ &- \int\limits_{\partial \mathrm{B}_{\mathrm{trac}}} \mathbf{t}^{*}\cdot(\tilde{\mathbf{u}} - \dot{\mathbf{u}})\, da - \int\limits_{\mathrm{B}} \mathbf{b}\cdot(\tilde{\mathbf{u}} - \dot{\mathbf{u}})\, dv \geq 0.\end{aligned} \tag{14.9}$$

basicVI

The *global variational formulation* (14.9) is to be understood as an inequality in the variables $\mathbf{u}$, $\vec{\gamma}$ and $\vec{\rho}$; thus the expression (13.8) is used for the stress $\mathbf{T}$ in this inequality. Summarizing, we have shown thus far that

(i) the constitutive relations for plastic flow,[30]

(ii) the macroscopic and microscopic virtual-power relations (2.36) and (13.2),

mmm (iii) and the boundary conditions (4.1),

together imply the global variational inequality (14.9).

We supplement the global variational inequality (14.9) with the *global microscopic virtual-power relation* (14.3), viz.

$$\int\limits_{\mathrm{B}} \mathbf{\Sigma}^{\alpha}\bullet\big(\tilde{\mathbf{\Gamma}}^{\alpha} - \dot{\mathbf{\Gamma}}^{\alpha}\big)\, dv = \int\limits_{\mathrm{B}} \tau^{\alpha}(\tilde{\gamma}^{\alpha} - \dot{\gamma}^{\alpha})\, dv \qquad \text{for all } \alpha. \tag{14.10}$$

microii

**Step 4: Energy balance.** It remains to formulate the global form of the energy equation (13.3). First, we define thermally admissible temperatures $\tilde{\vartheta}$ to be those that satisfy the *homogeneous* boundary condition $\tilde{\vartheta} = 0$ on $\partial\mathrm{B}_{\mathrm{temp}}$[31].

This is achieved by multiplying this equation by $\tilde{\vartheta}$, integrating over the body $B$, and integrating by parts the two terms involving divergences. Invoking also the assumption (10.4), these steps lead to the equation

$$\begin{aligned}\int\limits_{\mathrm{B}} c\dot{\vartheta}\tilde{\vartheta}\, dv + \int\limits_{\partial\mathrm{B}} \tilde{\vartheta}\mathbf{q}\cdot\mathbf{n}\, da - \int\limits_{\mathrm{B}} \mathbf{q}\cdot\nabla\tilde{\vartheta}\, dv - \int\limits_{\mathrm{B}} q\tilde{\vartheta}\, dv = \sum_{\alpha}\int\limits_{\mathrm{B}} \tilde{\vartheta}\tau^{\alpha}\dot{\gamma}^{\alpha}\, dv \\ - \sum_{\alpha}\int\limits_{\mathrm{B}} \Big(F^{\alpha}_{\mathrm{CW}} - \vartheta\,\frac{\partial F^{\alpha}_{\mathrm{CW}}}{\partial\vartheta}\Big)\dot{\rho}^{\alpha}\tilde{\vartheta}\, dv + \sum_{\alpha}\int\limits_{\partial\mathrm{B}} \dot{\gamma}^{\alpha}(\boldsymbol{\xi}^{\alpha}\cdot\mathbf{n})\tilde{\vartheta}\, da - \sum_{\alpha}\int\limits_{\mathrm{B}} \dot{\gamma}^{\alpha}\boldsymbol{\xi}^{\alpha}\cdot\nabla\tilde{\vartheta}\, dv\,.\end{aligned} \tag{14.11}$$

weaken1

[30] I. e., the elastic-range inequality $(7.48)_1$ and the flow rule (7.50) — or *equivalently* the inequality (7.54).

[31] Cf. (4.2).

Next, we use the boundary conditions (4.2) and $(4.8)_2$ so that the integrals on $\partial\mathrm{B}_{\text{temp}}$ disappear. This gives the final variational form of the energy equation:

$$\int\limits_{\mathrm{B}} c\dot{\vartheta}\tilde{\vartheta}\,dv + \int\limits_{\partial\mathrm{B}_{\text{flux}}} \tilde{\vartheta}q_n^*\,da - \int\limits_{\mathrm{B}} \mathbf{q}\cdot\nabla\tilde{\vartheta}\,dv - \int\limits_{\mathrm{B}} q\tilde{\vartheta}\,dv = \sum_\alpha \int\limits_{\mathrm{B}} \tilde{\vartheta}\tau^\alpha\dot{\gamma}^\alpha\,dv$$
$$- \sum_\alpha \int\limits_{\mathrm{B}} \Big(F^\alpha_{\text{CW}} - \vartheta\,\frac{\partial F^\alpha_{\text{CW}}}{\partial\vartheta}\Big)\,\dot{\rho}^\alpha\tilde{\vartheta}\,dv - \sum_\alpha \int\limits_{\mathrm{B}} \dot{\gamma}^\alpha\boldsymbol{\xi}^\alpha\cdot\nabla\tilde{\vartheta}\,dv\,. \qquad (14.12)$$ weaken2

Here it is understood that the functions $c$, $F_{\text{CW}}$, $\mathbf{q}$ and $\tau^\alpha$ are obtained as functions of $\mathbf{u}$, $\vartheta$, $\rho^\alpha$ and/or $\gamma^\alpha$ as appropriate via (13.5), (13.6), (13.10), (13.8) and (2.29). Furthermore, we note in respect of the last term on the right-hand side that the term $\dot{\gamma}^\alpha\boldsymbol{\xi}^\alpha$ is non-zero only when flow occurs, so that $\boldsymbol{\xi}^\alpha$ is given by the second component of (13.11), or equivalently by

$$\boldsymbol{\xi}^\alpha = (F^\alpha_{\text{CW}}(\vartheta,\vec{\rho})A^\alpha(\vartheta,\vec{\rho}) + Y^\alpha(\vec{\rho},\vartheta))\,\frac{\nabla^\alpha_{\tan}\dot{\gamma}^\alpha}{\dot{\Gamma}^\alpha_{\text{acc}}} \qquad (14.13)$$ xia3

in which $\dot{\Gamma}^\alpha_{\text{acc}} = \sqrt{(\dot{\gamma}^\alpha)^2 + \ell^2|\nabla^\alpha_{\tan}\dot{\gamma}^\alpha|^2}$.

The variational problem takes the following form.

Problem Var. Given the initial conditions (4.10) and (4.11), body force and surface traction $\mathbf{b}$ and $\mathbf{t}^*$ on B and $\partial\mathrm{B}_{\text{trac}}$ respectively, the heat flux $q_n^*$ on $\partial\mathrm{B}_{\text{flux}}$ and heat source $q$ on B, find the displacement $\mathbf{u}$, the slips $\gamma^\alpha$, the dislocation densities $\rho^\alpha$, the generalised microstress $\boldsymbol{\Sigma}^\alpha$, and the temperature $\vartheta$ that satisfy the global variational inequality (14.9), the microscopic virtual-power relation (14.10), the energy equation (14.12), the evolution equation (13.7), and the boundary conditions $(4.1)_1$ and $(4.2)_1$ for all admissible displacements $\tilde{\mathbf{u}}$, slips $\tilde{\gamma}^\alpha$ and temperatures $\tilde{\vartheta}$.

**Remark** Given that the dissipative microstress $\boldsymbol{\Sigma}^\alpha_{\text{dis}}$ is indeterminate in the elastic region, it would appear that is not possible to use $(13.12)_1$ to establish when flow takes place. This observation has been made earlier by Fleck and Willis (2009). The key to understanding this situation is to note that the flow relation makes sense only when considered as a *global* expression, for example in the form (14.9). Reddy (2011) has shown, for example, that when time-discretization is introduced, this inequality, in which the dissipative microstresses are absent, may be formulated as a well-posed *minimization* problem in $\mathbf{u}$ and $\vec{\gamma}$. Thus, while it is not possible to determine the elastic range pointwise, the elastic-plastic zones at any given time may be established a posteriori, once the solution has been obtained.

## 15 Specialization of the constitutive equations

specialization

The theory presented thus far is quite general. With a view toward applications, in this section we discuss a constitutive theory based on the following simplifying assumptions:

(i) The temperature $\vartheta$ is close to a fixed reference temperature $\vartheta_0$.

(ii) Recalling the additive free-energy (7.2), viz. $\psi = \psi^e(\mathbf{E}^e,\vartheta) + \hat{\psi}^p(\vartheta,\vec{\rho})$, we consider

(a) The elastic energy $\psi^e$ to be given by

$$\hat{\psi}^e(\mathbf{E}^e,\vartheta) = \frac{1}{2}\mathbf{E}^e : \mathbb{C}\mathbf{E}^e - (\vartheta-\vartheta_0)\mathbf{A} : \mathbb{C}\mathbf{E}^e + \frac{c}{2\vartheta_0}(\vartheta-\vartheta_0)^2, \qquad (15.1)$$ special1

where $\mathbb{C}$ is a symmetric, positive-definite linear transformation of symmetric tensors into symmetric tensors that represents the *elasticity tensor* at the reference temperature $\vartheta_0$, while $\mathbf{A}$ is the symmetric *thermal expansion tensor* at $\vartheta_0$, and $c > 0$ is a *constant* specific heat.

By $(7.15)_1$ the stress is then given by

$$\mathbf{T} = \mathbb{C}\big(\mathbf{E}^e - (\vartheta - \vartheta_0)\mathbf{A}\big). \tag{15.2}$$

special1a

(b) The defect energy $\psi^p$ to be given by

$$\hat{\psi}^p(\vartheta, \vec{\rho}) = \sum_\alpha E_{\rm CW}(\rho^\alpha) - \vartheta \sum_\alpha N_{\rm CW}(\rho^\alpha), \tag{15.3}$$

special2

a free-energy *which gives a heat capacity independent of* $\vec{\rho}$.

As discussed in Section 1.4 of Bever, Holt and Titchener (1973), the internal energy per unit length of a dislocation line may be estimated, using a line-tension model, as $a\mu b^2$, where $a$ is a constant approximately equal to 0.5, $\mu$ is the suitable shear modulus at $\vartheta_0$,[32] and $b$ is the magnitude of the Burgers vector. Hence for a dislocation density $\rho^\alpha$ (dislocation line length per unit volume), a simple estimate for $E_{\rm CW}(\rho^\alpha)$ is

$$E_{\rm CW}(\rho^\alpha) = a\mu b^2 \rho^\alpha. \tag{15.4}$$

special3

Also, as discussed in Bever, Holt and Titchener (1973), the entropy of dislocations has been estimated by Cottrell (1953) to be quite small, and that, at ordinary and low temperatures, the temperature-entropy product $\vartheta \sum_\alpha N_{\rm CW}(\rho^\alpha)$ may be *neglected* relative to the energetic contribution $\sum_\alpha E_{\rm CW}(\rho^\alpha)$ to the defect energy $\hat{\psi}^p(\vartheta, \vec{\rho})$. Accordingly, we take the defect energy to be given by the special form

$$\hat{\psi}^p(\vartheta, \vec{\rho}) = a\mu b^2 \sum_\alpha \rho^\alpha. \tag{15.5}$$

special4

Thus, by (15.1), (15.5) and $(7.15)_2$, the entropy is given by

$$\eta = \frac{c}{\vartheta_0}(\vartheta - \vartheta_0) + \mathbf{E}^e : \mathbb{C}\mathbf{A}. \tag{15.6}$$

special5

Further, using (15.5),

$$F^\alpha_{\rm CW}(\vartheta, \vec{\rho}) = \frac{\partial \hat{\psi}^p(\vartheta, \vec{\rho})}{\partial \rho^\alpha} = f_{\rm CW}(\rho^\alpha) = a\mu b^2 > 0. \tag{15.7}$$

special6

Hence, using (7.8), the generalized energetic stress $\boldsymbol{\Sigma}^\alpha_{\rm NR} = (\pi^\alpha_{\rm NR}, \ell^{-1}\boldsymbol{\xi}^\alpha_{\rm NR})$ is given by

$$\boldsymbol{\Sigma}^\alpha_{\rm NR} = (a\mu b^2) A^\alpha(\vartheta, \vec{\rho}) \frac{\dot{\boldsymbol{\Gamma}}^\alpha}{\dot{\Gamma}^\alpha_{\rm acc}}, \quad \text{for } \dot{\boldsymbol{\Gamma}}^\alpha \neq \mathbf{0}, \tag{15.8}$$

special7

where $\dot{\boldsymbol{\Gamma}}^\alpha = (\dot{\gamma}^\alpha, \ell \nabla^\alpha_{\rm tan} \dot{\gamma}^\alpha)$, and

$$\dot{\Gamma}^\alpha_{\rm acc} \stackrel{\rm def}{=} \sqrt{|\dot{\gamma}^\alpha|^2 + \ell^2 |\nabla^\alpha_{\rm tan} \dot{\gamma}^\alpha|^2}. \tag{15.9}$$

special8

[32] For cubic crystals, $\mu \equiv \sqrt{C_{44} \times (C_{11} - C_{12})/2}$, where the three non-zero $C_{ij}$ are the elastic constants in standard Voigt-notation. cubicshear

The generalized energetic stress (15.8) has the component form

$$\left.\begin{aligned} \pi^\alpha_{\rm NR} &= (a\mu b^2)A^\alpha(\vartheta,\vec\rho)\,\frac{\dot\gamma^\alpha}{\dot\Gamma^\alpha_{\rm acc}},\\ \boldsymbol{\xi}^\alpha_{\rm NR} &= (a\mu b^2)A^\alpha(\vartheta,\vec\rho)\,\frac{\ell^2\nabla^\alpha_{\rm tan}\dot\gamma^\alpha}{\dot\Gamma^\alpha_{\rm acc}}, \end{aligned}\right\} \quad \text{for } \dot{\mathbf{\Gamma}}^\alpha \neq \mathbf{0}. \tag{15.10}$$

special10

Hence, using (15.8) and equation (7.51) for $\mathbf{\Sigma}^\alpha_{\rm dis} = (\pi^\alpha_{\rm dis}, \ell^{-1}\boldsymbol{\xi}^\alpha_{\rm dis})$, the generalized stress $\mathbf{\Sigma}^\alpha = \mathbf{\Sigma}^\alpha_{\rm en} + \mathbf{\Sigma}^\alpha_{\rm dis} = (\pi^\alpha, \ell^{-1}\boldsymbol{\xi}^\alpha)$ has the component form

$$\left.\begin{aligned} \pi^\alpha &= \big((a\mu b^2)A^\alpha(\vartheta,\vec\rho)\, + Y^\alpha(\vec\rho,\vartheta)\big)\,\frac{\dot\gamma^\alpha}{\dot\Gamma^\alpha_{\rm acc}},\\ \boldsymbol{\xi}^\alpha &= \big((a\mu b^2)A^\alpha(\vartheta,\vec\rho) + Y^\alpha(\vec\rho,\vartheta)\big)\,\frac{\ell^2\nabla^\alpha_{\rm tan}\dot\gamma^\alpha}{\dot\Gamma^\alpha_{\rm acc}}, \end{aligned}\right\} \quad \text{for } \dot{\mathbf{\Gamma}}^\alpha \neq \mathbf{0}. \tag{15.11}$$

special11

(iii) A commonly used functional form for $Y^\alpha(\vec\rho,\vartheta)$ is

$$Y^\alpha(\vec\rho,\vartheta) = Y_0(\vartheta) + a\mu b\sqrt{\sum_\beta \rho^\beta}, \tag{15.12}$$

special12

where the first term on the right represents a lattice friction stress, and the second term, which depends on the square root of the total dislocation density, represents a resistance offered by "forest dislocations."

(iv) Recall from (2.22) that dislocation densities $\rho^\alpha$ are presumed to evolve according to

$$\dot\rho^\alpha = A^\alpha(\vartheta,\vec\rho)\,\dot\Gamma^\alpha_{\rm acc} - R^\alpha(\vartheta,\vec\rho) \quad \text{with} \quad \rho^\alpha\big|_{t=0} = \rho^\alpha_0. \tag{15.13}$$

disevolve

The evolution equation (15.13), in the "hardening-recovery" format, is based on ideas which have long been prevalent in the materials science literature on the creep of metals (cf., e.g., Bailey (1926), Orowan (1946)). To fix ideas:

(a) A simple form for the *dislocation accumulation modulus* $A^\alpha(\vartheta,\vec\rho)$ may be taken as

$$A^\alpha(\vartheta,\vec\rho) = A_0(\vartheta)\left(1 - \frac{\rho^\alpha}{\rho^\alpha_{\rm sat}}\right)^p, \tag{15.14}$$

satform

where $A_0(\vartheta) \geq 0$ is a temperature-dependent constant, and $\rho^\alpha_{\rm sat} \geq \rho^\alpha_0$ and $p > 0$ are additional constants. This is a *non-interacting* form for the accumulation-rate, in the sense it does not depend on the variables $\rho^\beta \neq \rho^\alpha$. Under circumstances in which $R^\alpha(\vartheta,\vec\rho) = 0$, the material parameter $\rho^\alpha_{\rm sat}$ represents a *saturation value* of $\rho^\alpha$; that is, as $\rho^\alpha$ approaches $\rho^\alpha_{\rm sat}$, the dislocation accumulation modulus $A^\alpha(\vartheta,\vec\rho)$ approaches zero and there is no further accumulation of $\rho^\alpha$ due to plastic flow.

(b) A simple non-interacting form for the recovery rate may be taken as

$$R^\alpha(\vartheta,\vec\rho) = R_0\,\exp\left(-\frac{Q_r}{k_B\vartheta}\right)\,\langle\rho^\alpha - \rho^\alpha_{\rm min}(\vartheta)\rangle^q, \tag{15.15}$$

recovery1

Here $R_0$, $Q_r$, $q$, are constants, with $Q_r$ representing an *activation energy* for static recovery, and $k_B$ is Boltzmann's constant. The quantity $\rho^\alpha_{\rm min}(\vartheta)$ represents a minimum defect density at a given temperature. Also, $\langle x\rangle$ denotes the ramp function with a value 0 if $x < 0$, and a value $x$ if $x \geq 0$.

Fig. 1 shows a plot of the evolution of $\rho^\alpha$, for a slip sytem $\alpha$, based on the evolution equation (2.22) with the special forms for $A^\alpha$ and $R^\alpha$ listed in (15.14) and (15.15). Fig. 1a corresponds to accumulation of dislocations at a plastic shear strain rate of $10^{-3}\,\mathrm{s}^{-1}$ for 50 seconds — that is for a total plastic shear strain of 5% — at a temperature of 293 K (20°C), while Fig. 1b corresponds to the decrease in the dislocation density due to a subsequent thermal annealing step in which the plastic strain-rate is set to zero and the temperature is increased to 423K (150°C), for an additional time of 4950 seconds. In producing this figure we have used the following illustrative values for the material parameters:[33]

$$A_0 = 3 \times 10^{16}\,\mathrm{m}^{-2} \quad \rho^\alpha_{\mathrm{sat}} = 10^{15}\,\mathrm{m}^{-2}, \quad p = 1, \quad \text{with} \quad \rho^\alpha_0 = 10^{12}\,\mathrm{m}^{-2},$$

and

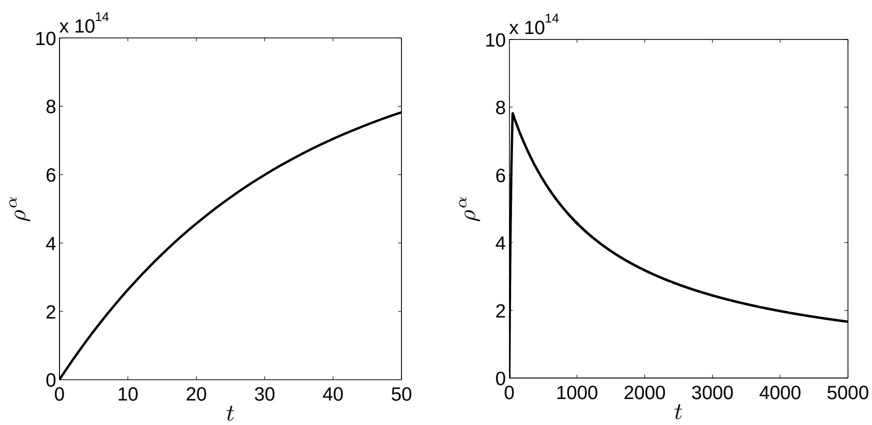
$$R_0 = 10^{-5}\,\mathrm{s}^{-1}, \quad Q_r = 1.75 \times 10^{-19}\,\mathrm{J}, \quad q = 2, \quad \text{with} \quad \rho^\alpha_{\mathrm{min}} = 0\,\mathrm{m}^{-2},$$

together with the Boltzmann's constant $k_B = 1.38 \times 10^{-23}\,\mathrm{J/K}$.

(v) Finally, as a constitutive equation for the heat flux we take *Fourier's law*

$$\mathbf{q} = -\mathbf{K}\nabla\vartheta, \tag{15.16}$$ special15

with $\mathbf{K}$, the thermal conductivity tensor at $\vartheta_0$, positive definite and symmetric.




(a) (b)

Figure 1: (a) Increase in dislocation density at a plastic shear strain rate of $10^{-3}\,\mathrm{s}^{-1}$ for 50 seconds, at a temperature of 293 K. (b) Decrease in dislocation density due to a subsequent thermal annealing step in which the plastic strain-rate is set to zero and the temperature is increased to 423 K, for an additional time of 4950 seconds. fig01

# 16 Concluding remarks

conclusions

We have formulated a *thermo-mechanically coupled gradient theory of rate-independent single-crystal plasticity* at low homologous temperatures, $\vartheta \lessapprox 0.35\,\vartheta_m$. Central to our

[33]For simplicity, the prameters $A_0$ and $\rho^\alpha_{\mathrm{min}}$ are taken to be temperature-independent.

continuum-mechanical theory is a defect energy

$$\hat{\psi}^p(\vartheta, \vec{\rho}) = \sum_\alpha E_{\rm CW}(\rho^\alpha) - \vartheta \sum_\alpha N_{\rm CW}(\rho^\alpha),$$

which represents an internal energy $\sum_\alpha E_{\rm CW}(\rho^\alpha)$ and an entropy $\sum_\alpha N_{\rm CW}(\rho^\alpha)$ associated with the accumulation of statistically-stored as well as geometrically-necessary dislocations — as represented by the dislocation densities $\rho^\alpha$, which are presumed to evolve according to

$$\dot{\rho}^\alpha = A^\alpha(\vartheta, \vec{\rho})\,\dot{\Gamma}^\alpha - R^\alpha(\vartheta, \vec{\rho}) \quad \text{with} \quad \rho^\alpha|_{t=0} = \rho_0^\alpha.$$

Our theory allows us to meaningfully discuss (cf. Section 11) the fraction of plastic stress-power that goes into heating, as well as the reduction of the dislocation density in a cold-worked material upon subsequent (or concurrent) thermal annealing.

The flow rule for the gradient theory is rate-independent, and takes the form of a yield function involving the dissipative generalized stress $\mathbf{\Sigma}^\alpha_{\rm dis}$, and an associated normality relation of Mises-Hill type for the generalized slip-rate $\dot{\mathbf{\Gamma}}^\alpha$. The flow relation may be expressed in equivalent form as an inequality involving the mechanical dissipation $D(\dot{\mathbf{\Gamma}}^\alpha, \vec{\rho})$. This inequality is central to the weak or variational formulation of the initial-boundary value problem: the resulting variational inequality incorporates the flow relation, the relation for the energetic generalized microstress $\mathbf{\Sigma}^\alpha_{\rm NR}$, and macroscopic equilibrium, and is supplemented by variational equations for microscopic forces and balance of energy.

The dissipative generalized microstress $\mathbf{\Sigma}^\alpha_{\rm dis}$ is indeterminate in the elastic region, so that the yield function may not be used pointwise to determine when flow takes place. The relation does however make sense within the variational setting in that the variational problem can be shown to be solvable[34], the solution providing a posteriori the elastic and plastic zones at each time-step.

We close by emphasizing that the purpose of this paper has been only to report on the formulation of our theory. We leave a report concerning its numerical implementation to future work. This is likely to follow an approach developed by Reddy, Wieners and Wohlmuth (2012) for a study in which the dissipative microstresses are absent and isothermal conditions are considered.

**Acknowledgements**

LA would like to gratefully acknowledge the support provided by NSF (CMMI Award No. 1063626). BDR acknowledges the support provided by the National Research Foundation through the South African Research Chair in Computational Mechanics.

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[34] E.g. by generalizing the approach taken by Reddy (2011) for the isothermal problem.

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