

BURGERS TENSOR FLOW ACCOUNTING FOR COLD WORK AND THERMAL ANNEALING

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ABSTRACT. This paper proposes a kinematical-thermal-based constitutive law for the evolution of Burgers tensor during cold work and upon subsequent thermal annealing of a polycrystalline. The proposal is based on the paper by Anand et al. [L. Anand., M. E. Gurtin., B. D. Reddy, *The stored energy of cold work, thermal annealing, and other thermodynamic issues in single crystal plasticity at small length scales*, Int. J. Plast. **64** (2015), 1–25]. The principle of virtual work and thermodynamic laws are employed to obtain balance of forces, balance of energy, and free-energy imbalance. Non-recoverable energetic microscopic stresses are obtained as features for materials that are cold-worked whenever the defect energy is dependent on Burgers tensor. Consequently, it is observed that internal-energetic plastic power is not less than entropic plastic power. The recovery rate during thermal annealing is shown to mimic dissipative behavior, leading to a reduction in the accumulation of dislocation densities. Furthermore, the free energy function –approximated as a quadratic form– is used to obtain the constitutive relations for the macroscopic and microscopic stresses.

1. Introduction

The visualization of a polycrystalline metal at the microstructural level often describes metal as an aggregate of grains with boundaries. The interiors of these grains have structures similar to single crystals, and their boundaries are called grain boundaries. At a temperature less than $0.35\theta_m$, where θ_m is the melting temperature of a metal, the plastic behavior involves a process known as cold working [3]. Within this temperature range, and for grain sizes with diameter greater than 100 nm , the plastic response of the entire polycrystalline metal is due to the plastic deformations of grain interiors with boundaries assumed to be perfectly bonded [17]. The carriers of these deformations are dislocations, which occur on crystallographic slip planes for each grain in the polycrystalline [28]. These give rise to strain hardening because such deformations for cold-worked materials

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are often accompanied by an increase in the number of dislocation densities, leading to resistance of plastic flows.

During cold working, a large portion of the plastic work performed is converted into heat, while a certain amount is stored as energy of cold work in the material. Experimental observations and theoretical studies on the stored energy of cold work have shown that the ratio of stored energy to plastic stress power for metals is often between 0 and 15% [7, 8, 23, 25]. This ratio plays a significant role in determining the fraction of plastic power that is converted into heating. Upon further heating to a temperature that is between $0.35\theta_m$ and $0.5\theta_m$, the cold-worked material undergoes a recovery process known as thermal annealing. During this process, there is a significant reduction in the accumulation of dislocation densities, thus allowing for plastic flow in the material. In this instance, the stored energy is released, which implies that the fraction of plastic power converted to heating changes with an increase in temperature, strain, and strain rates [3, 17, 19, 23].

A theory of polycrystalline plasticity under cold working should couple thermal effects with mechanical behavior in a thermodynamically consistent manner [1, 21]. Furthermore, such a theory should be capable of accounting –within the energy balance– for the increase in internal energy associated with the accumulation of dislocation densities [28]. Anand et al. [3] proposed a thermo-mechanical gradient theory of single-crystal plasticity for cold-worked materials, where a plastic internal energy that is dependent on dislocation densities is introduced. The proposed formulation expressed the evolution of the mean field of dislocation densities in terms of quantities associated with an increase in the accumulation of dislocation densities due to cold work, and quantities associated with a decrease in the accumulation of dislocation densities during thermal annealing.

Within the context of polycrystalline plasticity, the physical quantity that is known to measure dislocation densities is the Burgers tensor which can be expressed in terms of the distribution of edge and screw dislocation densities [15]. This paper aims to formulate a distortion gradient plasticity of a polycrystalline metal that accounts for the energy due to cold work and thermal annealing through a constitutively well-defined Burger tensor flow. In the paper of Borokinni et.al. [11] the Burgers tensor is assumed to be skew-symmetric, while its rate assumes no constitutive relation with the temperature, whereas in this paper, the Burgers tensor is not constrained to be skew-symmetric, but it is assumed to be constitutively dependent on the absolute temperature.

2. Basic kinematic relations

2.1. Decomposition of displacement gradient. Let \mathbf{u} be the displacement vector of a particle at a point \mathbf{x} and time t in a region B that corresponds to a plastic material. The displacement gradient of the material under small deformation admits the standard additive decomposition

$$(2.1) \quad \nabla \mathbf{u} = \mathbf{H}^e + \mathbf{H}^p$$

into elastic distortion \mathbf{H}^e and plastic distortion \mathbf{H}^p . The tensor \mathbf{H}^e measures the stretch and rotation of the underlying lattice structure of the plastic material,

while \mathbf{H}^p measures defects in the material structure arising from the formation and motion of dislocations. Plastic deformation, for most metals, does not incur changes in the volume of the material, thus we can assume the plastic incompressibility constraint

$$(2.2) \quad \text{tr } \mathbf{H}^p = 0.$$

The elastic and plastic strains \mathbf{E}^e and \mathbf{E}^p are defined as

$$\mathbf{E}^e = \frac{1}{2}(\mathbf{H}^e + \mathbf{H}^{eT}) \quad \text{and} \quad \mathbf{E}^p = \frac{1}{2}(\mathbf{H}^p + \mathbf{H}^{pT})$$

respectively. Also, the elastic and plastic rotations \mathbf{W}^e and \mathbf{W}^p are

$$\mathbf{W}^e = \frac{1}{2}(\mathbf{H}^e - \mathbf{H}^{eT}) \quad \text{and} \quad \mathbf{W}^p = \frac{1}{2}(\mathbf{H}^p - \mathbf{H}^{pT})$$

respectively. The tensor \mathbf{W}^e is called elastic rotation. It is the rotation of the underlying lattice structure associated with the skew-symmetric part of the elastic distortion tensor \mathbf{H}^e . The tensor \mathbf{W}^p is called plastic rotation arising from the formation and motion of dislocations. It is the skew-symmetric part of the plastic distortion tensor \mathbf{H}^p .

Clearly, \mathbf{E}^e and \mathbf{E}^p are the symmetric parts of \mathbf{H}^e and \mathbf{H}^p , respectively and \mathbf{W}^e and \mathbf{W}^p are the skew parts of \mathbf{H}^e and \mathbf{H}^p , respectively. The total strain \mathbf{E} and total rotation \mathbf{W} are given by

$$\mathbf{E} = \mathbf{E}^e + \mathbf{E}^p \quad \text{and} \quad \mathbf{W} = \mathbf{W}^e + \mathbf{W}^p$$

respectively. From eqs. (2.1) and (2.2), a basic kinematic rate equation is

$$(2.3) \quad \nabla \dot{\mathbf{u}} = \dot{\mathbf{H}}^e + \dot{\mathbf{H}}^p \quad \text{with} \quad \text{tr } \dot{\mathbf{H}}^p = 0,$$

where $\dot{\mathbf{A}}$ is the time-derivative of a physical quantity.

2.2. Burgers tensor. The Burgers tensor will be denoted as \mathbf{G} . This tensor is a local characterization of the Burgers vector which measures the closure failure of an infinitesimal circuit of a lattice on a plane with prescribed unit normal. The Burgers tensor \mathbf{G} is defined as¹

$$(2.4) \quad \mathbf{G} = \nabla \times \mathbf{H}^p \quad \text{or simply as} \quad G_{ij} = \varepsilon_{irs} H_{js,r}^p,$$

where ε_{irs} is the permutation symbol.

This definition in eq. (2.4) shows that a constitutive theory involving the Burgers tensor must account for plastic rotation \mathbf{W}^p through $\nabla \times \mathbf{W}^p$ except if one assumes from the outset that $\mathbf{W}^p = \mathbf{0}$. Constitutive theories for distortion gradient polycrystalline plasticity that account for plastic rotation will better approximate the single crystal gradient theories than those that ignore plastic rotation [2, 6, 9, 15]. Thus, in this paper, we make no assumption of plastic irrotationality.

¹ A_{ij} are the components of a second-order tensor \mathbf{A} . We denote $A_{j,s,r}$ as the partial derivative of $A_{j,s}$ with respect to x_r , where x_r are the components of the position vector \mathbf{x} .

2.3. Densities of edge and screw dislocations. The single crystal hypothesis allows the plastic distortion \mathbf{H}^p to be written as

$$(2.5) \quad \mathbf{H}^p = \sum_{\alpha} \gamma^{\alpha} \mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha},$$

where α indicates the slip system for a lattice with $\alpha = 1, 2, \dots, N$. Each slip system is described by a slip plane Π^{α} with normal \mathbf{m}^{α} . The vector \mathbf{s}^{α} is called slip direction and γ^{α} is the slip. The vectors \mathbf{s}^{α} and \mathbf{m}^{α} are unit, constant and orthogonal vectors i.e. $\mathbf{s}^{\alpha} \cdot \mathbf{m}^{\alpha} = 0$ and $|\mathbf{s}^{\alpha}| = |\mathbf{m}^{\alpha}| = 1$. With the choice of plastic distortion \mathbf{H}^p in eq. (2.5), it is observed that eq. (2.1) can be written as

$$\nabla \mathbf{u} = \mathbf{H}^e + \sum_{\alpha} \gamma^{\alpha} \mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha}.$$

Also, note that

$$\text{tr } \mathbf{H}^p = \text{tr} \left(\sum_{\alpha} \gamma^{\alpha} \mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha} \right) = \sum_{\alpha} \gamma^{\alpha} \mathbf{s}^{\alpha} \cdot \mathbf{m}^{\alpha} = 0.$$

Thus, the single-crystal theory naturally satisfies the plastic incompressibility constraint. Following Arsenlis and Parks [4], and within the framework of continuum mechanics, the quantities

$$(2.6) \quad \rho_E^{\alpha} := -\mathbf{s}^{\alpha} \cdot \nabla \gamma^{\alpha} \quad \text{and} \quad \rho_S^{\alpha} := (\mathbf{m}^{\alpha} \times \mathbf{s}^{\alpha}) \cdot \nabla \gamma^{\alpha}$$

mimic the edge and screw dislocation densities, respectively. Let $\mathbf{l}^{\alpha} = \mathbf{m}^{\alpha} \times \mathbf{s}^{\alpha}$, then the set $\{\mathbf{l}^{\alpha}, \mathbf{m}^{\alpha}, \mathbf{s}^{\alpha}\}$ forms an orthonormal basis in the three-dimensional Euclidean space. Thus, we have $\nabla \gamma^{\alpha} = -\rho_E^{\alpha} \mathbf{s}^{\alpha} + \rho_S^{\alpha} \mathbf{l}^{\alpha} + (\mathbf{m}^{\alpha} \cdot \nabla \gamma^{\alpha}) \mathbf{m}^{\alpha}$. The term $-\rho_E^{\alpha} \mathbf{s}^{\alpha} + \rho_S^{\alpha} \mathbf{l}^{\alpha}$ is known as the tangential slip gradient and is denoted as $\nabla_{\text{tan}}^{\alpha} \gamma^{\alpha}$, while the quantity $(\mathbf{m}^{\alpha} \cdot \nabla \gamma^{\alpha}) \mathbf{m}^{\alpha}$ is known as the normal slip gradient. The normal slip gradient is not a known measure of any macroscopic quantity that mimics dislocation density.

Using eqs. (2.5) and (2.6), the Burgers tensor can be written as

$$(2.7) \quad \mathbf{G} = \nabla \times \mathbf{H}^p = \sum_{\alpha} (\rho_E^{\alpha} \mathbf{l}^{\alpha} \otimes \mathbf{s}^{\alpha} + \rho_S^{\alpha} \mathbf{s}^{\alpha} \otimes \mathbf{s}^{\alpha}).$$

Eq. (2.7) shows that the Burgers tensor can be additively decomposed into the distribution of edge and screw dislocation densities on individual slip systems.

2.4. Constitutively defined flows of dislocation densities. In the paper written by Anand et al. [3], a dislocation density ρ^{α} representing the mean field of glide and geometrically necessary dislocation densities is defined through the initial-value problem

$$(2.8) \quad \dot{\rho}^{\alpha} = A^{\alpha}(\theta, \vec{\rho}) \dot{\Gamma}^{\alpha} - R^{\alpha}(\theta, \vec{\rho}) \quad \text{with} \quad \rho^{\alpha}(\mathbf{x}, 0) = \rho_o^{\alpha},$$

where $A^{\alpha}(\theta, \vec{\rho})$, $R^{\alpha}(\theta, \vec{\rho})$ and $\dot{\Gamma}^{\alpha}$ are dislocation-accumulation modulus, recovery rate and effective flow rate, respectively. The quantities θ and $\vec{\rho}$ are the absolute temperature and list of dislocation densities $(\rho^1, \rho^2, \dots, \rho^N)$ respectively. $A^{\alpha}(\theta, \vec{\rho})$ and $R^{\alpha}(\theta, \vec{\rho})$ satisfy

$$A^{\alpha}(\theta, \vec{\rho}) \geq 0, \quad \text{and} \quad R^{\alpha}(\theta, \vec{\rho}) \geq 0 \quad \text{with} \quad \frac{\partial R^{\alpha}}{\partial \theta} \geq 0 \quad \text{for all} \quad \theta > 0 \quad \text{and} \quad \vec{\rho}.$$

The effective flow rate is defined as $\dot{\Gamma} = \sqrt{|\dot{\gamma}^\alpha|^2 + l^2 |\nabla_{\tan}^\alpha \dot{\gamma}^\alpha|^2}$. We shall assume, for the moment, that dislocation densities (edge and screw) satisfy eq. (2.8) i.e.

$$(2.9) \quad \dot{\rho}_E^\alpha = A_E^\alpha(\theta, \vec{\rho}_E, \vec{\rho}_S, \vec{\rho}_G) \dot{\Gamma}^\alpha - R_E^\alpha(\theta, \vec{\rho}_E, \vec{\rho}_S, \vec{\rho}_G) \quad \text{with} \quad \rho_E^\alpha(\mathbf{x}, 0) = \rho_E^{*\alpha},$$

and

$$(2.10) \quad \dot{\rho}_S^\alpha = A_S^\alpha(\theta, \vec{\rho}_E, \vec{\rho}_S, \vec{\rho}_G) \dot{\Gamma}^\alpha - R_S^\alpha(\theta, \vec{\rho}_E, \vec{\rho}_S, \vec{\rho}_G) \quad \text{with} \quad \rho_S^\alpha(\mathbf{x}, 0) = \rho_S^\alpha,$$

where $\vec{\rho}_E$, $\vec{\rho}_S$ and $\vec{\rho}_G$ are the list of edge, screw, and glide dislocation densities, respectively. The quantities A_E^α and A_S^α are the dislocation-accumulation modulus associated with edge and screw dislocation densities, respectively. R_E^α and R_S^α are the recovery rates associated with edge and screw dislocation densities, respectively. Using eqs. (2.7), (2.9) and (2.10), the flow of Burgers tensor can be written as

$$(2.11) \quad \dot{\mathbf{G}} = \sum_{\alpha} \mathbf{A}^\alpha(\theta, \vec{\rho}_E, \vec{\rho}_S, \vec{\rho}_G) \dot{\Gamma}^\alpha - \sum_{\alpha} \mathbf{R}^\alpha(\theta, \vec{\rho}_E, \vec{\rho}_S, \vec{\rho}_G),$$

where, $\mathbf{A}^\alpha = A_E^\alpha \mathbf{I}^\alpha \otimes \mathbf{s}^\alpha + A_S^\alpha \mathbf{s}^\alpha \otimes \mathbf{s}^\alpha$ and $\mathbf{R}^\alpha = R_E^\alpha \mathbf{I}^\alpha \otimes \mathbf{s}^\alpha + R_S^\alpha \mathbf{s}^\alpha \otimes \mathbf{s}^\alpha$. Eq. (2.11) serves as a guide to obtaining the constitutive relation for the flow of Burgers tensor for a polycrystalline.

2.5. Burgers tensor rate for polycrystalline. It is not a basic assumption in polycrystalline theory that the plastic distortion takes the form in eq. (2.5). Thus, the single crystal and polycrystalline gradient theory are not the same [5, 12, 14]. However, a polycrystalline is an aggregate of grains –similar in structure to single-crystals– of different sizes and with grain boundaries. Hence, the constitutive relation for the Burgers tensor rate would be assumed in an average sense in concert with eq. (2.11). We propose a Burgers tensor rate $\dot{\mathbf{G}}$ of the form

$$(2.12) \quad \dot{\mathbf{G}} = \mathbf{A}(\theta, \mathbf{G}) d^p - \mathbf{R}(\theta, \mathbf{G}) \quad \text{with} \quad \mathbf{G}(\mathbf{x}, 0) = \mathbf{G}_o,$$

where $\mathbf{A}(\theta, \mathbf{G})$ and $\mathbf{R}(\theta, \mathbf{G})$ will be referred to as *accumulation modulus* and *recovery* tensors, respectively, which are assumed to be positive semi-definite. Here, the first term on the right-hand side of eq. (2.12) characterizes changes in Burgers tensor due to plastic flow, while the second term characterizes changes in Burgers tensor due to thermal annealing. The quantity d^p is the effective flow rate defined as

$$(2.13) \quad d^p = \sqrt{|\dot{\mathbf{H}}^p|^2 + l^2 |\nabla \dot{\mathbf{H}}^p|^2}.$$

3. Virtual power principle

The local macroscopic and microscopic force balances for plastic flow are often obtained as consequences of the principle of virtual power. Let P be an arbitrary region of the body B called a sub-body of B and with boundary ∂P . The external macroscopic forces on P are power-conjugate to velocity $\dot{\mathbf{u}}$. Let $\mathbf{t}(\mathbf{n})$ and \mathbf{b} be macro-traction on ∂P and body force on P , respectively, where \mathbf{n} is the outward unit normal on ∂P . Also, assume that a microscopic traction $\mathbf{K}(\mathbf{n})$ acts on ∂P

and it is power-conjugate to the plastic distortion rate $\dot{\mathbf{H}}^p$. The power $\mathcal{W}_{\text{ext}}(P)$ expended on P by these external forces for a quasi-static process is

$$\mathcal{W}_{\text{ext}}(P) = \int_{\partial P} \mathbf{t}(\mathbf{n}) \cdot \dot{\mathbf{u}} \, da + \int_P \mathbf{b} \cdot \dot{\mathbf{u}} \, dV + \int_{\partial P} \mathbf{K}(\mathbf{n}) : \dot{\mathbf{H}}^p \, da.$$

The external power expenditure on P is balanced by power expended within P . Consistent with the kinematic relation in eq. (2.3), the following can be assumed [13, 18, 24, 26, 27]:

- (i.) Macroscopic stress \mathbf{T} is power-conjugate to the elastic distortion rate $\dot{\mathbf{H}}^e$;
- (ii.) Plastic microscopic stress \mathbf{T}^p is deviatoric and power-conjugate to the plastic distortion rate $\dot{\mathbf{H}}^p$; and
- (iii.) A third-order polar microscopic stress \mathbb{K}^p is deviatoric in its first two indices and power-conjugate to the gradient of plastic distortion rate $\nabla \dot{\mathbf{H}}^p$.

The power $\mathcal{W}_{\text{int}}(P)$ expended within P is given by

$$\mathcal{W}_{\text{int}}(P) = \int_P [\mathbf{T} : \dot{\mathbf{H}}^e + \mathbf{T}^p : \dot{\mathbf{H}}^p + \mathbb{K}^p : \nabla \dot{\mathbf{H}}^p] \, dV.$$

Let $\nu = (\tilde{\mathbf{u}}, \tilde{\mathbf{H}}^e, \tilde{\mathbf{H}}^p)$ be a list of generalized virtual velocities consistent with

$$\nabla \tilde{\mathbf{u}} = \tilde{\mathbf{H}}^e + \tilde{\mathbf{H}}^p; \quad \text{tr } \tilde{\mathbf{H}}^p = 0.$$

The virtual power principle states that

$$\begin{aligned} \int_{\partial P} \mathbf{t}(\mathbf{n}) \cdot \tilde{\mathbf{u}} \, da + \int_P \mathbf{b} \cdot \tilde{\mathbf{u}} \, dV + \int_{\partial P} \mathbf{K}(\mathbf{n}) : \tilde{\mathbf{H}}^p \, da \\ = \int_P [\mathbf{T} : \tilde{\mathbf{H}}^e + \mathbf{T}^p : \tilde{\mathbf{H}}^p + \mathbb{K}^p : \nabla \tilde{\mathbf{H}}^p] \, dV. \end{aligned}$$

The consequences of the virtual power principle following Gurtin [15] and Anand et al. [3] are:

- (i.) Macroscopic force balance and macro-traction condition

$$\text{div } \mathbf{T} + \mathbf{b} = \mathbf{0} \quad \text{in } P \quad \text{and} \quad \mathbf{t}(\mathbf{n}) = \mathbf{T}\mathbf{n} \quad \text{on } \partial P$$

respectively.

- (ii.) Microscopic force balance and micro-traction condition

$$(3.1) \quad \mathbf{T}_o = \mathbf{T}^p - \text{div } \mathbb{K}^p \quad \text{in } P \quad \text{and} \quad \mathbf{K}(\mathbf{n}) = \mathbb{K}^p \mathbf{n} \quad \text{on } \partial P$$

respectively, where

$$\mathbf{T}_o = \mathbf{T} - \frac{1}{3}(\text{tr } \mathbf{T})\mathbf{I}$$

is the deviatoric part of \mathbf{T} and \mathbf{I} is the second order unit tensor.

Also, as a consequence of frame-indifferent, the macroscopic stress \mathbf{T} is symmetric (i.e. $\mathbf{T} = \mathbf{T}^T$) so that we obtain

$$\mathbf{T} : \dot{\mathbf{H}}^e = \mathbf{T} : \dot{\mathbf{E}}^e.$$

4. Balance of energy and free-energy imbalance

Balance of energy is simply a statement of the first law of thermodynamics which is written mathematically as

$$\int_P \dot{\epsilon} dv = \mathcal{W}_{\text{ext}}(P) - \int_{\partial P} \mathbf{q} \cdot \mathbf{n} da + \int_P q dv,$$

where ϵ is the internal energy measured per unit volume, \mathbf{q} is the heat flux through ∂P and q is the heat supply to P . Using the power balance principle and divergence theorem, the global energy balance can be written as

$$\int_P \dot{\epsilon} dv = \int_P [\mathbf{T} : \dot{\mathbf{E}}^e + \mathbf{T}^p : \dot{\mathbf{H}}^p + \mathbb{K}^p : \nabla \dot{\mathbf{H}}^p - \text{div } \mathbf{q} + q] dv.$$

Since, P is an arbitrary portion of B , the local form of the energy balance is

$$(4.1) \quad \dot{\epsilon} = \mathbf{T} : \dot{\mathbf{E}}^e + \mathbf{T}^p : \dot{\mathbf{H}}^p + \mathbb{K}^p : \nabla \dot{\mathbf{H}}^p - \text{div } \mathbf{q} + q.$$

The second law of thermodynamics is written as

$$\int_P \dot{\eta} dv \geq - \int_{\partial P} \frac{\mathbf{q}}{\theta} \cdot \mathbf{n} da + \int_P \frac{q}{\theta} dv,$$

where η is the entropy of P measured per unit volume and $\theta > 0$. Following the arbitrary nature of P , the entropy imbalance in local form is

$$\dot{\eta} \geq - \text{div} \left(\frac{\mathbf{q}}{\theta} \right) + \frac{q}{\theta}.$$

Introduce the free energy ψ defined via the Gibbs' relation

$$(4.2) \quad \psi = \epsilon - \theta \eta.$$

A combination of eqs. (4.1), (4.2) and the above inequality gives the local free-energy imbalance as

$$(4.3) \quad \dot{\psi} + \dot{\theta} \eta - \mathbf{T} : \dot{\mathbf{E}}^e - \mathbf{T}^p : \dot{\mathbf{H}}^p - \mathbb{K}^p : \nabla \dot{\mathbf{H}}^p + \frac{1}{\theta} \mathbf{q} \cdot \nabla \theta \leq 0.$$

This imbalance will be useful in obtaining thermodynamically consistent constitutive relations for the entropy, stresses, and heat flux.

5. Constitutive relations

Let the free energy be defined as $\psi = \hat{\psi}(\theta, \mathbf{E}^e, \mathbf{G})$, and assume a separable form $\hat{\psi}(\theta, \mathbf{E}^e, \mathbf{G}) = \hat{\psi}^e(\theta, \mathbf{E}^e) + \hat{\psi}^p(\theta, \mathbf{G})$ into elastic free energy ψ^e and defect energy ψ^p . With these choices, it is clear that

$$\dot{\psi} = \frac{\partial \hat{\psi}^e(\theta, \mathbf{E}^e)}{\partial \mathbf{E}^e} : \dot{\mathbf{E}}^e + \frac{\partial \hat{\psi}(\theta, \mathbf{E}^e, \mathbf{G})}{\partial \theta} \dot{\theta} + \frac{\partial \hat{\psi}^p(\theta, \mathbf{G})}{\partial \mathbf{G}} : \dot{\mathbf{G}}.$$

Let

$$\mathbf{S}^p = \mathbf{S}^p(\theta, \mathbf{G}) = \frac{\partial \hat{\psi}^p(\theta, \mathbf{G})}{\partial \mathbf{G}},$$

then by eq. (2.12), we have

$$(5.1) \quad \mathbf{S}^p : \dot{\mathbf{G}} = \mathbf{S}^p : \mathbf{A}(\theta, \mathbf{G}) d^p - \mathbf{S}^p : \mathbf{R}(\theta, \mathbf{G}).$$

Let $F(\theta, \mathbf{G})$ and $R(\theta, \mathbf{G})$ be defined as

$$(5.2) \quad F(\theta, \mathbf{G}) = \mathbf{S}^p(\theta, \mathbf{G}) : \mathbf{A}(\theta, \mathbf{G}) \quad \text{and} \quad R(\theta, \mathbf{G}) = \mathbf{S}^p(\theta, \mathbf{G}) : \mathbf{R}(\theta, \mathbf{G}),$$

and assume that $F(\theta, \mathbf{G}) \geq 0$. Using eqs. (2.13) and (5.2), we can write eq. (5.1) as

$$(5.3) \quad \mathbf{S}^p : \dot{\mathbf{G}} = \frac{F(\theta, \mathbf{G})}{d^p} [|\dot{\mathbf{H}}^p|^2 + l^2 |\nabla \dot{\mathbf{H}}^p|^2] - R(\theta, \mathbf{G}).$$

Now introduce the microscopic stresses \mathbf{T}_{NR}^p and \mathbb{K}_{NR}^p defined as

$$(5.4) \quad \mathbf{T}_{NR}^p = F(\theta, \mathbf{G}) \frac{\dot{\mathbf{H}}^p}{d^p} \quad \text{and} \quad \mathbb{K}_{NR}^p = l^2 F(\theta, \mathbf{G}) \frac{\nabla \dot{\mathbf{H}}^p}{d^p}, \quad \text{for } d^p \neq 0,$$

then eq. (5.3) can be written as

$$(5.5) \quad \mathbf{S}^p : \dot{\mathbf{G}} = \mathbf{T}_{NR}^p : \dot{\mathbf{H}}^p + \mathbb{K}_{NR}^p : \nabla \dot{\mathbf{H}}^p - R(\theta, \mathbf{G}).$$

Since, $F(\theta, \mathbf{G}) \geq 0$, then the stresses \mathbf{T}_{NR}^p and \mathbb{K}_{NR}^p are non-recoverable in the sense:

$$(5.6) \quad \mathbf{T}_{NR}^p : \dot{\mathbf{H}}^p + \mathbb{K}_{NR}^p : \nabla \dot{\mathbf{H}}^p \geq 0.$$

Eq. (5.4) holds provided $d^p \neq 0$. To accommodate $d^p = 0$, a scalar function ϕ is introduced and it is defined by $\phi(\theta, \mathbf{G}, d^p) = F(\theta, \mathbf{G})d^p$, for all $d^p \geq 0$. Clearly, when $d^p = 0$, we have $|\dot{\mathbf{H}}^p| = 0$ and $|\nabla \dot{\mathbf{H}}^p| = 0$. Given that $d^p \neq 0$ and

$$(5.7) \quad \mathbf{T}_{NR}^p : \tilde{\mathbf{H}}^p + \mathbb{K}_{NR}^p : \nabla \tilde{\mathbf{H}}^p \leq \phi(\theta, \mathbf{G}, \tilde{d}^p) \quad \text{for all } \tilde{d}^p \geq 0,$$

where $\tilde{d}^p = \sqrt{|\tilde{\mathbf{H}}^p|^2 + l^2 |\nabla \tilde{\mathbf{H}}^p|^2}$. Then by eqs. (5.4), (5.6), and (5.7), we obtain

$$(5.8) \quad \phi(\theta, \mathbf{G}, \tilde{d}^p) \geq \phi(\theta, \mathbf{G}, d^p) + \mathbf{T}_{NR}^p : (\tilde{\mathbf{H}}^p - \dot{\mathbf{H}}^p) + \mathbb{K}_{NR}^p : (\nabla \tilde{\mathbf{H}}^p - \nabla \dot{\mathbf{H}}^p)$$

for all $\tilde{d}^p \geq 0$. Using chain rule, it is clear that

$$\frac{\partial \phi}{\partial \dot{\mathbf{H}}^p} = \frac{\partial \phi}{\partial d^p} \frac{\partial d^p}{\partial \dot{\mathbf{H}}^p} = F(\theta, \mathbf{G}) \frac{\dot{\mathbf{H}}^p}{d^p}$$

and

$$\frac{\partial \phi}{\partial \nabla \dot{\mathbf{H}}^p} = \frac{\partial \phi}{\partial d^p} \frac{\partial d^p}{\partial \nabla \dot{\mathbf{H}}^p} = l^2 F(\theta, \mathbf{G}) \frac{\nabla \dot{\mathbf{H}}^p}{d^p} \quad \text{whenever } d^p \neq 0.$$

Hence, in terms of ϕ , the non-recoverable stresses can be written as

$$\mathbf{T}_{NR}^p = \frac{\partial \phi(\theta, \mathbf{G}, d^p)}{\partial \dot{\mathbf{H}}^p} \quad \text{and} \quad \mathbb{K}_{NR}^p = \frac{\partial \phi(\theta, \mathbf{G}, d^p)}{\partial \nabla \dot{\mathbf{H}}^p} \quad \text{provided } d^p \neq 0.$$

Following Anand et al. [3], we assume that the dissipative microscopic stresses \mathbf{T}_{dis}^p and \mathbb{K}_{dis}^p are defined through

$$(5.9) \quad \mathbf{T}_{dis}^p = \mathbf{T}^p - \mathbf{T}_{NR}^p \quad \text{and} \quad \mathbb{K}_{dis}^p = \mathbb{K}^p - \mathbb{K}_{NR}^p.$$

Thus, the free-energy imbalance eq. (4.3) can be written as

$$\left(\frac{\partial \hat{\psi}^e(\theta, \mathbf{E}^e)}{\partial \mathbf{E}^e} - \mathbf{T} \right) : \dot{\mathbf{E}}^e + \left(\frac{\partial \hat{\psi}(\theta, \mathbf{E}^e, \mathbf{G})}{\partial \theta} + \eta \right) \dot{\theta}$$

$$-R(\theta, \mathbf{G}) - \mathbf{T}_{\text{dis}}^p : \dot{\mathbf{H}}^p - \mathbb{K}_{\text{dis}}^p : \nabla \dot{\mathbf{H}}^p + \frac{1}{\theta} \mathbf{q} \cdot \nabla \theta \leq 0.$$

By Coleman–Noll procedure, we have the constitutive relations for the macroscopic stress and the entropy:

$$(5.10) \quad \mathbf{T} = \hat{\mathbf{T}}(\theta, \mathbf{E}^e) = \frac{\partial \hat{\psi}^e(\theta, \mathbf{E}^e)}{\partial \mathbf{E}^e} \quad \text{and} \quad \eta = \hat{\eta}(\theta, \mathbf{E}^e, \mathbf{G}) = -\frac{\partial \hat{\psi}(\theta, \mathbf{E}^e, \mathbf{G})}{\partial \theta}.$$

The dissipation inequality is given as

$$R(\theta, \mathbf{G}) + \mathbf{T}_{\text{dis}}^p : \dot{\mathbf{H}}^p + \mathbb{K}_{\text{dis}}^p : \nabla \dot{\mathbf{H}}^p - \frac{1}{\theta} \mathbf{q} \cdot \nabla \theta \geq 0.$$

As a constitutive choice, consistent with literature [3, 17], we assume that $\mathbf{q} = \hat{\mathbf{q}}(\theta, \nabla \theta)$, where $\mathbf{T}_{\text{dis}}^p$, $\mathbb{K}_{\text{dis}}^p$ and $R(\theta, \mathbf{G})$ are independent of temperature gradient, then it is clear that we have the heat-conduction inequality to be given as

$$\hat{\mathbf{q}}(\theta, \nabla \theta) \cdot \nabla \theta \leq 0 \quad \text{for all } \nabla \theta, \dot{\mathbf{H}}^p, \nabla \dot{\mathbf{H}}^p, \text{ and } \mathbf{G}.$$

Because $\nabla \theta$ can be chosen arbitrarily independent of $\dot{\mathbf{H}}^p$, $\nabla \dot{\mathbf{H}}^p$ and \mathbf{G} , then we have the mechanical dissipation inequality given as $R(\theta, \mathbf{G}) + \mathbf{T}_{\text{dis}}^p : \dot{\mathbf{H}}^p + \mathbb{K}_{\text{dis}}^p : \nabla \dot{\mathbf{H}}^p \geq 0$. Consistent with Gurtin et al. [17] for rate-independent plastic materials, we assume the constitutive forms:

$$\mathbf{T}_{\text{dis}}^p = \hat{\mathbf{T}}_{\text{dis}}^p(\theta, \mathbf{e}^p, \dot{\mathbf{H}}^p, \nabla \dot{\mathbf{H}}^p) \quad \text{and} \quad \mathbb{K}_{\text{dis}}^p = \hat{\mathbb{K}}_{\text{dis}}^p(\theta, \mathbf{e}^p, \dot{\mathbf{H}}^p, \nabla \dot{\mathbf{H}}^p),$$

where \mathbf{e}^p is an hardening variable satisfying the equation $\dot{\mathbf{e}}^p = d^p$ with $\mathbf{e}^p(\mathbf{x}, 0) = 0$. With these constitutive choices, it is clear that $\mathbf{T}_{\text{dis}}^p$ and $\mathbb{K}_{\text{dis}}^p$ are independent of \mathbf{G} . Thus, for arbitrary choices of $\dot{\mathbf{H}}^p$ and $\nabla \dot{\mathbf{H}}^p$ we have the important result

$$(5.11) \quad R(\theta, \mathbf{G}) \geq 0 \quad \text{for all } \mathbf{G}.$$

The mechanical dissipation is defined as

$$\delta := \mathbf{T}_{\text{dis}}^p : \dot{\mathbf{H}}^p + \mathbb{K}_{\text{dis}}^p : \nabla \dot{\mathbf{H}}^p.$$

Consistent with Anand et al. [3], we assume that the material is strongly dissipative in the sense that the mechanical dissipation δ satisfies $\delta \geq 0$ for all d^p , and $\delta > 0$ for all $d^p \neq 0$.

REMARK 5.1. The inequality (5.11) shows that if defect microscopic force \mathbf{S}^p and recovery tensor \mathbf{R} are not orthogonal, then the recovery mimics a dissipative process and will characterize a decrease in dislocation densities due to thermal annealing.

6. Associative flow for dissipative microscopic stresses

Assume the material under consideration is rate-independent [16, 22]. We define the yield function $F(\theta, \mathbf{e}^p, \mathbf{T}_{\text{dis}}^p, \mathbb{K}_{\text{dis}}^p)$ by

$$F(\theta, \mathbf{e}^p, \mathbf{T}_{\text{dis}}^p, \mathbb{K}_{\text{dis}}^p) = \sqrt{|\mathbf{T}_{\text{dis}}^p|^2 + l^{-2} |\mathbb{K}_{\text{dis}}^p|^2} - Y(\theta, \mathbf{e}^p),$$

where $Y(\theta, \mathbf{e}^p)$ is the flow resistance defined as $Y(\theta, \mathbf{e}^p) = \frac{\delta}{\dot{\mathbf{e}}^p}$ for all $\dot{\mathbf{e}}^p \neq 0$. Following the assumption of strict dissipativity (i.e. $\delta > 0$ whenever $\dot{\mathbf{e}}^p \neq 0$), then $Y(\theta, \mathbf{e}^p) > 0$.

For associative flow, the following normality relations hold:

$$\frac{\dot{\mathbf{H}}^p}{\dot{\epsilon}^p} = \frac{\mathbf{T}_{\text{dis}}^p}{\sqrt{|\mathbf{T}_{\text{dis}}^p|^2 + l^{-2}|\mathbb{K}_{\text{dis}}^p|^2}} \quad \text{and} \quad \frac{l\nabla\dot{\mathbf{H}}^p}{\dot{\epsilon}^p} = \frac{l^{-1}\mathbb{K}_{\text{dis}}^p}{\sqrt{|\mathbf{T}_{\text{dis}}^p|^2 + l^{-2}|\mathbb{K}_{\text{dis}}^p|^2}} \quad \text{for } \dot{\epsilon}^p \neq 0.$$

For plastic flow $\dot{\epsilon}^p \neq 0$, the yield criterion $F(\theta, \mathbf{e}^p, \dot{\mathbf{H}}^p, \nabla\dot{\mathbf{H}}^p) = 0$ is satisfied, so that we have

$$\sqrt{|\mathbf{T}_{\text{dis}}^p|^2 + l^{-2}|\mathbb{K}_{\text{dis}}^p|^2} = Y(\theta, \mathbf{e}^p) \quad \text{whenever } \dot{\epsilon}^p \neq 0.$$

The consequences of the normality relations are the following constitutive relations for dissipative microscopic stresses:

$$\mathbf{T}_{\text{dis}}^p = Y(\theta, \mathbf{e}^p) \frac{\dot{\mathbf{H}}^p}{d^p} \quad \text{and} \quad \mathbb{K}_{\text{dis}}^p = l^2 Y(\theta, \mathbf{e}^p) \frac{\nabla\dot{\mathbf{H}}^p}{d^p} \quad \text{for } d^p \neq 0.$$

The elastic range is given as $F(\theta, \mathbf{e}^p, \dot{\mathbf{H}}^p, \nabla\dot{\mathbf{H}}^p) \leq 0$ for all $\dot{\epsilon}^p \geq 0$. The no flow condition is given by $\dot{\epsilon}^p = 0$ whenever $F(\theta, \mathbf{e}^p, \dot{\mathbf{H}}^p, \nabla\dot{\mathbf{H}}^p) < 0$.

Suppressing other arguments, the dissipation δ is defined as

$$(6.1) \quad \delta = \delta(\dot{\epsilon}^p) = Y(\theta, \mathbf{e}^p) \dot{\epsilon}^p \quad \text{for all } \dot{\epsilon}^p \geq 0.$$

According to the principle of maximum plastic dissipation, fields evolve so as to maximize dissipation in the sense [10]

$$(6.2) \quad \delta(\tilde{\epsilon}^p) \geq \mathbf{T}_{\text{dis}}^p : \tilde{\mathbf{H}}^p + \mathbb{K}_{\text{dis}}^p : \nabla\tilde{\mathbf{H}}^p \quad \text{for all } \tilde{\epsilon}^p \geq 0.$$

Combining eqs. (6.1) and (6.2), we have

$$(6.3) \quad \delta(\tilde{\epsilon}^p) \geq \delta(\dot{\epsilon}^p) + \mathbf{T}_{\text{dis}}^p : (\tilde{\mathbf{H}}^p - \dot{\mathbf{H}}^p) + \mathbb{K}_{\text{dis}}^p : (\nabla\tilde{\mathbf{H}}^p - \nabla\dot{\mathbf{H}}^p).$$

Also, observe from eq. (6.1) that

$$\mathbf{T}_{\text{dis}}^p = \frac{\partial\delta(\dot{\epsilon}^p)}{\partial\dot{\mathbf{H}}^p} \quad \text{and} \quad \mathbb{K}_{\text{dis}}^p = \frac{\partial\delta(\dot{\epsilon}^p)}{\partial\nabla\dot{\mathbf{H}}^p} \quad \text{for all } \dot{\mathbf{H}}^p \neq \mathbf{0} \quad \text{and} \quad \nabla\dot{\mathbf{H}}^p \neq \mathbf{0}.$$

7. Energy balance in terms of heat capacity: Energy and entropy of cold work

It is known that for many metals, dislocation changes do not contribute much to changes in the heat capacity. Following Lubliner [20], Rosakis et al. [23], and Anand et al. [3], we assume the heat capacity is independent of the Burgers tensor \mathbf{G} . If c denotes the heat capacity, then constitutively, we write $c = c(\theta, \mathbf{E}^e)$. The heat capacity is defined as

$$(7.1) \quad c(\theta, \mathbf{E}^e) = \frac{\partial\hat{\epsilon}(\theta, \mathbf{E}^e, \mathbf{G})}{\partial\theta},$$

where $\epsilon = \hat{\epsilon}(\theta, \mathbf{E}^e, \mathbf{G})$ is the internal energy satisfying the Gibbs' relation

$$(7.2) \quad \hat{\epsilon}(\theta, \mathbf{E}^e, \mathbf{G}) = \hat{\psi}(\theta, \mathbf{E}^e, \mathbf{G}) + \theta\hat{\eta}(\theta, \mathbf{E}^e, \mathbf{G}).$$

Using eqs. (7.1) and (7.2), the energy balance eq. (4.1) can be written as

$$\begin{aligned} c\dot{\theta} + \frac{\partial\epsilon}{\partial\mathbf{E}^e} : \dot{\mathbf{E}}^e + \frac{\partial\epsilon}{\partial\mathbf{G}} : \dot{\mathbf{G}} &= \mathbf{T} : \dot{\mathbf{E}}^e + \mathbf{T}^p : \dot{\mathbf{H}}^p + \mathbb{K}^p : \nabla\dot{\mathbf{H}}^p - \text{div } \mathbf{q} + q \\ \implies c\dot{\theta} - \theta \frac{\partial\mathbf{T}}{\partial\theta} : \dot{\mathbf{E}}^e - R(\theta, \mathbf{G}) - \theta \frac{\partial\mathbf{S}^p}{\partial\theta} : \dot{\mathbf{G}} &= \mathbf{T}_{\text{dis}}^p : \dot{\mathbf{H}}^p + \mathbb{K}_{\text{dis}}^p : \nabla\dot{\mathbf{H}}^p - \text{div } \mathbf{q} + q. \end{aligned}$$

Also, observe that by eqs. (3.1), (5.5) and (5.9), we have

$$\begin{aligned} \mathbf{T}_{\text{dis}}^p &: \dot{\mathbf{H}}^p + \mathbb{K}_{\text{dis}}^p \cdot \nabla \dot{\mathbf{H}}^p + R(\theta, \mathbf{G}) + \theta \frac{\partial \mathbf{S}^p}{\partial \theta} : \dot{\mathbf{G}} \\ &= \mathbf{T} : \dot{\mathbf{H}}^p + \text{div}(\mathbb{K}^p \dot{\mathbf{H}}^p) - \left(\mathbf{S}^p - \theta \frac{\partial \mathbf{S}^p}{\partial \theta} \right) : \dot{\mathbf{G}}, \end{aligned}$$

where the component of $\mathbb{K}^p \dot{\mathbf{H}}^p$ is given by $(\mathbb{K}^p \dot{\mathbf{H}}^p)_k = K_{ijk}^p \dot{H}_{ij}^p$. The components of \mathbb{K}^p and $\dot{\mathbf{H}}^p$ are K_{ijk}^p and \dot{H}_{ij}^p , respectively. The stress-temperature modulus tensor \mathbf{M} is defined as

$$\mathbf{M} = \mathbf{M}(\theta, \mathbf{E}^e) = \frac{\partial \mathbf{T}}{\partial \theta}.$$

The energy balance can thus be written as

$$(7.3) \quad c\dot{\theta} + \text{div} \mathbf{q} - q = \mathbf{T} : \dot{\mathbf{H}}^p + \text{div}(\mathbb{K}^p \dot{\mathbf{H}}^p) - \left(\mathbf{S}^p - \theta \frac{\partial \mathbf{S}^p}{\partial \theta} \right) : \dot{\mathbf{G}} + \theta \mathbf{M} : \dot{\mathbf{E}}^e.$$

Since $c = \hat{c}(\theta, \mathbf{E}^e)$, we can assume that the internal energy ϵ has the additive decomposition $\hat{\epsilon}(\theta, \mathbf{E}^e, \mathbf{G}) = \hat{\epsilon}^e(\theta, \mathbf{E}^e) + \hat{\epsilon}^p(\mathbf{G})$ into elastic part $\hat{\epsilon}^e(\theta, \mathbf{E}^e)$ and plastic part $\hat{\epsilon}^p(\mathbf{G})$, where

$$\hat{c}(\theta, \mathbf{E}^e) = \frac{\partial \hat{\epsilon}^e(\theta, \mathbf{E}^e)}{\partial \theta} \quad \text{and} \quad \frac{\partial \hat{\epsilon}^p(\mathbf{G})}{\partial \theta} = 0.$$

From eqs. (7.1) and (7.2), it is observed that

$$\mathbf{0} = \frac{\partial c(\theta, \mathbf{E}^e)}{\partial \mathbf{G}} = \frac{\partial}{\partial \mathbf{G}} \left(\theta \frac{\partial \hat{\eta}(\theta, \mathbf{E}^e, \mathbf{G})}{\partial \theta} \right) = -\theta \frac{\partial^2}{\partial \theta^2} \left(\frac{\partial \psi}{\partial \mathbf{G}} \right).$$

This implies that there exist tensor functions $\mathbf{P}(\mathbf{G})$ and $\mathbf{Q}(\mathbf{G})$ such that

$$(7.4) \quad \frac{\partial \psi}{\partial \mathbf{G}} = \frac{\partial \hat{\psi}^p(\theta, \mathbf{G})}{\partial \mathbf{G}} = \mathbf{S}^p = \mathbf{P}(\mathbf{G}) - \theta \mathbf{Q}(\mathbf{G}).$$

Suppose $\hat{\psi}^p(\theta, \mathbf{0}) = 0$, then upon integration, there exist functions $E = E(\mathbf{G})$ and $N = N(\mathbf{G})$ such that $\hat{\psi}^p(\theta, \mathbf{G}) = E(\mathbf{G}) - \theta N(\mathbf{G})$. Based on the structure of the free-energy in relation to the internal energy and entropy, we assume that the plastic internal energy $\hat{\epsilon}^p(\mathbf{G})$ is defined as

$$(7.5) \quad \hat{\epsilon}^p(\mathbf{G}) = \hat{\psi}^p(\theta, \mathbf{G}) + \theta \hat{\eta}^p(\mathbf{G}),$$

where $\hat{\eta}^p(\mathbf{G})$ is the plastic entropy assumed to be a function of the Burgers tensor \mathbf{G} . This structure implies that $E(\mathbf{G}) = \hat{\epsilon}^p(\mathbf{G})$ and $N(\mathbf{G}) = \hat{\eta}^p(\mathbf{G})$.

It follows that by eqs. (7.4) and (7.5), we have

$$(7.6) \quad \mathbf{P}(\mathbf{G}) = \frac{\partial \hat{\epsilon}^p(\mathbf{G})}{\partial \mathbf{G}} \quad \text{and} \quad \mathbf{Q}(\mathbf{G}) = \frac{\partial \hat{\eta}^p(\mathbf{G})}{\partial \mathbf{G}}.$$

Also, by eqs. (4.2) and (7.5), the entropy must admit the additive decomposition

$$\hat{\eta}(\theta, \mathbf{E}^e, \mathbf{G}) = \hat{\eta}^e(\theta, \mathbf{E}^e) + \hat{\eta}^p(\mathbf{G})$$

into elastic part $\hat{\eta}^e(\theta, \mathbf{E}^e)$ and the plastic part $\hat{\eta}^p(\mathbf{G})$. Consequently, the plastic entropy in terms of the plastic free-energy, and the heat capacity in terms of the elastic entropy are defined as

$$\hat{\eta}^p(\mathbf{G}) = \frac{\partial \hat{\psi}^p(\theta, \mathbf{G})}{\partial \theta} \quad \text{and} \quad c(\theta, \mathbf{E}^e) = \theta \frac{\partial \hat{\eta}^e(\theta, \mathbf{E}^e)}{\partial \theta}.$$

Furthermore, it is observed that by eqs. (5.1), (5.2), (5.4), and (7.4), we obtain $\mathbf{T}_{NR}^p : \dot{\mathbf{H}}^p + \mathbb{K}_{NR}^p \cdot \nabla \dot{\mathbf{H}}^p = \mathbf{P}(\mathbf{G}) : \mathbf{A}(\theta, \mathbf{G})d^p - \theta \mathbf{Q}(\mathbf{G}) : \mathbf{A}(\theta, \mathbf{G})d^p$, where the terms $\mathbf{P}(\mathbf{G}) : \mathbf{A}(\theta, \mathbf{G})d^p$ and $\theta \mathbf{Q}(\mathbf{G}) : \mathbf{A}(\theta, \mathbf{G})d^p$ are the internal-energetic plastic power, and the entropic plastic power respectively. An immediate consequence of inequality in eq. (5.6) is

$$\text{Internal-energetic plastic power} \geq \text{Entropic plastic power}.$$

We note that the definition of \mathbf{S}^p through eq. (7.4) implies that

$$\frac{\partial \mathbf{S}^p}{\partial \theta} = -\mathbf{Q}(\mathbf{G}) \quad \text{and} \quad \mathbf{S}^p - \theta \frac{\partial \mathbf{S}^p}{\partial \theta} = \mathbf{P}(\mathbf{G}).$$

Clearly by eq. (7.6), we have

$$\left(\mathbf{S}^p - \theta \frac{\partial \mathbf{S}^p}{\partial \theta} \right) : \dot{\mathbf{G}} = \mathbf{P} : \dot{\mathbf{G}} = \frac{\partial \hat{\epsilon}^p(\mathbf{G})}{\partial \mathbf{G}} : \dot{\mathbf{G}} = \dot{\epsilon}^p(\mathbf{G}).$$

Thus, the energy balance eq. (7.3) in terms of heat capacity and internal energy due to cold work has the form

$$c(\theta, \mathbf{E}^e) \dot{\theta} + \operatorname{div} \mathbf{q} - q = \mathbf{T} : \dot{\mathbf{H}}^p - \dot{\epsilon}^p(\mathbf{G}) + \theta \mathbf{M} : \dot{\mathbf{E}}^e + \operatorname{div}(\mathbb{K}^p \dot{\mathbf{H}}^p).$$

Upon integration over the domain B occupied by the body, we have (where $\epsilon^p = \hat{\epsilon}^p(\mathbf{G})$)

$$\begin{aligned} \int_B c \dot{\theta} dv + \int_{\partial B} \mathbf{q} \cdot \mathbf{n} da - \int_B q dv \\ = \int_B \mathbf{T} : \dot{\mathbf{H}}^p dv - \int_B \dot{\epsilon}^p dv + \int_B \theta \mathbf{M} : \dot{\mathbf{E}}^p dv + \int_{\partial B} \mathbb{K} \dot{\mathbf{H}}^p \cdot \mathbf{n} da. \end{aligned}$$

If thermal expansion is neglected (i.e. $\mathbf{M} : \dot{\mathbf{E}}^e \approx 0$), and dividing through by

$$\int_B \mathbf{T} : \dot{\mathbf{H}}^p dv + \int_{\partial B} \mathbb{K} \dot{\mathbf{H}}^p \cdot \mathbf{n} da,$$

we have

$$(7.7) \quad \beta_B = 1 - \frac{\int_B \dot{\epsilon}^p dv}{\int_B \mathbf{T} : \dot{\mathbf{H}}^p dv + \int_{\partial B} \mathbb{K} \dot{\mathbf{H}}^p \cdot \mathbf{n} da},$$

where

$$\beta_B = \frac{\int_B c \dot{\theta} dv + \int_{\partial B} \mathbf{q} \cdot \mathbf{n} da - \int_B q dv}{\int_B \mathbf{T} : \dot{\mathbf{H}}^p dv + \int_{\partial B} \mathbb{K} \dot{\mathbf{H}}^p \cdot \mathbf{n} da}$$

is the global fraction of plastic power that goes into heating. By eq. (7.7), it is clear that β_B deviates from unity provided that there is a temporal change in the global plastic internal energy.

8. Complete initial and boundary value problem

Evolution of Burgers tensor \mathbf{G} . The Burgers tensor $\mathbf{G} = \mathbf{G}(\mathbf{x}, t)$ is assumed to satisfy the evolution equation $\dot{\mathbf{G}} = \mathbf{A}(\theta, \mathbf{G}) d^p - \mathbf{R}(\theta, \mathbf{G})$ with initial condition $\mathbf{G}(\mathbf{x}, 0) = \mathbf{G}_o$.

Macroscopic force balance and associated boundary conditions. The macroscopic force balance and macro-traction condition are given as

$$(8.1) \quad \operatorname{div} \mathbf{T} + \mathbf{b} = \mathbf{0} \quad \text{in } B \quad \text{and} \quad \mathbf{T} \mathbf{n} = \mathbf{t}^*(\mathbf{n}) \quad \text{on } \partial B_{\text{trac}},$$

where $\mathbf{t}^*(\mathbf{n})$ is prescribed on ∂B_{trac} a portion of ∂B .

Given the free energy $\psi = \hat{\psi}^e(\theta, \mathbf{E}^e)$, the stress \mathbf{T} is defined constitutively by

$$\mathbf{T} = \frac{\partial \psi^e(\theta, \mathbf{E}^e)}{\partial \mathbf{E}^e},$$

where $\mathbf{E}^e = \mathbf{E} - \mathbf{E}^p$ and $\mathbf{E} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$. We shall assume that the displacement \mathbf{u} is specified on a portion ∂B_u of ∂B in the sense

$$(8.2) \quad \mathbf{u}(\mathbf{x}, t) = \mathbf{u}_o \quad \text{on } \partial B_u,$$

where ∂B_u and ∂B_{trac} are complementary subsurfaces of ∂B .

Microscopic force balance and constitutive relation for microscopic stresses.

The microscopic force balance is given as

$$(8.3) \quad \mathbf{T}_o = \mathbf{T}^p - \operatorname{div} \mathbb{K}^p \quad \text{in } B.$$

The Cauchy stress and microscopic forces are constitutively defined as follows

$$\mathbf{T} = \frac{\partial \psi^e(\theta, \mathbf{E}^e)}{\partial \mathbf{E}^e};$$

and

$$(8.4) \quad \mathbf{T}^p = (F(\theta, \mathbf{G}) + Y(\theta, \mathbf{e}^p)) \frac{\dot{\mathbf{H}}^p}{d^p} \quad \text{and} \quad \mathbb{K}^p = l^2 (F(\theta, \mathbf{G}) + Y(\theta, \mathbf{e}^p)) \frac{\nabla \dot{\mathbf{H}}^p}{d^p}$$

for $d^p \neq 0$, where $Y(\theta, \mathbf{G})$ is the flow resistance and

$$F(\theta, \mathbf{G}) = \frac{\partial \hat{\psi}^p(\theta, \mathbf{G})}{\partial \mathbf{G}} : A(\theta, \mathbf{G}) \geq 0.$$

By substituting constitutive relations eq. (8.4) into the microscopic force balance eq. (8.3) gives what is known as the plastic flow rule. The flow rule is to be accompanied by appropriate initial and boundary conditions.

Initial-boundary conditions of flow rule. For the initial condition of the flow rule, we assume that $\mathbf{H}^p(\mathbf{x}, 0) = \mathbf{0}$ for all $\mathbf{x} \in B$. For the boundary conditions, it is assumed that the body B is made up of time-dependent complementary sub-bodies $B^e(t)$ and $B^p(t)$ called the elastic and plastic region, respectively. These sub-bodies share an interface $\mathcal{I}(t)$ in the sense:

$$B = B^e(t) \cup B^p(t) \quad \text{and} \quad B^e(t) \cap B^p(t) = \mathcal{I}(t).$$

Let $\partial B^p(t)$ be the boundary of $B^p(t)$. We define the surface $S^p(t)$ by

$$S^p(t) = \partial B^p(t) \cap \partial B.$$

Now, suppose $\partial B_{\text{hard}}^{ev}$ and $\partial B_{\text{free}}^{ev}$ are complementary subsurfaces of ∂B , such that $\partial B_{\text{hard}}^{ev}$ is the portion of ∂B that does not allow flow of dislocation, and $\partial B_{\text{free}}^{ev}$ is that portion of ∂B that allows flow of dislocation. We shall define the microscopic hard surface $S_{\text{hard}}^p(t)$ and microscopic free surface $S_{\text{free}}^p(t)$ as

$$S_{\text{hard}}^p(t) = S^p(t) \cap \partial B_{\text{hard}}^{ev} \quad \text{and} \quad S_{\text{free}}^p(t) = S^p(t) \cap \partial B_{\text{free}}^{ev}.$$

The microscopic-hard and microscopic-free boundary conditions specified on these microscopic surfaces are given by

$$(8.5) \quad \dot{\mathbf{H}}^p(\mathbf{x}, t) = \mathbf{0} \quad \text{on } S_{\text{hard}}^p(t) \quad \text{and} \quad \mathbb{K}^p \mathbf{n} = \mathbf{0} \quad \text{on } S_{\text{free}}^p(t)$$

respectively.

Balance of energy and associated initial-boundary conditions. The balance of energy is given as

$$c(\theta, \mathbf{E}^e) \dot{\theta} + \operatorname{div} \mathbf{q} - q = \mathbf{T} : \dot{\mathbf{H}}^p - \dot{\epsilon}^p + \theta \mathbf{M} : \dot{\mathbf{E}}^e + \operatorname{div}(\mathbb{K}^p \dot{\mathbf{H}}^p),$$

where,

$$c(\theta, \mathbf{E}^e) = -\theta \frac{\partial^2 \hat{\psi}(\theta, \mathbf{E}^e, \mathbf{G})}{\partial \theta^2}, \quad \mathbf{M} = \frac{\partial \mathbf{T}(\theta, \mathbf{E}^e)}{\partial \theta} \quad \text{and}$$

$$\dot{\epsilon}^p = \left(\frac{\partial \hat{\psi}^p(\theta, \mathbf{G})}{\partial \mathbf{G}} - \theta \frac{\partial^2 \hat{\psi}^p(\theta, \mathbf{G})}{\partial \theta \partial \mathbf{G}} \right) : \dot{\mathbf{G}}.$$

Given a known function $\theta_o(\mathbf{x})$, the initial condition for the temperature distribution is assumed to take the form $\hat{\theta}(\mathbf{x}, 0) = \theta_o(\mathbf{x}) \forall \mathbf{x} \in B$. Also, given the functions θ^* defined on portion ∂B_θ of the boundary ∂B and q_n defined on portions ∂B_q of the boundary ∂B , we choose as boundary conditions the following: $\theta(\mathbf{x}, t) = \theta^*$ on ∂B_θ and $\mathbf{q} \cdot \mathbf{n} = q_n$ on ∂B_q , where ∂B_θ and ∂B_q are complementary sub-surfaces of ∂B .

9. Weak formulation of the coupled problem

Let $\tilde{\mathbf{u}}$, $\tilde{\mathbf{H}}^p$ and $\nabla \tilde{\mathbf{H}}^p$ be kinematically admissible variables consistent with the boundary conditions eqs. (8.2) and (8.5), and $\tilde{\theta}$ be a thermally admissible variable in the sense that $\tilde{\theta} = 0$ on ∂B_θ .

From eq. (8.1), the macroscopic force balance satisfies [3, 16, 22]

$$\int_B ((\tilde{\mathbf{u}} - \dot{\mathbf{u}}) \cdot \operatorname{div} \mathbf{T} + \mathbf{b} \cdot (\tilde{\mathbf{u}} - \dot{\mathbf{u}})) dv = 0.$$

By Gauss divergence theorem, we have

$$(9.1) \quad \int_B \mathbf{T} : (\mathbf{E}(\tilde{\mathbf{u}}) - \mathbf{E}(\dot{\mathbf{u}})) dv - \int_{\partial B_t} \mathbf{t}^*(\mathbf{n}) \cdot (\tilde{\mathbf{u}} - \dot{\mathbf{u}}) da - \int_B \mathbf{b} \cdot (\tilde{\mathbf{u}} - \dot{\mathbf{u}}) dv = 0,$$

where $\dot{\mathbf{E}} = \mathbf{E}(\dot{\mathbf{u}}) = \frac{1}{2}[\nabla \dot{\mathbf{u}} + (\nabla \dot{\mathbf{u}})^T]$ and $\tilde{\mathbf{E}} = \mathbf{E}(\tilde{\mathbf{u}}) = \frac{1}{2}[\nabla \tilde{\mathbf{u}} + (\nabla \tilde{\mathbf{u}})^T]$.

From eq. (8.3), the microscopic force balance satisfies the equation

$$\int_B \mathbf{T} : (\tilde{\mathbf{H}}^p - \dot{\mathbf{H}}^p) dv = \int_B \mathbf{T}^p : (\tilde{\mathbf{H}}^p - \dot{\mathbf{H}}^p) dv - \int_B (\tilde{\mathbf{H}}^p - \dot{\mathbf{H}}^p) : \operatorname{div} \mathbb{K}^p dv.$$

Applying the Gauss divergence theorem and the use of eq. (8.5), we have

$$(9.2) \quad \int_B [\mathbf{T}^p : (\tilde{\mathbf{H}}^p - \dot{\mathbf{H}}^p) + \mathbb{K}^p : (\nabla \tilde{\mathbf{H}}^p - \nabla \dot{\mathbf{H}}^p)] dv - \int_B \mathbf{T} : (\tilde{\mathbf{H}}^p - \dot{\mathbf{H}}^p) dv = 0.$$

Integrate eqs. (5.8) and (6.3) over B , and add to the sum of eqs. (9.1) and (9.2), we obtain

$$(9.3) \quad \int_B (\hat{\delta}(\tilde{\epsilon}^p) + \hat{\phi}(\tilde{\epsilon}^p)) dv - \int_B (\hat{\delta}(\dot{\epsilon}^p) + \hat{\phi}(\dot{\epsilon}^p)) dv \\ + \int_B \mathbf{T} : ((\mathbf{E}(\tilde{\mathbf{u}}) - \tilde{\mathbf{H}}^p) - (\mathbf{E}(\dot{\mathbf{u}}) - \dot{\mathbf{H}}^p)) dv \\ - \int_{\partial B_t} \mathbf{t}^*(\mathbf{n}) \cdot (\tilde{\mathbf{u}} - \dot{\mathbf{u}}) da - \int_B \mathbf{b} \cdot (\tilde{\mathbf{u}} - \dot{\mathbf{u}}) dv \geq 0.$$

Hence, the macroscopic and microscopic force balances in eqs. (8.1)₁ and (8.3), the constitutive relations for the macroscopic stress \mathbf{T} , the microscopic stresses \mathbf{T}^p and \mathbb{K}^p together with the natural boundary conditions in eqs. (8.1)₂ and (8.5)₂ are equivalent to the weak form represented as a variational inequality in eq. (9.3).

The weak form of the energy equation is simply given as

$$\int_B c \dot{\theta} \tilde{\theta} dv + \int_{\partial B_q} \tilde{\theta} q_n da - \int_B \mathbf{q} \cdot \nabla \tilde{\theta} dv - \int_B q \tilde{\theta} dv \\ = \int_B \mathbf{T} : \dot{\mathbf{H}}^p \tilde{\theta} dv - \int_B \tilde{\theta} \dot{\epsilon}^p dv + \int_{\partial B} \mathbb{K}^p \mathbf{n} : \dot{\mathbf{H}}^p \tilde{\theta} da \\ - \int_B \mathbb{K}^p \dot{\mathbf{H}}^p \cdot \nabla \tilde{\theta} dv + \int_B \tilde{\theta} \dot{\theta} \mathbf{M} : \dot{\mathbf{E}}^c dv,$$

where $\int_B \tilde{\theta} \operatorname{div} \mathbf{q} dv = - \int_B \mathbf{q} \cdot \nabla \tilde{\theta} dv + \int_{\partial B_q} \tilde{\theta} q_n da$, $q_n = \mathbf{q} \cdot \mathbf{n}$ on ∂B_q and $\tilde{\theta} = 0$ on ∂B_θ .

10. Constitutive relation in a reference configuration natural for a fixed temperature

Let $\omega = \hat{\omega}(\theta, \mathbf{E}^e, \mathbf{G})$ be Gibbs function defined as

$$\hat{\omega}(\theta, \mathbf{E}^e, \mathbf{G}) = \hat{\psi}(\theta, \mathbf{E}^e, \mathbf{G}) + (\theta - \theta_o)\hat{\eta}(\theta, \mathbf{E}^e, \mathbf{G}),$$

where θ_o is a fixed temperature.

By definition, a reference configuration is said to be *natural* for a fixed temperature θ_o if $\hat{\omega}(\theta, \mathbf{E}^e, \mathbf{G})$ has a minimum at $(\theta, \mathbf{E}^e, \mathbf{G}) = (\theta_o, \mathbf{0}, \mathbf{0})$ (Gurtin et.al., [17]). The consequences of this definition are:

- (i.) The Cauchy stress \mathbf{T} vanishes at $(\theta_o, \mathbf{0}, \mathbf{0})$;
- (ii.) The elasticity tensor $\frac{\partial \mathbf{T}}{\partial \mathbf{E}^e} = \frac{\partial^2 \psi}{\partial \mathbf{E}^e \partial \mathbf{E}^e}$ is positive semi-definite at $(\theta_o, \mathbf{0}, \mathbf{0})$;
- (iii.) The specific heat capacity $c = c(\theta, \mathbf{E}^e)$ is non-negative at $\theta = \theta_o$ and $\mathbf{E}^e = \mathbf{0}$.

For small deformation, let ε be define as

$$\varepsilon := \sqrt{|\mathbf{E}^e|^2 + |\mathbf{H}^p|^2 + l^2|\mathbf{G}|^2 + \frac{(\theta - \theta_o)^2}{\theta_o^2} + L^2 \frac{|\nabla \theta|^2}{\theta_o^2}},$$

where l and L are length scales.

Given an arbitrary field $\Phi = \Phi(\theta, \mathbf{E}^e, \mathbf{G})$. We shall denote the value of Φ at $(\theta_o, \mathbf{0}, \mathbf{0})$ as $\Phi|_0$ and assume that at this virgin state, Gibb's function ω , free energy ψ , and entropy η satisfy

$$(10.1) \quad \omega|_0 = \psi|_0 = \eta|_0 = 0.$$

By Taylor's series expansion, the free energy is expanded about $(\theta_o, \mathbf{0}, \mathbf{0})$ as

$$(10.2) \quad \begin{aligned} \hat{\psi}(\theta, \mathbf{E}^e, \mathbf{G}) &= \psi|_0 + \frac{\partial \psi}{\partial \mathbf{E}^e}|_0 : \mathbf{E}^e + \frac{\partial \psi}{\partial \theta}|_0 (\theta - \theta_o) + \frac{\partial \psi}{\partial \mathbf{G}}|_0 : \mathbf{G} \\ &+ \frac{1}{2} \mathbf{E}^e : \left(\frac{\partial^2 \psi}{\partial \mathbf{E}^e \partial \mathbf{E}^e} \right)|_0 \mathbf{E}^e + \frac{1}{2} \mathbf{G} : \left(\frac{\partial^2 \psi}{\partial \mathbf{G} \partial \mathbf{G}} \right)|_0 \mathbf{G} + \frac{1}{2} \frac{\partial^2 \psi}{\partial \theta^2}|_0 (\theta - \theta_o)^2 \\ &+ \frac{\partial^2 \psi}{\partial \theta \partial \mathbf{E}^e}|_0 : \mathbf{E}^e (\theta - \theta_o) + \frac{\partial^2 \psi}{\partial \theta \partial \mathbf{G}}|_0 : \mathbf{G} (\theta - \theta_o) + o(\varepsilon^2) \quad \text{as } \varepsilon \rightarrow 0, \end{aligned}$$

where,

$$\frac{\partial^2 \psi}{\partial \mathbf{E}^e \partial \mathbf{G}} = \mathbf{0} \quad \text{since } \psi = \hat{\psi}^e(\theta, \mathbf{E}^e) + \hat{\psi}^p(\theta, \mathbf{G}).$$

Recall that at $(\theta_o, \mathbf{0}, \mathbf{0})$, ω is a minimum, so that we have

$$(10.3) \quad \frac{\partial \omega}{\partial \mathbf{E}^e}|_0 = \mathbf{0} = \frac{\partial \psi}{\partial \mathbf{E}^e}|_0, \quad \frac{\partial \omega}{\partial \mathbf{G}}|_0 = \mathbf{0} = \frac{\partial \psi}{\partial \mathbf{G}}|_0 \quad \text{and} \quad \frac{\partial \psi}{\partial \theta}|_0 = 0.$$

The elasticity tensor \mathbb{C} , specific heat capacity c_o , coefficient of thermal expansion tensor due to elasticity \mathbf{M} , a coefficient of thermal expansion due to defectiveness \mathbf{W} and a defective modulus \mathbb{B} at $(\theta_o, \mathbf{0}, \mathbf{0})$ are given as

$$\mathbb{C} = \frac{\partial^2 \psi}{\partial \mathbf{E}^e \partial \mathbf{E}^e}|_0, \quad c_o = -\frac{\partial^2 \psi}{\partial \theta^2}|_0, \quad \mathbf{M} = \frac{\partial^2 \psi}{\partial \theta \partial \mathbf{E}^e}|_0, \quad \mathbf{W} = \frac{\partial^2 \psi}{\partial \theta \partial \mathbf{G}}|_0 \quad \text{and} \quad \mathbb{B} = \frac{\partial^2 \psi}{\partial \mathbf{G} \partial \mathbf{G}}|_0$$

respectively.

By eqs. (10.1) and (10.3), and ignoring higher-order terms in eq. (10.2), the free-energy ψ has the quadratic form

$$(10.4) \quad \hat{\psi}(\theta, \mathbf{E}^e, \mathbf{G}) = \frac{1}{2} \mathbf{E}^e : \mathbb{C} \mathbf{E}^e - \frac{c_o}{2\theta_o} (\theta - \theta_o)^2 + (\theta - \theta_o) \mathbf{M} : \mathbf{E}^e$$

$$+ \frac{1}{2} \mathbf{G} : \mathbb{B} \mathbf{G} + (\theta - \theta_o) \mathbf{W} : \mathbf{G}.$$

It is clear that the elastic free energy ψ^e and the plastic free energy ψ^p are given as the quadratic forms

$$(10.5) \quad \begin{aligned} \hat{\psi}^e(\theta, \mathbf{E}^e) &= \frac{1}{2} \mathbf{E}^e : \mathbb{C} \mathbf{E}^e - \frac{c_o}{2\theta_o} (\theta - \theta_o)^2 + (\theta - \theta_o) \mathbf{M} : \mathbf{E}^e, \\ \hat{\psi}^p(\theta, \mathbf{G}) &= \frac{1}{2} \mathbf{G} : \mathbb{B} \mathbf{G} + (\theta - \theta_o) \mathbf{W} : \mathbf{G}. \end{aligned}$$

By eqs. (5.10), (7.4), (10.4), and (10.5) the Cauchy stress \mathbf{T} , the microscopic stress \mathbf{S}^p and the entropy η are given as

$$\begin{aligned} \mathbf{T} &= \mathbb{C} \mathbf{E}^e + (\theta - \theta_o) \mathbf{M}, & \mathbf{S}^p &= \mathbb{B} \mathbf{G} + (\theta - \theta_o) \mathbf{W}, & \text{and} \\ \hat{\eta}(\theta, \mathbf{E}^e, \mathbf{G}) &= \frac{c_o}{\theta_o} (\theta - \theta_o) - \mathbf{M} : \mathbf{E}^e - \mathbf{W} : \mathbf{G}. \end{aligned}$$

11. Conclusion

In this paper, a report on a thermo-mechanically coupled theory of polycrystalline distortion gradient plasticity for cold working has been presented. A constitutively well-defined Burger tensor rate, in terms of an accumulation modulus tensor $\mathbf{A}(\theta, \mathbf{G})$ and a recovery rate tensor $\mathbf{R}(\theta, \mathbf{G})$ are proposed. It is observed that the Burgers tensor flow is associated with changes in dislocation densities arising from cold working and thermal annealing. The recovery rate tensor is shown to mimic a dissipative behavior, thus resulting in a decrease in the accumulation of dislocation densities during thermal annealing. Also, it is obtained that the non-recoverable energetic microscopic stresses have well-defined constitutive relations during cold working whenever the effective flow rate does not vanish. Other features associated with cold-worked polycrystalline are the plastic internal energy and entropy which are obtained as functions of the Burgers tensor.

This proposed theory is shown to be thermodynamically consistent. Numerical implementations of this theory using benchmark problems have been left for future work.

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**БУРГЕРСОВ ТЕНЗОР ПРОТОКА, ХЛАДНИ РАД И
ТЕРМИЧКО ЖАРЕЊЕ**

РЕЗИМЕ. У овом раду се предлаже кинематичко-термички конститутивни закон еволуције Бургерсовог тензора током хладног рада и након накнадног термичког жарења поликристала. Предлог је заснован на раду L. Anand, M. E. Gurtin, B. D. Reddy, *The stored energy of cold work, thermal annealing, and other thermodynamic issues in single crystal plasticity at small length scales*, Int. J. Plast. **64** (2015), 1–25. Принцип виртуелног рада и термодинамички закони се користе за постизање равнотеже сила, равнотеже енергије и неравнотеже слободне енергије. Неповратни енергетски микроскопски напони се добијају као карактеристике материјала који се обрађују хладно кад год је енергија дефекта зависна од Бургерсовог тензора. Сходно томе, примећује се да унутрашња енергетска пластична снага није мања од ентропијске пластичне снаге. Показано је да стопа опоравка током термичког жарења опонаша дисипативно понашање, што доводи до смањења акумулације густине дислокација. Штавише, слободна енергија – апроксимирана квадратном формом – се користи за добијање конститутивних релација за макроскопске и микроскопске напоне.

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