

*Research Paper***Two-Temperature Continuum Model for Metal Plasticity**

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A physically based continuum plasticity model for metals from the consideration of non-equilibrium thermodynamics is presented. The modeling is accomplished in a two-temperature framework that appears naturally by considering the thermodynamic system to be composed of two weakly interacting subsystems, namely the kinetic vibrational and configurational subsystems. While the atomic vibrations of plastically deforming metals form the kinetic vibrational subsystem, much slower degrees of freedom in terms of the motion of defects constitute the configurational subsystem. Both subsystems assume their own temperatures and fall out of equilibrium from each other because of the externally imposed driving. Dislocation density characterising the configurational subsystem is considered to be the state variable for the present development. The continuum model accommodates finite deformation and describes plastic deformation in a yield-free framework via a microforce balance along with the conventional macroforce balance.

Keywords: Metal Viscoplasticity; Non-Equilibrium Thermodynamics; Two-Temperature Framework; Dislocation Density

Introduction

The physical process of plastic/viscoplastic deformation of metals is extremely complex and inherently irreversible. It originates from the motion of microscopic defects, more specifically the crystallographic slip caused by dislocations. Even though, several other mechanisms including twinning, grain boundary sliding, void growth and so on influence the plastic deformation, we would only consider the most important component – the dislocation motion and evolution – as the sole micromechanism responsible for metal plasticity. The motion of dislocations through lattice requires overcoming an energy barrier with the aid of a combination of applied driving force and thermal fluctuation. The crystal lattice configuration, namely face-centered cubic (FCC), body-centered cubic (BCC), hexagonal close-packed (HCP), plays an important role in determining the effect of thermal activation in mechanical response and consequently plastic deformation of metals differs from one another depending on their crystal structure.

A crystalline material with dislocations, when driven by an external protocol, falls out of equilibrium because of self-energy of dislocations. Langer *et al.* (2010) argued that a macroscopic system undergoing plastic deformation may be considered to be composed of slow *configurational degrees of freedom* describing infrequent and intermittent atomic rearrangement responsible for plastic flow and *kinetic-vibration degrees of freedom* that describe the thermal and vibrational motion of atom. Consequently, the system may be divided into a configuration subsystem and a kinetic-vibration subsystem. Self-energy of dislocations, i.e. the energy of the configurational subsystem, along with its own entropy defines a new temperature – the configurational temperature or effective temperature – which is different from the thermal or kinetic-vibrational temperature. As plastic deformation progresses under the expenditure of external work, the effective temperature evolves differently from the thermal temperature and establishes a current of heat from configurational subsystem to kinetic-vibrational

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subsystem. Consequently, a large fraction of the external work input that generates dislocation and keeps them in motion, gets dissipated as heat. This makes the highly irreversible and dissipative nature of plastic deformation evident and also indicates the configurational rearrangements to be far from equilibrium.

In continuum mechanics, a desirable, albeit challenging, goal is to develop predictive viscoplasticity models accounting for the complex phenomena of dislocation evolution and motion. The models should be applicable to a wide range of temperature and strain rates as the deformation response of metals depends, to a large extent, on these two parameters. More importantly, several engineering applications of metals at high strain rates, e.g., high speed machining, impact on armor systems, metal forming etc. demand the understanding of the underlying micromechanism of plastic deformation and incorporation of them into the predictive model in order to optimize and enhance the operations and design of such systems. Over the years, there has been a significant progress in the development of theories of plasticity and viscoplasticity that attempts at representing inelastic constitutive properties phenomenologically. Theory of local equilibrium thermodynamics with internal state variables has been utilized to characterize the irreversible process of viscoplasticity. At another remove, there have been a number of efforts towards developing physically based theory for viscoplastic deformation. These models typically do not take recourse to thermodynamic principles, instead postulate the constitutive relations in terms of the evolution equations of dislocation densities. These equations explicitly contain terms describing several microscopic phenomena, e.g., dislocation multiplication, annihilation, grain size effect, effect of cell boundaries, twinning, interaction with lattice and so on. In a refined level, such physically based models even distinguish among different types of dislocation, namely mobile, immobile, statistically stored and geometrically necessary dislocations. They describe evolution of each of these separately taking into account their mutual interactions.

For the present work on viscoplasticity formulation for metals, we would only consider the mechanisms of dislocation motion and evolution to be responsible for plastic deformation. Following Langer

et al. (2010), the dislocations are assumed to form the configurational subsystem where the changes occur, due to plastic deformation, much more slowly compared to the kinetic vibration of the atomic lattice. Along with the usual forms of force balance, energy balance etc., we would apply second law of thermodynamics to derive constitutive restrictions and evolution equation of dislocation density (ρ). Again, continuum formulation for viscoplasticity can be achieved in different formats, namely consistency viscoplasticity, Perzyna type model (see Lubliner, 2008; Simo and Hughes, 2006, for both the formats), yield free theories (Gurtin, Fried and Anand, 2010; Bodner and Partom, 1975) etc. We would formulate the present theory in a yield-free set up following Gurtin *et al.* (2010).

Kinematics

Let $\mathcal{B}_0 \subset \mathbb{R}^3$ be the reference configuration of a body at time t_0 . Macroscopically, each material point \mathbf{x} of this continuum deforms elasto-viscoplastically to \mathbf{y} in its spatial configuration, \mathcal{B}_t , at time t . This deformation is represented by a smooth map χ as $\mathbf{y} = \chi(\mathbf{x}, t)$.

χ is a one-one and onto map; therefore possesses a unique inverse. The deformation gradient (\mathbf{F}), velocity (\mathbf{v}) and velocity gradient (\mathbf{L}) fields are defined as follows.

$$\mathbf{F} := \nabla_{\mathbf{x}} \chi, \quad \mathbf{v} := \dot{\chi}, \quad \mathbf{L} := \nabla_{\mathbf{y}} \mathbf{v} = \dot{\mathbf{F}}\mathbf{F}^{-1}, \quad (1)$$

where $\nabla_{\mathbf{x}}, \nabla_{\mathbf{y}}$ and superposed dot respectively denote the gradient operation with respect to the material coordinate \mathbf{x} , gradient with respect to the spatial coordinate \mathbf{y} and the material time derivative.

In order to separate out the elastic and viscoplastic parts of \mathbf{F} , we opt for its multiplicative decomposition as follows.

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p \quad (2)$$

where, $\mathbf{F}^p(\mathbf{x})$, a local plastic deformation at \mathbf{x} , carries the material to a coherent structure residing in the relaxed intermediate configuration space at \mathbf{x} and $\mathbf{F}^e(\mathbf{x})$ represents the subsequent rotation and stretching of the coherent structure. With the decomposition given in Eq. (2), the velocity gradient \mathbf{L} can be shown to admit the following decomposition.

$$\mathbf{L} = \mathbf{L}^e + \mathbf{F}^e \mathbf{L}^p \mathbf{F}^{e-1}, \quad (3)$$

where, $\mathbf{L}^e = \dot{\mathbf{F}}^e \mathbf{F}^{e-1}$ and $\mathbf{L}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1}$. Elastic and viscoplastic rate of deformation tensors (\mathbf{D}^e and \mathbf{D}^p) and spin tensors (\mathbf{W}^e and \mathbf{W}^p) are defined as follows.

$$\begin{aligned} \mathbf{D}^e &= \text{sym}(\mathbf{L}^e), \quad \mathbf{D}^p = \text{sym}(\mathbf{L}^p) \\ \mathbf{W}^e &= \text{skew}(\mathbf{L}^e), \quad \text{and} \quad \mathbf{W}^p = \text{skew}(\mathbf{L}^p) \end{aligned} \quad (4)$$

We take two kinematical assumptions concerning the plastic flow: *incompressibility* and *irrotationality*. These two assumptions, translate to the following conditions.

$$\det \mathbf{F}^p = 1, \quad \text{tr} \mathbf{L}^p = 0, \quad \mathbf{W}^p = 0 \quad (5)$$

Plastic irrotationality implies $\mathbf{L}^p = \mathbf{D}^p$ and consequently $\mathbf{F}^p = \mathbf{F}^p \mathbf{D}^p$. Defining a scalar ν^p and a tensor quantity \mathbf{N}^p as

$$\nu^p = |\mathbf{D}^p| \quad \text{and} \quad \mathbf{N}^p = \frac{\mathbf{D}^p}{\nu^p} \quad \text{when} \quad \nu^p > 0 \quad (6)$$

Eq. (1) may be recast as

$$\nabla_y \mathbf{v} = \mathbf{L} = \mathbf{L}^e + \nu^p \mathbf{F}^e \mathbf{N}^p \mathbf{F}^{e-1} \quad (7)$$

Following the definition of Green-Lagrange strain tensor in elasticity, we define for the present case the elastic strain tensor \mathbf{E}^e as

$$\mathbf{E}^e = \frac{1}{2} (\mathbf{F}^{eT} \mathbf{F}^e - \mathbf{I}) = \frac{1}{2} (\mathbf{C}^e - \mathbf{I}) \quad (8)$$

Since \mathcal{B}_t evolves through an observable space, a change of observer (i.e., a change of reference frame $F \rightarrow F^*$), therefore, relates the observed spatial coordinates \mathbf{y} and \mathbf{y}^* as follows.

$$\begin{aligned} \mathbf{y}^* &= \boldsymbol{\chi}^*(\mathbf{x}, t) = \mathbf{Q}(t) \boldsymbol{\chi}(\mathbf{x}, t) + \mathbf{r}(t) \\ &= \mathbf{Q}(t) \mathbf{y} + \mathbf{r}(t) = \boldsymbol{\phi}(\mathbf{y}) \end{aligned} \quad (9)$$

Consequently, several tensorial quantities defined above transform as follows.

$$\begin{aligned} \mathbf{F}^* &= \mathbf{Q} \mathbf{F}, \quad \dot{\mathbf{F}}^* = \dot{\mathbf{Q}} \mathbf{F} + \mathbf{Q} \dot{\mathbf{F}}, \quad \mathbf{L}^* = \dot{\mathbf{Q}} \mathbf{Q}^T + \mathbf{Q} \mathbf{L} \mathbf{Q}^T, \\ \mathbf{F}^{e*} &= \mathbf{Q} \mathbf{F}^e, \quad \mathbf{F}^{p*} = \mathbf{F}^p, \quad \mathbf{L}^{p*} = \mathbf{L}^p, \quad \mathbf{D}^{p*} = \mathbf{D}^p, \\ \mathbf{L}^{e*} &= \dot{\mathbf{Q}} \mathbf{Q}^T + \mathbf{Q} \mathbf{L}^e \mathbf{Q}^T, \quad \mathbf{D}^{e*} = \mathbf{Q} \mathbf{D}^e \mathbf{Q}^T, \\ \mathbf{W}^{e*} &= \dot{\mathbf{Q}} \mathbf{Q}^T + \mathbf{Q} \mathbf{W}^e \mathbf{Q}^T \end{aligned} \quad (10)$$

Equations of Motion

An essential ingredient of continuum mechanics is the equation describing the motion of the body. It is, generally, via Cauchy's hypothesis on the existence of traction vector, use of laws of linear and angular momentum balance and a subsequent localization leading to the derivation of equations of motion. However, following Gurtin *et al.* (2010), in this paper, we take the balance of virtual power as a basic postulate and derive the equations of motion from there as presented below.

Let \mathcal{P}_t denotes an arbitrary subregion of \mathcal{B}_t and $\partial \mathcal{P}_t$ is its bounding surface with outward normal \mathbf{n} . Principle of virtual power is based on the balance between the external power expenditure $\mathcal{W}_{\text{ext}}(\mathcal{P}_t)$ on \mathcal{P}_t and internal power expended $\mathcal{W}_{\text{int}}(\mathcal{P}_t)$ within \mathcal{P}_t . The rate quantities that expend power are \mathbf{v} , \mathbf{L}^e and ν^p . However, these rates are not independent, rather constrained by Eq. (7). Considering an elastic stress \mathbf{S}^e and a scalar plastic stress π , the internal power expenditure within \mathcal{P}_t is given by

$$\mathcal{W}_{\text{int}}(\mathcal{P}_t) = \int_{\mathcal{P}_t} (\mathbf{S}^e : \mathbf{L}^e + J^{-1} \pi \nu^p) dv \quad (11)$$

where $J = \det \mathbf{F} = \det \mathbf{F}^e$. π and ν^p being quantities defined on intermediate configurations, J^{-1} is used to bring the plastic power expressed in per unit volume of intermediate configuration to per unit volume of current configuration.

Given traction force vector $\mathbf{t}(\mathbf{n})$ working on the boundary, density of body force \mathbf{b}_0 and inertial force $\rho_m \dot{\mathbf{v}}$ with ρ_m to be the mass density, the external power input $\mathcal{W}_{\text{ext}}(\mathcal{P}_t)$ is given by the following.

$$\mathcal{W}_{\text{ext}}(\mathcal{P}_t) = \int_{\partial\mathcal{P}_t} \mathbf{t}(\mathbf{n}) \cdot \mathbf{v} ds + \int_{\mathcal{P}_t} (\mathbf{b}_0 - \rho_m \dot{\mathbf{v}}) \cdot \mathbf{v} dv \quad (12)$$

We will henceforth denote $(\mathbf{b}_0 - \rho_m \dot{\mathbf{v}})$ by \mathbf{b} .

Considering virtual rate fields, $\tilde{\mathbf{v}}, \tilde{\mathbf{L}}^e$ and $\tilde{\mathbf{v}}^p$, consistent with the restriction

$$\nabla_y \tilde{\mathbf{v}} = \tilde{\mathbf{L}}^e + \tilde{\mathbf{v}}^p \mathbf{F}^e \mathbf{N}^p \mathbf{F}^{e-1} \quad (13)$$

principle of virtual power balance for the region \mathcal{P}_t is stated as

$$\mathcal{W}_{\text{ext}}(\mathcal{P}_t, \mathcal{V}) = \mathcal{W}_{\text{int}}(\mathcal{P}_t, \mathcal{V}) \quad \forall \mathcal{V} \quad (14)$$

where \mathcal{V} is the list of virtual velocities: $\mathcal{V} = (\tilde{\mathbf{v}}, \tilde{\mathbf{L}}^e, \tilde{\mathbf{v}}^p)$.

Besides the virtual power principle, the invariance of $\mathcal{W}_{\text{int}}(\mathcal{P}_t, \mathcal{V})$ under change of observer should also get satisfied. This leads to the following.

$$\mathcal{W}_{\text{int}}(\mathcal{P}_t, \mathcal{V}) = \mathcal{W}_{\text{int}}^*(\mathcal{P}_t^*, \mathcal{V}^*) \quad (15)$$

Using the definition given in Eq. (11), Eq. (15) is rewritten as

$$\begin{aligned} \int_{\mathcal{P}_t} (\mathbf{S}^e : \tilde{\mathbf{L}}^e + J^{-1} \pi \tilde{\mathbf{v}}^p) dv(y) \\ = \int_{\mathcal{P}_t^*} (\mathbf{S}^{e*} : \tilde{\mathbf{L}}^{e*} + J^{*-1} \pi^* \tilde{\mathbf{v}}^{p*}) dv(y^*) \end{aligned} \quad (16)$$

Under change of observer $\pi \nu^p$ remains invariant. Therefore Eq. (16) takes the following form.

$$\begin{aligned} \int_{\mathcal{P}_t} \mathbf{S}^e(y) : \tilde{\mathbf{L}}^e(y) dv(y) &= \int_{\mathcal{P}_t^*} \mathbf{S}^{e*}(y^*) : \tilde{\mathbf{L}}^{e*}(y^*) dv(y^*) \\ &= \int_{\mathcal{P}_t^*} \mathbf{S}^{e*}(y^*) : (\dot{\mathbf{Q}}\mathbf{Q}^T + \mathbf{Q}\tilde{\mathbf{L}}^e(\phi^{-1}(y^*))\mathbf{Q}^T) dv(y^*) \\ &= \int_{\mathcal{P}_t} \mathbf{S}^{e*}(\phi(y)) : (\dot{\mathbf{Q}}\mathbf{Q}^T + \mathbf{Q}\tilde{\mathbf{L}}^e(\phi^{-1}(y^*))\mathbf{Q}^T) dv(y) \end{aligned} \quad (17)$$

Equivalently one may write the following local

form exploiting the arbitrariness of \mathcal{P}_t .

$$\begin{aligned} \mathbf{S}^e : \tilde{\mathbf{L}}^e &= \mathbf{S}^{e*} : (\dot{\mathbf{Q}}\mathbf{Q}^T + \mathbf{Q}\tilde{\mathbf{L}}^e\mathbf{Q}^T) \\ &= \mathbf{Q}^T \mathbf{S}^{e*} \mathbf{Q} : \tilde{\mathbf{L}}^e + \mathbf{S}^{e*} : \dot{\mathbf{Q}}\mathbf{Q}^T \end{aligned} \quad (18)$$

Without loss of generality, choosing a change of frame such that \mathbf{Q} is constant, one concludes from Eq. (18) that

$$\mathbf{S}^{e*} = \mathbf{Q}\mathbf{S}^e\mathbf{Q}^T \quad (19)$$

Substituting Eq. (19) in Eq. (18), we get $\mathbf{S}^{e*} : \dot{\mathbf{Q}}\mathbf{Q}^T = 0$. For arbitrary \mathbf{Q} , $\dot{\mathbf{Q}}\mathbf{Q}^T$ is an arbitrary skew tensor and thus we conclude $\mathbf{S}^{e*} = \mathbf{S}^{e*T}$ and hence using Eq. (19),

$$\mathbf{S}^e = \mathbf{S}^{eT} \quad (20)$$

Macroscopic Force Balance

To derive macroscopic force balance, let us consider virtual velocity associated with viscoplastic deformation to be zero, i.e., $\tilde{\mathbf{v}}^p = 0$. Following, Eq. (13), admissible virtual elastic distortion rate $\tilde{\mathbf{L}}^e$ is given by

$$\nabla_y \tilde{\mathbf{v}} = \tilde{\mathbf{L}}^e, \quad (21)$$

where $\tilde{\mathbf{v}}$ is arbitrary. Virtual power balance (see Eq. (14)), in this case, takes the following form.

$$\int_{\partial\mathcal{P}_t} \mathbf{t}(\mathbf{n}) \cdot \tilde{\mathbf{v}} ds + \int_{\mathcal{P}_t} \mathbf{b} \cdot \tilde{\mathbf{v}} dv = \int_{\mathcal{P}_t} \mathbf{S}^e : \nabla_y \tilde{\mathbf{v}} dv \quad (22)$$

Using divergence theorem to the integral in the right hand side of Eq. (22), the equation may be recast as

$$\int_{\partial\mathcal{P}_t} (\mathbf{t}(\mathbf{n}) - \mathbf{S}^e \mathbf{n}) \cdot \tilde{\mathbf{v}} ds + \int_{\mathcal{P}_t} (\nabla_y \cdot \mathbf{S}^e + \mathbf{b}) \cdot \tilde{\mathbf{v}} dv = \mathbf{0}, \quad (23)$$

which upon localization because of the arbitrariness of \mathcal{P}_t , leads to the macroscopic force balance and traction-stress relation as follows.

$$\nabla_y \cdot \mathbf{S}^e + \mathbf{b} = \mathbf{0} \quad (24)$$

$$\mathbf{S}^e \mathbf{n} = \mathbf{t}(\mathbf{n}) \quad (25)$$

Note that arbitrariness of virtual velocity $\tilde{\mathbf{v}}$ is also used to write Eq. (24) and (25). The elastic stress \mathbf{S}^e satisfying Eq. (24) and (25) along with the properties given in Eq. (19) and (20) can be identified with the classical Cauchy stress \mathbf{T} and therefore in what follows we would replace \mathbf{S}^e by \mathbf{T} .

Microscopic Force Balance

The microscopic force balance can be derived considering $\tilde{\mathbf{v}} = \mathbf{0}$. Eq. (13) and virtual power balance Eq. (14), in this case, take the following forms.

$$\tilde{\mathbf{L}}^e = -\tilde{\mathbf{v}}^p \mathbf{F}^e \mathbf{N}^p \mathbf{F}^{e-1} \quad (26)$$

$$\int_{\mathcal{P}_i} (\mathbf{T} : \tilde{\mathbf{L}}^e + J^{-1} \pi \tilde{\mathbf{v}}^p) dV = 0 \quad (27)$$

Arbitrariness of \mathcal{P}_i again allows localization of Eq. (27), which upon using Eq. (26), takes the following form.

$$\begin{aligned} J^{-1} \pi \tilde{\mathbf{v}}^p &= -\mathbf{T} : \tilde{\mathbf{L}}^e = -\mathbf{T} : (-\tilde{\mathbf{v}}^p \mathbf{F}^e \mathbf{N}^p \mathbf{F}^{e-1}) \\ &= (\mathbf{F}^{eT} \mathbf{T} \mathbf{F}^{e-T} : \mathbf{N}^p) \tilde{\mathbf{v}}^p \\ &= (\mathbf{F}^{eT} \mathbf{T}_0 \mathbf{F}^{e-T} : \mathbf{N}^p) \tilde{\mathbf{v}}^p \end{aligned} \quad (28)$$

The last equality in Eq. (28), follows using the fact that $\text{tr} \mathbf{N}^p = 0$. In this last terms \mathbf{T}_0 is the deviatoric part of \mathbf{T} . $\tilde{\mathbf{v}}^p$ being arbitrary, Eq. (28) leads to the following microscopic force balance.

$$\pi = J \mathbf{F}^{eT} \mathbf{T}_0 \mathbf{F}^{e-T} : \mathbf{N}^p \quad (29)$$

Apart from Cauchy stress \mathbf{T} , one may also define second Piola-Kirchhoff type stress \mathbf{T}^e and Mendel stress \mathbf{M}^e as

$$\mathbf{T}^e := J \mathbf{F}^{e-1} \mathbf{T} \mathbf{F}^{e-T} \quad \text{and} \quad \mathbf{M}^e := \mathbf{C}^e \mathbf{T}^e \quad (30)$$

In terms of Mendel stress, the microscopic force balance Eq. (29) takes the following form.

$$\pi = \mathbf{M}_0^e : \mathbf{N}^p \quad (31)$$

Here \mathbf{M}_0^e is the deviatoric part of \mathbf{M}^e .

Constitutive Relations

Constitutive relation plays a crucial role in continuum modelling of material. It provides closure to the equations of motion via describing stress-strain relationship for the given material. It is through constitutive relation that the material behaviour, e.g. viscoplasticity in the present case, enters the continuum formulation. Presently, we base our constitutive theory of viscoplasticity of metals on dislocation dynamics described through a single parameter– the dislocation density ρ . We would not distinguish among different types of dislocations, rather would consider ρ to present their effects in an average sense. The goal of constitutive modelling here is to express \mathbf{T} and π in terms of the kinematic quantities and material parameters, and also to find out the evolution equation of dislocation density and heat flux-temperature relation.

First and Second Laws of Thermodynamics

As mentioned in introduction, we take recourse to two-temperature thermodynamics to model viscoplastic deformation in metals. To start with, we state the first law of thermodynamics or the internal energy balance as

$$\rho_m \dot{e} = p_{\text{int}} - \nabla_y \cdot \mathbf{q}, \quad (32)$$

where e , p_{int} and \mathbf{q} are respectively the specific internal energy, the internal power density and heat flux vector. We have neglected the external heat source in describing the first law. The internal power density is given by

$$\begin{aligned} p_{\text{int}} &:= \mathbf{T} : \mathbf{L}^e + J^{-1} \pi \mathbf{v}^p = \mathbf{T} : \mathbf{D}^e + J^{-1} \pi \mathbf{v}^p \\ &= J^{-1} \mathbf{T}^e : \mathbf{E}^e + J^{-1} \pi \mathbf{v}^p \end{aligned} \quad (33)$$

Recalling that the total internal energy density e and heat flux \mathbf{q} are composed of contributions from two distinct sources, namely the configurational subsystem and kinetic-vibrational subsystem, we consider the following additive decomposition

$$e = e_c + e_k \quad \text{and} \quad \mathbf{q} = \mathbf{q}_c + \mathbf{q}_k, \quad (34)$$

where the subscripts c and k denote respectively the configurational and kinetic-vibrational contributions. Following Kamrin and Bouchbinder (2014), we separate the energy balance equation given by Eq. (32) between two subsystems as

$$\rho_m \dot{e}_c = J^{-1} \mathbf{T}^e : \dot{\mathbf{E}}^e + J^{-1} \pi v^p - q_{ck} - \nabla_y \cdot \mathbf{q}_c, \quad (35)$$

and

$$\rho_m \dot{e}_k = q_{ck} - \nabla_y \cdot \mathbf{q}_k, \quad (36)$$

Here q_{ck} designates a scalar heat flux that gets established between the configurational and kinetic-vibrational subsystems as the system is driven out of equilibrium because of the imposed external load. q_{ck} in fact acts as a source of heat for the kinetic-vibrational system. It is easy to see that, when added, Eq. (35) and (36) recover the energy balance for the entire system (see Eq. (32)).

The constitutive relations must be compatible with the second law of thermodynamics too. With the hypothesis of local equilibrium, the second law inequality, in absence of external entropy source, may be stated as

$$\rho_m \dot{\eta} + \nabla_y \cdot \mathbf{j} \geq 0 \quad (37)$$

where η is the specific entropy and \mathbf{j} is the entropy flux. Again we adopt the additive decompositions: $\eta = \eta_c + \eta_k$ and $\mathbf{j} = \mathbf{j}_c + \mathbf{j}_k$. Considering the decomposed entropy fluxes to be given by the following relations

$$\mathbf{j}_c = \frac{\mathbf{q}_c}{\theta_c} \quad \text{and} \quad \mathbf{j}_k = \frac{\mathbf{q}_k}{\theta_k}, \quad (38)$$

where by θ_c and θ_k respectively we denote the configurational or the effective and the kinetic-vibrational or the ordinary temperature, we may write the entropy inequality as follows.

$$\rho_m \dot{\eta}_c + \rho_m \dot{\eta}_k + \nabla_y \cdot \left(\frac{\mathbf{q}_c}{\theta_c} \right) + \nabla_y \cdot \left(\frac{\mathbf{q}_k}{\theta_k} \right) \geq 0 \quad (39)$$

Substituting for $\nabla_y \cdot \mathbf{q}_c$ and $\nabla_y \cdot \mathbf{q}_k$ from Eq. (35) and (36), Eq. (39) is rewritten as

$$\begin{aligned} & \rho_m \dot{\eta}_c + \rho_m \dot{\eta}_k \\ & + \frac{1}{\theta_c} \left[J^{-1} \left(\mathbf{T}^e : \dot{\mathbf{E}}^e + \pi v^p \right) - q_{ck} - \rho_m \dot{e}_c \right] \\ & + \frac{1}{\theta_k} \left[q_{ck} - \rho_m \dot{e}_k \right] - \frac{1}{\theta_c^2} \mathbf{q}_c \cdot \nabla_y \theta_c \\ & - \frac{1}{\theta_k^2} \mathbf{q}_k \cdot \nabla_y \theta_k \geq 0 \end{aligned} \quad (40)$$

Eq. (40) is a spatial description of entropy inequality. Now we transform this inequality to intermediate frame representation by denoting

$\rho_m^I = J \rho_m$ as the mass density of the intermediate configuration and defining the quantities relative to volumes, areas and lengths of this intermediate space as

$$\begin{aligned} e_c^I &= \rho_m^I e_c, \quad e_k^I = \rho_m^I e_k, \quad \eta_c^I = \rho_m^I \eta_c, \quad \eta_k^I \\ &= \rho_m^I \eta_k, \quad q_{ck}^I = J q_{ck}, \quad \mathbf{q}_c^I = \mathcal{J} \mathbf{F}^{e-1} \mathbf{q}_c, \quad \mathbf{q}_k^I \\ &= \mathcal{J} \mathbf{F}^{e-1} \mathbf{q}_k, \quad \mathbf{g}_c^I = \mathbf{F}^{eT} \nabla_y \theta_c, \quad \mathbf{g}_k^I = \mathbf{F}^{eT} \nabla_y \theta_k \end{aligned} \quad (41)$$

For ease of exposition, we drop the superscript I from the notation, and write the intermediate space description of entropy imbalance as following.

$$\begin{aligned} & \eta_c + \eta_k + \frac{1}{\theta_c} \left[\mathbf{T}^e : \dot{\mathbf{E}}^e + \pi v^p - q_{ck} - \dot{e}_c \right] \\ & + \frac{1}{\theta_k} \left[q_{ck} - \dot{e}_k \right] - \frac{1}{\theta_c^2} \mathbf{q}_c \cdot \mathbf{g}_c - \frac{1}{\theta_k^2} \mathbf{q}_k \cdot \mathbf{g}_k \geq 0 \end{aligned} \quad (42)$$

Intermediate space representations of Eq. (35) and (36) take the following forms.

$$\dot{e}_c = \mathbf{T}^e : \dot{\mathbf{E}}^e + \pi v^p - q_{ck} - \nabla \cdot \mathbf{q}_c, \quad (43)$$

$$\dot{e}_k = q_{ck} - \nabla \cdot \mathbf{q}_k, \quad (44)$$

Here, $\nabla \cdot$ is the divergence operator defined on the intermediate space and its relation with spatial divergence is given by $\nabla \cdot \mathbf{u} = J \nabla_y \cdot (J^{-1} \mathbf{F}^e \mathbf{u})$ for any vector field \mathbf{u} defined on intermediate space.

Constitutive Relations and Evolution Equations

We assume e_c, e_k, \mathbf{E}^e along with the dislocation density ρ act as the independent variables and describe the state of the viscoplasticity deforming metal. We also consider the following dependencies

$$\eta_c = \hat{\eta}_c(e_c, \mathbf{E}^e, \rho), \quad \eta_k = \hat{\eta}_k(e_k), \quad \mathbf{T}^e = \hat{\mathbf{T}}^e(\mathbf{E}^e), \quad (45)$$

which allows to expand Eq. (42) as follows.

$$\begin{aligned}
& \left(\frac{\partial \hat{\eta}_c}{\partial e_c} - \frac{1}{\theta_c} \right) \dot{e}_c + \left(\frac{\partial \hat{\eta}_k}{\partial e_k} - \frac{1}{\theta_k} \right) \dot{e}_k \\
& + \left(\frac{\partial \hat{\eta}_c}{\partial \mathbf{E}^e} + \frac{1}{\theta_c} \mathbf{T}^e \right) : \dot{\mathbf{E}}^e + \frac{\partial \hat{\eta}_c}{\partial \rho} \dot{\rho} \\
& + \frac{1}{\theta_c} \pi v^p + \left(\frac{1}{\theta_k} - \frac{1}{\theta_c} \right) q_{ck} \\
& - \frac{1}{\theta_c^2} \mathbf{q}_c \cdot \mathbf{g}_c - \frac{1}{\theta_k^2} \mathbf{q}_k \cdot \mathbf{g}_k \geq 0
\end{aligned} \quad (46)$$

The first three terms of the inequality (46), being linear in the independent rate quantities \dot{e}_c , \dot{e}_k and $\dot{\mathbf{E}}^e$, the usual Coleman-Noll type argument (Coleman and Noll, 1963) to ensure the non-negativity leads to the following.

$$\frac{1}{\theta_c} = \frac{\partial \hat{\eta}_c}{\partial e_c}, \quad \frac{1}{\theta_k} = \frac{\partial \hat{\eta}_k}{\partial e_k}, \quad (47)$$

and

$$\text{Sym} \left(\frac{\partial \hat{\eta}_c}{\partial \mathbf{E}^e} + \frac{1}{\theta_c} \mathbf{T}^e \right) = \mathbf{0} \quad (48)$$

By $\text{Sym}(\mathbf{A})$ we denote symmetric part of the tensor \mathbf{A} . However, \mathbf{E}^e and \mathbf{T}^e both being symmetric

tensors, $\left(\frac{\partial \hat{\eta}_c}{\partial \mathbf{E}^e} + \frac{1}{\theta_c} \mathbf{T}^e \right)$ itself is symmetric and therefore, Eq. (48) leads to the following.

$$\mathbf{T}^e = -\theta_c \frac{\partial \hat{\eta}_c}{\partial \mathbf{E}^e} \quad (49)$$

Substituting Eq. (47) and (49) into (46), the entropy imbalance reduces to

$$\begin{aligned}
& \frac{\partial \hat{\eta}_c}{\partial \rho} \dot{\rho} + \frac{1}{\theta_c} \pi v^p + \left(\frac{1}{\theta_k} - \frac{1}{\theta_c} \right) q_{ck} \\
& - \frac{1}{\theta_c^2} \mathbf{q}_c \cdot \mathbf{g}_c - \frac{1}{\theta_k^2} \mathbf{q}_k \cdot \mathbf{g}_k \geq 0.
\end{aligned} \quad (50)$$

Let us now assume that $\hat{\eta}_c$ admits the following decomposition.

$$\begin{aligned}
\hat{\eta}_c(e_c, \mathbf{E}^e, \rho) &= \hat{\eta}_\rho(\rho) + \hat{\eta}_{\text{surr}}(e_{\text{surr}}) \\
\text{with } e_{\text{surr}} &:= e_c - \hat{e}_\rho(\rho) - \hat{e}_e(\mathbf{E}^e)
\end{aligned} \quad (51)$$

The configurational entropy density and energy density associated with dislocations, i.e., $\hat{\eta}_\rho(\rho)$ and $\hat{e}_\rho(\rho)$, may be given by the following (Langer, 2015).

$$\begin{aligned}
\hat{\eta}_\rho(\rho) &= \frac{\rho}{L} - \frac{\rho}{L} \ln(a^2 \rho) \quad \text{and} \\
\hat{e}_\rho(\rho) &= \frac{e_D \rho}{L}
\end{aligned} \quad (52)$$

Here L , a and e_D are respectively a characteristic length of dislocation, a length of order atomic spacing and the energy per dislocation. The elastic energy $\hat{e}_e(\mathbf{E}^e)$ may be considered to be

$$\hat{e}_e(\mathbf{E}^e) = \frac{1}{2} \lambda \left(\text{tr}(\mathbf{E}^e) \right)^2 + \mu \mathbf{E}^e : \mathbf{E}^e, \quad (53)$$

where λ and μ are the Lamé parameters. Using Eq.

(51)-(52), and the fact that $\frac{\partial \hat{\eta}_{\text{surr}}}{\partial e_{\text{surr}}} = \frac{1}{\theta_c}$, Eq. (50) may be recast as

$$\begin{aligned}
& -\frac{1}{L} \left(\frac{e_D}{\theta_c} + \ln(a^2 \rho) \right) \dot{\rho} + \frac{1}{\theta_c} \pi v^p + \left(\frac{1}{\theta_k} - \frac{1}{\theta_c} \right) q_{ck} \\
& - \frac{1}{\theta_c^2} \mathbf{q}_c \cdot \mathbf{g}_c - \frac{1}{\theta_k^2} \mathbf{q}_k \cdot \mathbf{g}_k \geq 0.
\end{aligned} \quad (54)$$

Heat Flux-temperature Relations

To ensure the non-negativity of entropy production, we demand all the five terms appearing in the left hand side of (54) to be individually non-negative. Choice of the constitutive relations for the heat fluxes in form Fourier's type law, as given in Eq. (55), ensures the non-negativity of the last three terms.

$$\begin{aligned}
\mathbf{q}_c &= -k_c \mathbf{g}_c, \quad k_c = \hat{k}_c(\theta_c, \nu^p) \geq 0 \\
\mathbf{q}_k &= -k_k \mathbf{g}_k, \quad k_k = \hat{k}_k(\theta_k) \geq 0 \\
q_{ck} &= k_{ck}(\theta_c - \theta_k), \quad k_{ck} = \hat{k}_{ck}(\theta_c, \theta_k, \nu^p) \geq 0
\end{aligned} \quad (55)$$

Dislocation Density Evolution

With the ensured non-negativity of the last three terms in (54), it only remains to ensure the same for the first two terms. Evolution of dislocation density in the way given in Eq. (55) would guarantee the non-negativity of the first term.

$$\begin{aligned}
\dot{\rho} &= -\mathcal{M} \left(\frac{e_D}{\theta_c} + \ln(a^2 \rho) \right), \\
\mathcal{M} &= \hat{\mathcal{M}}(\theta_c, \theta_k, \nu^p, \rho) \geq 0
\end{aligned} \quad (56)$$

Eq. (56) may be approximated as

$$\dot{\rho} = \mathcal{M} \left(1 - \frac{\rho}{\rho_0} \right), \quad (57)$$

where $\rho_0 = \frac{1}{a^2} \exp\left(-\frac{e_D}{\theta_c}\right)$. As suggested by

Langer (2015), we consider $\hat{\mathcal{M}} =$

$$k_p \frac{\hat{\pi}(\theta_c, \theta_k, \nu^p, \rho) \nu^p}{\gamma_D}, \text{ where } k_p \text{ is a non-negative}$$

number, $\hat{\pi}$ is the constitutive function for the micro stress π and $\gamma_D = e_D / L$ is energy of dislocation per unit length.

Constitutive Relation for π

It is now remaining to ensure $\frac{1}{\theta_c} \pi \nu^p \geq 0$. By

definition (see Eq. (6)), ν^p is non-negative and this is true for θ_c too. Therefore the only requirement is that constitutive relation for π should be such that it is always non-negative. To find out this constitutive relation for π , we take recourse to the theory of thermal activation of dislocation. For the present work, we only focus on FCC metals. The kinetic equation

relating ν^p and π for FCC metals can be given in the following Arrhenius form.

$$\nu^p = \frac{\rho b l^*}{\tau_0} \exp\left[-\frac{k_B T_p}{\theta_k} \exp\left(-\frac{\pi}{\pi_T}\right)\right] \quad (58)$$

Here l^* is some mean free path or average distance between dislocations, b the magnitude of Burgers vector, τ_0^{-1} a microscopic attempt frequency of the order of 10^{12} per second. $k_B T_p$ is the thermal barrier of the potential in which the dislocation is trapped in absence of external driving. k_B refers to the Boltzmann constant. π_T is the Taylor stress given as $\pi_T = \mu_T b \sqrt{\rho}$, where μ_T is proportional to shear modulus μ . For further details see Langer *et al.* (2010). Inverting Eq. (58), we get the constitutive relation for π as

$$\pi = \mu_T b \sqrt{\rho} \left[\ln\left(\frac{k_B T_p}{\theta_k}\right) - \ln\left\{\frac{1}{2} \ln\left(\frac{\rho b^2}{\tau_0^2 \nu^{p2}}\right)\right\} \right] \quad (59)$$

Temperature Evolution

From Eq. (43) and (44), evolution equations for effective temperature and kinetic-vibrational temperature may be derived. Towards this, we assume the dependencies $e_k = \hat{e}_k(\theta_k)$ and $e_c = \hat{e}_c(\theta_c, \mathbf{E}^e, \rho)$ which allows to compute the energy rates as follows.

$$\dot{e}_k = \frac{\partial \hat{e}_k}{\partial \theta_k} \dot{\theta}_k = \hat{c}_k(\theta_k) \dot{\theta}_k \quad (60)$$

$$\dot{e}_c = \frac{\partial \hat{e}_c}{\partial \theta_c} \dot{\theta}_c + \frac{\partial \hat{e}_c}{\partial \mathbf{E}^e} : \dot{\mathbf{E}}^e + \frac{\partial \hat{e}_c}{\partial \rho} \dot{\rho} \quad (61)$$

Taking partial derivative of Eq. (51) with respect to \mathbf{E}^e , we get

$$\frac{\partial \hat{\eta}_c}{\partial \mathbf{E}^e} = \frac{\partial \hat{\eta}_{\text{surr}}}{\partial e_{\text{surr}}} \left(-\frac{\partial \hat{e}_c(\mathbf{E}^e)}{\partial \mathbf{E}^e} \right) = -\frac{1}{\theta_c} \frac{\partial \hat{e}_c}{\partial \mathbf{E}^e} \quad (62)$$

We rewrite Eq. (61) using Eq. (49), (52) and (62) as

$$\dot{\epsilon}_c = \hat{c}_c \dot{\theta}_c + \mathbf{T}^e : \dot{\mathbf{E}}^e + \gamma_D \dot{\rho} \quad (63)$$

In Eq. (60) and (63), \hat{c}_k and \hat{c}_c respectively denote the specific heat of kinetic-vibrational subsystem and configurational subsystem. Using Eq. (60), (63) and (55), the energy balance equations given by Eq. (43) and (44) can be written in the form of temperature evolution equations as

$$\hat{c}_c \dot{\theta}_c = \pi \mathbf{v}^p - \gamma_D \dot{\rho} - k_{ck} (\theta_c - \theta_k) + \nabla \cdot (k_c \mathbf{g}_c) \quad (64)$$

and

$$\hat{c}_k \dot{\theta}_k = k_{ck} (\theta_c - \theta_k) + \nabla \cdot (k_k \mathbf{g}_k) \quad (65)$$

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Concluding Remarks

We have derived a two-temperature viscoplasticity model, based on the principles of nonequilibrium thermodynamics, for polycrystalline solids. The proposed model extends the original development by Langer *et al.* (2010) to a full-fledged three dimensional continuum formulation allowing for spatial variations of fields – an aspect not explored so far. Another special feature of the present model is that it is derived in a yield-free format in which the usual flow rule is replaced by a microscopic force balance. The constitutive modelling is done in a physically consistent way considering dislocation motion and evolution. Though presently restricted to only FCC metals, an extension of the present model to BCC metals could be readily accomplished.

