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# On the thermo-mechanical theory of field dislocations in transient heterogeneous temperature fields

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## **Abstract**

A strong coupling between the field theory of dislocation mechanics and heat conduction is proposed. The novel model, called the thermal field dislocation mechanics (T-FDM) model, is designed to study the dynamics of dislocations during rapid or gradual temperature changes in a body having a heterogeneous temperature distribution; for example, such conditions occur in a heat-affected crystalline solid during an additive manufacturing process. It is based on the principles of rational thermodynamics whose main assumptions include respecting local thermodynamic equilibrium and imposing the classical Clausius-Kelvin-Planck formulation of the second law of thermodynamics. The T-FDM model is designed to operate at the length scale of individual dislocations and temperature-dependent crystallographic dislocation driving forces are derived based on global dissipation considerations. The advantages and consequences of the assumptions of the T-FDM model under rapidly changing temperatures, both spatially and temporally, are discussed. Local thermodynamic equilibrium is found to be a reasonable assumption even for high rates of change of temperature such as those occurring during an additive manufacturing process.

## **Highlights**

- Strong temperature gradients during 3D-printing can trigger dislocation dynamics
- A novel fully-coupled dislocation dynamics and heat conduction model is proposed
- Proposed model can deal with high temperature rates during additive manufacturing
- Local thermodynamic equilibrium is respected even under strong temperature rates

**Keywords:** dislocations, dynamics, thermal stress, constitutive behavior, additive manufacturing

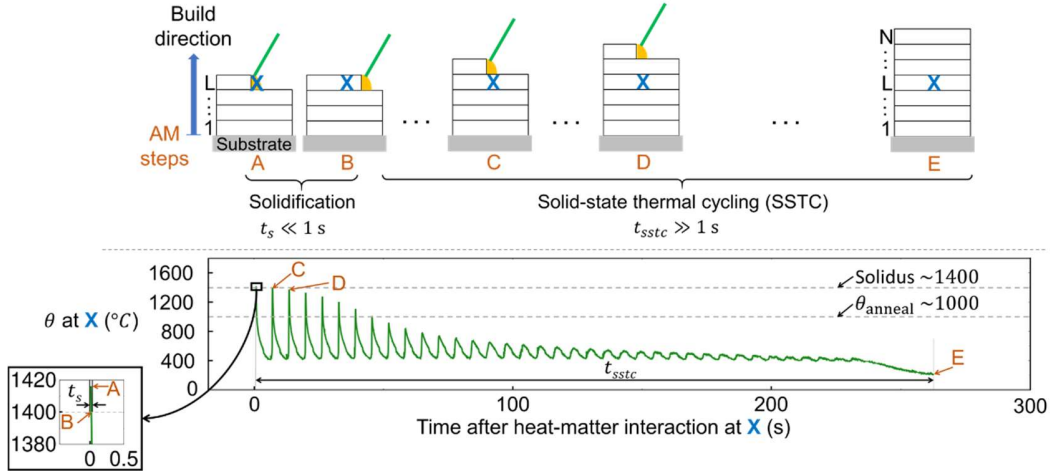
## **1. Introduction**

### **1.1 Motivation**

In this work, we are interested in developing a thermodynamically rigorous model to study dislocation dynamics, at the length scale of individual dislocations, within a body having a heterogeneous temperature distribution and undergoing rapid and/or gradual temperature changes.

The main motivation for the development of such a model is to study dislocation structure evolution in a heat-affected crystalline solid during an additive manufacturing (also known as 3D-printing) process. During an additive manufacturing process, just after local deposition due to a moving heat-source, a liquid material rapidly solidifies within a few milliseconds. Following solidification, as the building continues, the material is subjected to multiple cooling-heating cycles in the solid-state, i.e. solid-state thermal cycling, at varying temperature rates and amplitudes. An illustration of varying temperature rates and amplitudes at a material point during the 3D-printing of a metal/alloy wall is shown in Fig. 1. During initial stages of solid-state thermal cycling, temperature amplitudes higher than annealing points and temperature rates of the order of  $10^6$  K/s can be encountered due to localized heat-matter interactions. Consequently, large transient temperature gradients are formed, which result in strong transient thermal stresses due to internal and/or external constraints. Such rapidly varying temperatures and thermal stresses can result in significant

changes in the microstructure, including dislocation structure evolution via dislocation dynamics. During later stages of solid-state thermal cycling, a nearly steady-state heat conduction occurs at relatively high temperatures with respect to room temperature. These relatively high temperatures along with internal stresses due to a metastable microstructure can also result in additional dislocation dynamics, including recovery mechanisms. The existing dislocation dynamics models are unable to handle temperature change driven dislocation dynamics.



**Figure 1:** An illustration of temperature ( $\theta$ ) vs time ( $t$ ) evolution at a material point X during additive manufacturing of a wall.  $t = 0$  corresponds to the moment the heat-matter interactions occur at X in a layer  $L < N$ , where  $N$  is the total number of layers.

## 1.2 State-of-the-art, aim and structure of the paper

Most existing dislocation dynamics models, both discrete and continuous kind, are designed to study dislocation motion and interactions under isothermal and/or adiabatic conditions. Indeed, there exist couplings between heat conduction and phenomenological elastic-plastic theory (Simo and Miehe, 1992) as well as between heat conduction and dislocation mechanics theory (Acharya, 2011; Ghoniem et al., 2000; Kratochvil and Dillon, 1969). In (Kratochvil and Dillon, 1969), scalar parameters were introduced to represent dislocation arrangements of different kinds and phenomenological time evolution laws were proposed. However, due to the phenomenological nature of the evolution laws, it is difficult to connect the modeling approach with crystallography of materials. In (Ghoniem et al., 2000), following the thermo-mechanical developments, temperature effects were however neglected when deriving dislocation driving forces. In (Acharya, 2011), although a coupling was proposed between a dislocation mechanics model and heat conduction, however, the modeling approach focused at the length scale where crystal plasticity models operate (Acharya and Roy, 2006) and not at the length scale of individual dislocations. Furthermore, explicit temperature dependent constitutive relationships were not proposed. To the author's knowledge, none of the existing dislocation dynamics models account for temperature change induced crystallographic dislocation driving forces.

To that end, in this work, a strong coupling between the field dislocation mechanics (FDM) approach, developed by Acharya (Acharya, 2004, 2003, 2001), and the heat conduction problem at the length scale of individual dislocations is proposed.

FDM is a thermo-mechanically rigorous model for the dynamics of continuously-represented dislocations. It finds its roots in the elastic theory of continuously distributed dislocations (Bilby et al., 1955; Fox, 1966; Kosevich, 1979; Kröner, 1981, 1958; Mura, 1963; Willis, 1967), which started from the seminal work of Nye (Nye, 1953). Unlike the earlier models that employed the eigenstrain approach

(Eshelby and Peierls, 1957) to solve the mechanical problem for a dislocation, FDM uses the Stokes-Helmholtz orthogonal decomposition of the elastic/plastic distortion fields into compatible and incompatible components. This approach uniquely determines the elastic/plastic distortion fields associated with a prescribed areal dislocation density. The incompatible part of the elastic/plastic distortion is related to the curl of the prescribed areal dislocation density field, which makes FDM a non-local model. Nevertheless, it does not require using higher-order stress or boundary conditions, which are typical in gradient plasticity models (for example (Forest, 2008)) or micro-stress/micro-traction conditions (for example, (Gurtin, 2002, 2000)). The thermodynamic considerations in FDM straightforwardly result in dislocation driving forces that are crystallographic in nature. In light of the above, FDM is a highly appropriate approach for the desired coupling with heat conduction.

This paper is structured as follows. The notations and tensorial operations used in this work are presented in section 2 along with important properties and relationships of the Stokes-Helmholtz decomposition of a second-order tensor, proposed by Acharya (Acharya, 2004, 2001). In section 3, the proposed model, henceforth known as the thermal-FDM (T-FDM) model, is developed. The model development involves a thorough consideration of the kinematics of the FDM model and the thermodynamics of both the FDM model and the heat conduction problem. In the discussion section 4, the consequences of the thermodynamic considerations adopted during the development of the T-FDM model are critically analyzed. In addition, ideas for possible future work are presented. The conclusions of this work are presented in section 5 and the bibliography in section 6.

## 2. Notations and tensorial operations

A bold letter or symbol with overhead bars denotes a tensor. The number of overhead bars denote the order of a tensor; for example, a first order tensor has one overhead bar, a second order tensor has two overhead bars and so on. Only the differential operator  $\nabla$  is presented without an overhead bar. Scalars (zeroth order tensors) are denoted with regular font and no overhead bars. The summation convention will be implied for operations between tensorial quantities; in this section, it is used to understand different tensorial operations considered in this work. Consider two 1<sup>st</sup> order tensors, i.e. vectors,  $\bar{\mathbf{a}}$  and  $\bar{\mathbf{b}}$ , two second order tensors  $\bar{\bar{\mathbf{A}}}$  and  $\bar{\bar{\mathbf{B}}}$ , and rectangular Cartesian basis unit vectors  $\hat{\mathbf{e}}$ . In this work, we will use the following operations (demonstrated in the rectangular Cartesian frame).

Tensorial (outer) product:

$$\begin{aligned}(\bar{\mathbf{a}} \otimes \bar{\mathbf{b}})_{ij} &= a_i b_j \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j \\(\bar{\mathbf{a}} \otimes \bar{\bar{\mathbf{B}}})_{ijk} &= a_i B_{jk} \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j \otimes \hat{\mathbf{e}}_k \\(\bar{\bar{\mathbf{A}}} \otimes \bar{\mathbf{b}})_{ijk} &= A_{ij} b_k \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j \otimes \hat{\mathbf{e}}_k \\(\bar{\bar{\mathbf{A}}} \otimes \bar{\bar{\mathbf{B}}})_{ijkl} &= A_{ij} B_{kl} \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j \otimes \hat{\mathbf{e}}_k \otimes \hat{\mathbf{e}}_l\end{aligned}$$

Inner (dot) product between tensors:

$$\begin{aligned}(\bar{\mathbf{a}} \cdot \bar{\mathbf{b}}) &= (\bar{\mathbf{b}} \cdot \bar{\mathbf{a}}) = a_i b_i \\(\bar{\bar{\mathbf{A}}} \cdot \bar{\bar{\mathbf{B}}})_{ij} &= A_{ik} B_{kj} \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j \\(\bar{\mathbf{a}} \cdot \bar{\bar{\mathbf{B}}})_j &= a_i B_{ij} \hat{\mathbf{e}}_j \\(\bar{\bar{\mathbf{A}}} \cdot \bar{\mathbf{b}})_i &= A_{ij} b_j \hat{\mathbf{e}}_i \\(\bar{\bar{\mathbf{A}}} : \bar{\bar{\mathbf{B}}}) &= A_{ij} B_{ij}\end{aligned}$$

where “:” is the symbol for a double dot product.

Cross product between tensors:

$$\begin{aligned}
(\bar{\mathbf{a}} \times \bar{\mathbf{b}})_i &= e_{ijk} a_j b_k \hat{\mathbf{e}}_i \\
(\bar{\mathbf{A}} \times \bar{\mathbf{b}})_{ij} &= e_{jlk} A_{il} b_k \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j \\
(\bar{\mathbf{a}} \times \bar{\mathbf{B}})_{ij} &= e_{ilk} a_l B_{kj} \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j
\end{aligned}$$

where  $e_{ijk}$  is a component of the third order Levi-Cevita permutation tensor  $\bar{\bar{\mathbf{X}}}$ .

For tensorial operations involving the differential operator  $\nabla$ , we will follow the convention used by Salencon (Salencon, 2001) and Acharya (Acharya, 2003):

$$\begin{aligned}
(\nabla \bar{\mathbf{a}})_{ij} &= (\mathbf{grad} \bar{\mathbf{a}})_{ij} = a_{i,j} \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j \\
(\nabla \bar{\mathbf{A}})_{ijk} &= (\mathbf{grad} \bar{\mathbf{A}})_{ijk} = A_{ij,k} \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j \otimes \hat{\mathbf{e}}_k \\
(\nabla \cdot \bar{\mathbf{a}}) &= (\mathbf{div} \bar{\mathbf{a}}) = a_{i,i} \\
(\nabla \cdot \bar{\mathbf{A}})_i &= (\mathbf{div} \bar{\mathbf{A}})_i = A_{ij,j} \hat{\mathbf{e}}_i \\
(\nabla \times \bar{\mathbf{a}})_i &= (\mathbf{curl} \bar{\mathbf{a}})_i = e_{ijk} a_{k,j} \hat{\mathbf{e}}_i \\
(\nabla \times \bar{\mathbf{A}})_{ij} &= (\mathbf{curl} \bar{\mathbf{A}})_{ij} = e_{jkl} A_{il,k} \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j
\end{aligned}$$

Of key importance in FDM theory is the establishment of a relationship between the local slip distortion rate, a second order tensor, produced by the motion of an areal dislocation density tensor, another second order tensor, to the overall plastic distortion rate in a manner that does not violate any thermodynamic considerations. This requires using the Stokes-Helmholtz decomposition of a second order tensor employed by Acharya (Acharya, 2004, 2003, 2001) based on the work of Weyl (Weyl, 1940).

If we suppose that  $D$  is the set of all square-integrable matrix fields on a domain  $\mathcal{B}$  having the property of the double dot product, then any second order tensor field  $\bar{\mathbf{A}} \in D$  can be uniquely decomposed (Stokes-Helmholtz decomposition) into a curl-free component  $\bar{\mathbf{A}}^{\parallel}$  (denoted with a superscript “ $\parallel$ ”) and a divergence-free component  $\bar{\mathbf{A}}^{\perp}$  (denoted with a superscript “ $\perp$ ”) as:

$$\bar{\mathbf{A}} = \bar{\mathbf{A}}^{\parallel} + \bar{\mathbf{A}}^{\perp} \quad (2.1)$$

such that  $\bar{\mathbf{A}}^{\parallel} : \bar{\mathbf{A}}^{\perp} = 0$ . Relationship (2.1) additionally satisfies the following conditions:

- (i)  $\bar{\mathbf{A}}^{\parallel}$  belongs to  $N(\mathbf{curl}) \subset D$ ; where  $N(\mathbf{curl})$  is the null-space of the curl operator.
- (ii)  $\bar{\mathbf{A}}^{\perp}$  belongs to  $N^{\perp}(\mathbf{curl}) = \{B \in D \text{ such that } \int_{\mathcal{B}} B : \nabla dv = 0, \forall \nabla \in N(\mathbf{curl})\}$ .
- (iii)  $\int_{\mathcal{B}} \bar{\mathbf{A}} : \bar{\mathbf{B}} dv = \int_{\mathcal{B}} \bar{\mathbf{A}}^{\parallel} : \bar{\mathbf{B}}^{\parallel} dv + \int_{\mathcal{B}} \bar{\mathbf{A}}^{\perp} : \bar{\mathbf{B}}^{\perp} dv$
- (iv) For every  $\bar{\mathbf{A}} \in D$ , there exists a  $\bar{\mathbf{W}}_A \in D$  that satisfies

$$\int_{\mathcal{B}} \bar{\mathbf{W}}_A : \nabla \times \bar{\mathbf{Q}} dv = \int_{\mathcal{B}} \bar{\mathbf{A}}^{\perp} : \bar{\mathbf{Q}} dv, \quad \forall \bar{\mathbf{Q}} \in T \text{ with } \bar{\mathbf{W}}_A = 0 \text{ on } \partial \mathcal{B} \quad (2.3)$$

where  $T$  is the set of all test functions that vanish on the boundary  $\partial \mathcal{B}$  of the domain  $\mathcal{B}$ . Then,  $\bar{\mathbf{W}}_A$  in (2.3) can be determined by solving:

$$\left. \begin{aligned}
\nabla \times \bar{\mathbf{W}}_A &= \bar{\mathbf{A}}^{\perp} \\
\nabla \cdot \bar{\mathbf{W}}_A &= 0 \\
\bar{\mathbf{W}}_A &= 0 \text{ on } \partial \mathcal{B}
\end{aligned} \right\} \text{ on } \mathcal{B} \quad (2.4)$$

Relationships (2.1) – (2.4) are of key importance to the development of the original FDM model, and hence, also in the present work. A detailed mathematical formulation of these relationships can be found in (Acharya, 2003, 2001).

### 3. The T-FDM model

In essence, the T-FDM model is a generalization of the isothermal and adiabatic FDM model of Acharya (Acharya, 2004, 2003, 2001) to a transient heterogeneous temperature distribution case via a strong coupling with the heat conduction problem. FDM has been constructed within a continuum framework whose main assumptions are based on the principles of rational thermodynamics (RT) (Coleman, 1964; Coleman and Noll, 1960; Coleman and Owen, 1975; Gurtin, 1968; Truesdell, 1984, 1968; Truesdell and Noll, 2004). We shall also perform this coupling in a rational thermodynamics (RT) framework.

When dealing with heat conduction, the role of entropy and temperature becomes crucial and these entities need to be treated carefully. Following the proofs by Coleman, Owen and Serrin (Coleman et al., 1981; Coleman and Owen, 1974; Serrin, 1979), we know that for cyclic processes and for approximately cyclic processes described within an RT framework, there exists (i) an entropy that is a state function and (ii) an empirical absolute temperature scale. We will assume that all the intended applications of the T-FDM model fall within the category of cyclic or approximately cyclic processes, and hence the aforementioned entropy and temperature always exist. This assumption is sufficient for the development of the T-FDM model, and its implications will be discussed in section 4.

#### 3.1 Theory of continuously represented stationary dislocations in a heterogeneous temperature field

Let us consider a body  $\mathcal{B}$  with surface  $\partial\mathcal{B}$  to be a thermodynamically closed system, i.e. it is allowed to exchange heat and work with its surroundings but not matter. We will suppose that  $\mathcal{B}$  has a heterogeneous temperature distribution due to some combination of steady-state heat-flux and/or constant temperature on  $\partial\mathcal{B}$  as well as some *a priori* unknown steady-state heat sources within  $\mathcal{B}$ . We shall further assume that the local temperature  $\theta(\bar{\mathbf{x}})$  is always below solidus at any given instant in time anywhere in  $\mathcal{B}$ . We will use  $\theta_0$  to denote the reference temperature.

It is clear that globally  $\mathcal{B}$  is not in thermal equilibrium. However, we shall adopt the local thermodynamic equilibrium hypothesis, which is the basic tenet of any RT based model. According to this hypothesis, we assume that every material point in  $\mathcal{B}$  is in thermodynamic (thermal, mechanical and chemical) equilibrium, even though globally  $\mathcal{B}$  may not be in thermodynamic equilibrium.

We will assume that  $\mathcal{B}$  is a simply connected body, i.e. voids and cracks are not allowed to exist/form within the body. Furthermore, we will assume that  $\mathcal{B}$  is a single crystal.

Let  $\mathcal{B}$  contain an arbitrary distribution of continuously represented stationary dislocations and we shall focus on the thermo-mechanics of stationary dislocations within  $\mathcal{B}$  far from the boundary  $\partial\mathcal{B}$ . Quantities presented in the derivations below will be assumed to be spatially “local” unless explicitly mentioned otherwise. However, these quantities may depend either on the local temperature  $\theta$  at  $\bar{\mathbf{x}}$  or on a temperature distribution  $\mathcal{T}(\theta)$  in a suitable neighborhood around  $\bar{\mathbf{x}}$ . In other words, they may have a non-local dependence on temperature. In the following,  $\eta(\theta)$  and  $\eta(\mathcal{T}(\theta))$  shall be used to denote the dependence of any variable  $\eta$  either on local  $\theta$  or on  $\mathcal{T}(\theta)$ . Note that the usage of these notations does not imply that a variable  $\eta$  is solely dependent on  $\theta$  or  $\mathcal{T}(\theta)$ .

In order to facilitate the coupling between FDM and heat conduction, we will restrict ourselves to the case of small displacements and small strains but allow large temperature differences.

The simply connected nature of  $\mathcal{B}$  implies that the total displacement field  $\bar{\mathbf{u}}(\theta)$  is continuously differentiable everywhere in  $\mathcal{B}$  at any instant in time. Note that the presence of a heterogeneous temperature distribution does not preclude such a definition. The total distortion field  $\bar{\mathbf{U}}(\theta)$ , defined as the gradient of total displacement:

$$\bar{\mathbf{U}}(\theta) = \nabla \bar{\mathbf{u}}(\theta), \quad (3.1)$$

is a compatible (curl-free) field, i.e.  $\bar{\mathbf{U}}(\theta) = \bar{\mathbf{U}}^{\parallel}(\theta)$  and satisfies

$$\nabla \times \bar{\mathbf{U}}(\theta) = 0 \quad (3.2)$$

everywhere in  $\mathcal{B}$ . Equation (3.2) is a necessary condition for integrability of  $\bar{\mathbf{u}}(\theta)$  and a compatibility condition for  $\bar{\mathbf{U}}(\theta)$ . The total strain  $\bar{\boldsymbol{\epsilon}}(\theta)$ , defined as the symmetric component of  $\bar{\mathbf{U}}(\theta)$ :

$$\bar{\boldsymbol{\epsilon}}(\theta) = \bar{\boldsymbol{\epsilon}}^{\parallel}(\theta) = \text{sym}(\bar{\mathbf{U}}(\theta)) = \frac{1}{2}(\nabla \bar{\mathbf{u}}(\theta) + (\nabla \bar{\mathbf{u}}(\theta))^T), \quad (3.3)$$

is also compatible and it satisfies:

$$\nabla \times \bar{\boldsymbol{\epsilon}}(\theta) \times \nabla = 0 \quad (3.4)$$

The temperature difference  $\Delta\theta = \theta - \theta_0$  induces a local compatible thermal (inelastic) strain  $\bar{\boldsymbol{\epsilon}}^{\theta}(\theta)$  such that:

$$\bar{\boldsymbol{\epsilon}}^{\theta}(\theta) = \bar{\boldsymbol{\epsilon}}^{\theta\parallel}(\theta) = \bar{\boldsymbol{\gamma}}(\theta)\Delta\theta \quad (3.5)$$

where  $\bar{\boldsymbol{\gamma}}(\theta)$  is the local thermal expansion coefficient tensor, which is symmetric.

In the presence of dislocations in a heterogeneous temperature field,  $\bar{\mathbf{U}}(\theta)$  can be additively decomposed into elastic  $\bar{\mathbf{U}}^e(\theta)$  and inelastic  $\bar{\mathbf{U}}^{in}(\theta)$  components:

$$\bar{\mathbf{U}}(\theta) = \bar{\mathbf{U}}^e(\theta) + \bar{\mathbf{U}}^{in}(\theta), \quad (3.6)$$

Similarly, the total strain  $\bar{\boldsymbol{\epsilon}}(\theta)$  can be additively decomposed into elastic  $\bar{\boldsymbol{\epsilon}}^e(\theta)$  and inelastic  $\bar{\boldsymbol{\epsilon}}^{in}(\theta)$  components as:

$$\bar{\boldsymbol{\epsilon}}(\theta) = \bar{\boldsymbol{\epsilon}}^e(\theta) + \bar{\boldsymbol{\epsilon}}^{in}(\theta) = \bar{\boldsymbol{\epsilon}}^m(\theta) + \bar{\boldsymbol{\epsilon}}^{\theta}(\theta), \quad (3.7)$$

with  $\bar{\boldsymbol{\epsilon}}^e = \text{sym}(\bar{\mathbf{U}}^e)$ ,  $\bar{\boldsymbol{\epsilon}}^{in} = \text{sym}(\bar{\mathbf{U}}^{in})$ , and  $\bar{\boldsymbol{\epsilon}}^m = \bar{\boldsymbol{\epsilon}}^e + \bar{\boldsymbol{\epsilon}}^p$  with  $\bar{\boldsymbol{\epsilon}}^p$  being the plastic strain tensor.

$\bar{\mathbf{U}}^{in}(\theta)$  and  $\bar{\boldsymbol{\epsilon}}^{in}(\theta)$  can be additively decomposed into:

$$\bar{\mathbf{U}}^{in}(\theta) = \bar{\boldsymbol{\epsilon}}^{\theta}(\theta) + \bar{\mathbf{U}}^p(\theta), \quad (3.8)$$

$$\bar{\boldsymbol{\epsilon}}^{in}(\theta) = \bar{\boldsymbol{\epsilon}}^{\theta}(\theta) + \bar{\boldsymbol{\epsilon}}^p(\theta), \quad (3.9)$$

where  $\bar{\mathbf{U}}^p(\theta)$  is the plastic distortion tensor. By invoking the Stokes-Helmholtz decomposition, it is possible to decompose both  $\bar{\mathbf{U}}^e(\theta)$  and  $\bar{\mathbf{U}}^p(\theta)$  into compatible (curl-free) and incompatible (divergence-free) components such that

$$\bar{\mathbf{U}}^i(\theta) = \bar{\mathbf{U}}^{i\parallel}(\theta) + \bar{\mathbf{U}}^{i\perp}(\theta); i = e \text{ or } in \quad (3.10)$$

Equations (3.5), (3.8), (3.9) and (3.10) imply that

$$\bar{\mathbf{U}}^{e\perp}(\theta) + \bar{\mathbf{U}}^{p\perp}(\theta) = 0 \quad (3.11)$$

along with  $\bar{\mathbf{U}}^{in\perp}(\theta) = \bar{\mathbf{U}}^{p\perp}(\theta)$ .

Consider an arbitrary material surface  $S$  inside  $\mathcal{B}$  and let an ensemble of dislocations thread this surface. The presence of dislocations precludes a unique definition of the elastic (and plastic) displacement fields. If we were to draw an arbitrary circuit  $\mathcal{C}$  on the surface  $S$  surrounding the dislocation, then a constant discontinuity  $\bar{\mathbf{b}}$  in the form of a jump in the elastic displacement  $\llbracket \bar{\mathbf{u}}^e \rrbracket$  manifests itself as a closure defect along the circuit  $\mathcal{C}$  such that:

$$\bar{\mathbf{b}} = \llbracket \bar{\mathbf{u}}^e \rrbracket = \int_C \bar{\mathbf{U}}^e(\theta) \cdot d\bar{\mathbf{L}}(\theta) \quad (3.12)$$

where  $d\bar{\mathbf{L}}$  is the local tangent to  $C$ .  $C$  is referred to as the Burgers circuit and  $\bar{\mathbf{b}}$  as the Burgers vector of the dislocation ensemble. When determining  $\bar{\mathbf{b}}$  for an ensemble of dislocations under strong temperature gradients, attention must be given to the size of surface  $S$  and circuit  $C$ . Their sizes will determine whether  $\bar{\mathbf{b}}$  depends only on the local temperature  $\theta$ , i.e.  $\bar{\mathbf{b}} = \bar{\mathbf{b}}(\theta)$  or on the temperature distribution in the neighborhood within  $S$  (delimited by  $C$ ), i.e.  $\bar{\mathbf{b}} = \bar{\mathbf{b}}(\mathcal{J}(\theta))$ . The former and latter scenarios occur at length scales where dislocation dynamics models and polycrystalline plasticity models operate, respectively. Since we are concerned with the former case, the size of  $S$  has to be such that only one dislocation or a few dislocations traverse it and all quantities depend on local temperature  $\theta$ .

Next, using the Stokes' theorem in equation (3.12) we get

$$\bar{\mathbf{b}}(\theta) = \int_S \nabla \times \bar{\mathbf{U}}^e(\theta) \cdot \hat{\mathbf{n}} dS = \int_S \nabla \times \bar{\mathbf{U}}^{e\perp}(\theta) \cdot \hat{\mathbf{n}} dS, \quad (3.13)$$

where  $\hat{\mathbf{n}}$  is a unit normal to the surface  $S$ . Defining a pointwise continuous tensor field  $\bar{\boldsymbol{\alpha}}(\theta)$  as

$$\bar{\boldsymbol{\alpha}}(\theta) = \nabla \times \bar{\mathbf{U}}^e(\theta) = \nabla \times \bar{\mathbf{U}}^{e\perp}(\theta) \quad (3.14)$$

we get

$$\bar{\mathbf{b}}(\theta) = \int_S \bar{\boldsymbol{\alpha}}(\theta) \cdot \hat{\mathbf{n}} dS \quad (3.15)$$

$\bar{\boldsymbol{\alpha}}(\theta)$  is a continuous areal dislocation density field referred to as the Nye's dislocation density tensor (Nye, 1953). A non-zero  $\bar{\boldsymbol{\alpha}}(\theta)$  implies the presence of geometrically necessary dislocations. Note that in the theory of continuously represented dislocations, a non-zero  $\bar{\boldsymbol{\alpha}}(\theta)$  is sufficient to characterize a dislocation. However, when it comes to determining  $\bar{\mathbf{U}}^{e\perp}$  from  $\bar{\boldsymbol{\alpha}}(\theta)$ , equation (3.14) is insufficient because it does not ensure that  $\bar{\mathbf{U}}^{e\perp}$  is equal to zero in the absence of  $\bar{\boldsymbol{\alpha}}(\theta)$ , which should be the case since it is only the presence of dislocations that induces  $\bar{\mathbf{U}}^{e\perp}$ . Following Jiang (Jiang, 1998), equation (3.14) needs to be augmented with additional conditions,

$$\nabla \cdot \bar{\mathbf{U}}^{e\perp}(\theta) = 0 \quad \text{and} \quad \bar{\mathbf{U}}^{e\perp}(\theta) \cdot \hat{\mathbf{n}} = 0 \text{ on } \partial\mathcal{B} \quad (3.16)$$

In equation set (3.16), the latter condition is imposed on the surface  $\partial\mathcal{B}$  with unit normal  $\hat{\mathbf{n}}$  to ensure that its solution does not contain a gradient term. Taking curl of equation (3.14) we get

$$\nabla \times \bar{\boldsymbol{\alpha}}(\theta) = \nabla \times \nabla \times \bar{\mathbf{U}}^{e\perp}(\theta) = \nabla \left( \nabla \cdot \bar{\mathbf{U}}^{e\perp}(\theta) \right) - \nabla \cdot \nabla \bar{\mathbf{U}}^{e\perp}(\theta) \quad (3.17)$$

Using equation (3.16) we get,

$$\nabla \cdot \nabla \bar{\mathbf{U}}^{e\perp}(\theta) = -\nabla \times \bar{\boldsymbol{\alpha}}(\theta) \quad \text{and} \quad \bar{\mathbf{U}}^{e\perp}(\theta) \cdot \hat{\mathbf{n}} = 0 \text{ on } \partial\mathcal{B} \quad (3.18)$$

The left-hand side of equation (3.18) is a Poisson type equation whose solution for  $\bar{\mathbf{U}}^{e\perp}(\theta)$  under the given boundary condition vanishes when  $\bar{\boldsymbol{\alpha}}(\theta) = 0$ . Note that using the relationship (3.6) and (3.8), equations (3.14) and (3.18) can be reformulated as

$$\bar{\boldsymbol{\alpha}}(\theta) = -\nabla \times \bar{\mathbf{U}}^{in}(\theta) = -\nabla \times \bar{\mathbf{U}}^p(\theta) = -\nabla \times \bar{\mathbf{U}}^{p\perp}(\theta) \quad (3.19)$$

$$\nabla \cdot \nabla \bar{\mathbf{U}}^{p\perp}(\theta) = \nabla \times \bar{\boldsymbol{\alpha}}(\theta) \quad \text{and} \quad \bar{\mathbf{U}}^{p\perp}(\theta) \cdot \hat{\mathbf{n}} = 0 \text{ on } \partial\mathcal{B} \quad (3.20)$$

Following (3.19), we obtain the following condition,

$$\nabla \cdot \bar{\boldsymbol{\alpha}}(\theta) = 0, \quad (3.21)$$

which implies that dislocation lines do not originate or end in the bulk material.



Since we are interested in resolving individual dislocations, it is important to account for the crystallography of the material. Let  $\bar{\alpha}^\beta(\theta)$  define the field density of a single dislocation on slip system  $\beta$ . If this dislocation crosses a surface  $S$ , then from equation (3.15) we get the Burgers vector of this dislocation as:

$$\bar{\mathbf{b}}^\beta(\theta) = \int_S \bar{\alpha}^\beta(\theta) \cdot \hat{\mathbf{n}} dS \quad (3.22)$$

Let  $\bar{\mathbf{l}}^\beta$  define the local tangent to this dislocation line;  $\bar{\mathbf{l}}^\beta$  is also a function of  $\theta$ . The dislocation density tensor  $\bar{\alpha}^\beta(\theta)$  can also be written as:

$$\bar{\alpha}^\beta(\theta) = \frac{1}{V} \left( \bar{\mathbf{b}}^\beta(\theta) \otimes \bar{\mathbf{l}}^\beta(\theta) \right) \quad (3.23)$$

where  $V$  is a reference volume that should be chosen such that variations in  $\theta$  within this volume are negligible.

If there are multiple dislocations on the same slip system  $\beta$  that traverse  $S$ , then  $\bar{\mathbf{b}}^\beta(\theta)$  and  $\bar{\alpha}^\beta(\theta)$  determine the Burgers vector and dislocation density tensor, respectively, of the ensemble of these dislocations. If multiple dislocations from different slip systems traverse  $S$ , then the net local Burgers vector  $\bar{\mathbf{b}}(\theta) = \sum_{i=1}^N \bar{\mathbf{b}}^{\beta_i}(\theta) = \sum_{i=1}^N \int_S \bar{\alpha}^{\beta_i}(\theta) \cdot \hat{\mathbf{n}} dS = \int_S \left( \sum_{i=1}^N \bar{\alpha}^{\beta_i}(\theta) \right) \cdot \hat{\mathbf{n}} dS = \int_S \bar{\alpha}(\theta) \cdot \hat{\mathbf{n}} dS$ . Note here that this relationship is only valid for small  $S$ .

### 3.2 Kinematics

Let us now assume that  $\mathcal{B}$  is subjected to an elastic-plastic deformation under the action of some traction and/or displacement boundary conditions. Let us consider that a single dislocation (or multiple dislocations) on a slip system  $\beta$  traverses a material surface  $S$  bounded by a closed circuit  $C$ . Let  $\bar{\mathbf{f}}^\beta(\theta)$  be the flux field of these dislocations. It is a measure of the rate of inflow of dislocation lines into  $S$ , carrying along with them their corresponding Burgers vectors  $\bar{\mathbf{b}}^\beta(\theta)$  through a line element  $d\bar{\mathbf{x}}$  of circuit  $C$ . Let  $\bar{\mathbf{s}}^\beta(\theta)$  be the dislocation source term on slip system  $\beta$ . Then the conservation of Burgers' vector content requires respecting the following equation:

$$\frac{d\bar{\mathbf{b}}^\beta(\theta)}{dt} = \frac{d}{dt} \int_S \bar{\alpha}^\beta(\theta) \cdot \hat{\mathbf{n}} dS = \int_C \bar{\mathbf{f}}^\beta(\theta) \cdot d\bar{\mathbf{x}} + \int_S \bar{\mathbf{s}}^\beta(\theta) \cdot \hat{\mathbf{n}} dS \quad (3.24)$$

As mentioned in section 3.1, the surface  $S$  and circuit  $C$  are small such that along with  $\bar{\mathbf{b}}^\beta(\theta)$  and  $\bar{\alpha}^\beta(\theta)$ ,  $\int_C \bar{\mathbf{f}}^\beta(\theta) \cdot d\bar{\mathbf{x}}$  and  $\int_S \bar{\mathbf{s}}^\beta(\theta) \cdot \hat{\mathbf{n}} dS$  are also solely dependent on the local temperature  $\theta$ . From Stokes' theorem, the point-wise statement of equation (3.24) is given as

$$\dot{\bar{\alpha}}^\beta(\theta) = \nabla \times \bar{\mathbf{f}}^\beta(\theta) + \bar{\mathbf{s}}^\beta(\theta) \quad (3.25)$$

Let  $\bar{\mathbf{v}}^\beta(\theta)$  be the velocity of dislocations relative to the crystal. Then, the rate of inflow of Burgers vectors across a surface  $dS = \left| \bar{\mathbf{l}}^\beta(\theta) \times d\bar{\mathbf{x}}(\theta) \right|$  with unit normal  $\hat{\mathbf{n}} = \bar{\mathbf{l}}^\beta(\theta) \times d\bar{\mathbf{x}} / \left| \bar{\mathbf{l}}^\beta(\theta) \times d\bar{\mathbf{x}} \right|$  is  $\bar{\mathbf{f}}^\beta(\theta) \cdot d\bar{\mathbf{x}} = \frac{1}{V} (\bar{\mathbf{v}}^\beta(\theta) \cdot \hat{\mathbf{n}}) \bar{\mathbf{b}}^\beta(\theta) dS$ . After some algebra, we get  $\bar{\mathbf{f}}^\beta(\theta) = -\frac{1}{V} \bar{\mathbf{b}}^\beta(\theta) \otimes \bar{\mathbf{l}}^\beta(\theta) \times \bar{\mathbf{v}}^\beta(\theta) = -\bar{\alpha}^\beta(\theta) \times \bar{\mathbf{v}}^\beta(\theta)$ . Substituting this expression into equation (3.25) gives:

$$\dot{\bar{\alpha}}^\beta(\theta) = -\nabla \times \left( \bar{\alpha}^\beta(\theta) \times \bar{\mathbf{v}}^\beta(\theta) \right) + \bar{\mathbf{s}}^\beta(\theta) \quad (3.26)$$

Equation (3.26) is the transport equation for field dislocations. Let  $\bar{\bar{\mathbf{U}}}^{p,\beta}(\theta)$  define the slip distortion tensor resulting from dislocations on slip system  $\beta$ . Taking the time derivative of equation (3.19) and comparing with equation (3.26) gives:

$$\dot{\bar{\bar{\mathbf{U}}}}^{p,\beta}(\theta) = \bar{\bar{\boldsymbol{\alpha}}}^\beta(\theta) \times \bar{\mathbf{V}}^\beta(\theta), \quad (3.27)$$

which is unique up to a gradient term.

The net slip distortion tensor rate due to all the dislocations on all slip systems is given as:

$$\dot{\bar{\bar{\mathbf{U}}}}^p(\theta) = \sum_\beta \dot{\bar{\bar{\mathbf{U}}}}^{p,\beta}(\theta) = \sum_\beta \left( \bar{\bar{\boldsymbol{\alpha}}}^\beta(\theta) \times \bar{\mathbf{V}}^\beta(\theta) \right) \quad (3.28)$$

Due to the presence of the inelastic strain tensor  $\bar{\boldsymbol{\epsilon}}^\theta(\theta)$ , following equations (3.6), (3.8) and (3.11), the compatible part of the overall inelastic distortion  $\bar{\bar{\mathbf{U}}}^{in}(\theta)$  and the plastic distortion  $\bar{\bar{\mathbf{U}}}^p(\theta)$  are respectively redefined as:

$$\bar{\bar{\mathbf{U}}}^{in||}(\theta) = \bar{\bar{\mathbf{U}}}^{p||}(\theta) + \bar{\boldsymbol{\epsilon}}^\theta(\theta) \quad (3.29)$$

$$\bar{\bar{\mathbf{U}}}^p(\theta) = \bar{\bar{\mathbf{U}}}^{p||}(\theta) \quad (3.30)$$

Finally, if there is no dislocation motion relative to the crystal and no dislocations are generated, then the following condition should be satisfied:

$$\frac{d}{dt} \int_S \bar{\bar{\boldsymbol{\alpha}}}^\beta(\theta) \cdot \hat{\mathbf{n}} dS = 0 \quad (3.31)$$

for all surfaces  $S$  in  $\mathcal{B}$ .

### 3.3 Boundary conditions

For simplicity, in the following, the arguments of constitutive variables are presented only when it is necessary.

Let  $\mathcal{B}$  undergo the aforementioned elastic-plastic deformation under the action of evolving traction  $\bar{\mathbf{T}}$  on surface  $\partial\mathcal{B}_T$  and displacement  $\bar{\mathbf{u}}$  on surface  $\partial\mathcal{B}_d$ , and transient temperature changes under the action of heat flux  $\bar{\mathbf{q}}$  on surface  $\partial\mathcal{B}_q$  and evolving temperature  $\theta$  boundary conditions on surface  $\partial\mathcal{B}_\theta$ .

$$\bar{\mathbf{T}} = \bar{\boldsymbol{\sigma}} \cdot \hat{\mathbf{n}}, \forall \bar{\mathbf{x}} \in \partial\mathcal{B}_T \quad (3.32a)$$

$$\bar{\mathbf{u}} = \bar{\mathbf{u}}_d, \forall \bar{\mathbf{x}} \in \partial\mathcal{B}_d \quad (3.32b)$$

$$\bar{\mathbf{q}} = \bar{\mathbf{q}}_h, \forall \bar{\mathbf{x}} \in \partial\mathcal{B}_q \quad (3.32c)$$

$$\theta = \theta', \forall \bar{\mathbf{x}} \in \partial\mathcal{B}_\theta \quad (3.32d)$$

where  $\bar{\boldsymbol{\sigma}}$  is the symmetric Cauchy stress tensor. Note that  $\partial\mathcal{B}_T \cap \partial\mathcal{B}_d = \emptyset$  and  $\partial\mathcal{B}_q \cap \partial\mathcal{B}_\theta = \emptyset$  must be respected. However,  $\partial\mathcal{B}_T \cap \partial\mathcal{B}_q$ ,  $\partial\mathcal{B}_T \cap \partial\mathcal{B}_\theta$ ,  $\partial\mathcal{B}_d \cap \partial\mathcal{B}_q$  or  $\partial\mathcal{B}_d \cap \partial\mathcal{B}_\theta$  may not be empty sets.

### 3.4 Balance of linear momentum

Under the sudden application of a large  $\bar{\mathbf{q}}$  or  $\theta$  on  $\partial\mathcal{B}_q$  or  $\partial\mathcal{B}_\theta$  for a short duration of time, a large temperature gradient field is generated in the material that can result in very rapid changes in local momentum during this short interval in time. The displacements and strains nevertheless remain small. In such a case, we can write the local form of the balance of linear momentum as:

$$\rho \frac{d}{dt} \dot{\bar{\mathbf{u}}} = \nabla \cdot \bar{\boldsymbol{\sigma}} + \rho \bar{\mathbf{f}} \quad (3.33)$$

Note that  $\rho$ ,  $\bar{\mathbf{f}}$  and  $\bar{\boldsymbol{\sigma}}$  also depend on  $\theta$ . The term  $\frac{d}{dt} \dot{\mathbf{u}}$  can be rewritten as  $\frac{d}{dt} \dot{\mathbf{u}} = \frac{\partial \dot{\mathbf{u}}}{\partial t} + \dot{\mathbf{u}} \cdot \nabla \dot{\mathbf{u}}$ , where  $\frac{\partial}{\partial t}$  is the Eulerian derivative and  $\dot{\mathbf{u}} \cdot \nabla \dot{\mathbf{u}}$  is the convective derivative term. Under a small strain and small displacement assumption, we neglect the convective derivative term and use the Eulerian description. For simplicity, we shall denote  $\frac{\partial}{\partial t}$  with an overhead dot; note that the same is true for all the equations presented in section 3.2 and the equations that shall appear in the remainder of the article. Then, we have:

$$\rho \ddot{\mathbf{u}} = \nabla \cdot \bar{\boldsymbol{\sigma}} + \rho \bar{\mathbf{f}} \quad (3.34)$$

The left-hand side term in equation (3.34) importantly accounts for inertial effects.

### 3.5 Balance of energy

From the first law of thermodynamics, we obtain the following expression for the local form of the rate of change of internal energy density ( $u$ ):

$$\rho \dot{u} = -\nabla \cdot \bar{\mathbf{q}} + \bar{\boldsymbol{\sigma}} : \dot{\boldsymbol{\epsilon}}^m + \rho r \quad (3.35)$$

where  $\dot{\boldsymbol{\epsilon}}^m = \dot{\boldsymbol{\epsilon}}^e + \dot{\boldsymbol{\epsilon}}^p$  and  $\rho r$  is representative of internal heat sources, losses to the surroundings, etc. For example, heat loss due to plastic deformation via dislocation motion can be accounted for via  $\rho r$ . Note that the convective derivative of the internal energy is neglected in the small strain framework.

Assuming  $\dot{u} = c_v \dot{\theta}$  ( $c_v$  is the specific heat capacity at constant volume) and substituting it into equation (3.35), we get the following expression for the rate of change of temperature:

$$\rho c_v \dot{\theta} = -\nabla \cdot \bar{\mathbf{q}} + \bar{\boldsymbol{\sigma}} : \dot{\boldsymbol{\epsilon}}^m + \rho r \quad (3.36)$$

From the above equation, one can deduce that an elastic loading and/or plastic activity will result in local temperature evolution.

### 3.6 Thermo-mechanical dissipation (Second law of thermodynamics)

In order to obtain constitutive relationships for  $\bar{\mathbf{q}}$  and  $\bar{\boldsymbol{\sigma}}$  as well as the driving forces for slip-system dislocation velocities, we need to perform a dissipation analysis. Prior to doing that, we need to appropriately formulate our problem to be consistent with the second law of thermodynamics.

Thus far, the developments were performed under the assumption that there may exist any arbitrarily large temperature and/or stress gradients under the action of boundary conditions listed in equation set (3.32), which may evolve in time. We now impose that these gradients are large to the extent that the assumption of local thermodynamic equilibrium is respected at any given instant in time at every material point in  $\mathcal{B}$ . In other words, we assume that the time required for a material point to adjust to any thermal and/or mechanical changes occurring under the action of boundary conditions (3.31) is negligibly small in comparison to the timespan during which the boundary conditions evolve. Note that this condition does not impose that the overall system  $\mathcal{B}$  has to be in thermal equilibrium. However, the second basic tenet of an RT based model is that it applies the second law in the form of the classical Clausius-Kelvin-Planck inequality, which formulates the entropy change for a system undergoing an irreversible process that brings it from one *equilibrium state* A to another *equilibrium state* B such that:

$$\Delta S \geq \int_A^B \frac{\delta Q}{\theta} \quad (3.37)$$

where  $\Delta S$  is the entropy change in  $\mathcal{B}$ , and  $\delta Q$  is the path dependent heat exchanged between  $\mathcal{B}$  and its surroundings.

Since the total quantity of heat  $\delta Q$  results from the exchange with the surroundings through the boundaries and the presence of internal sources, equation (3.37) can be rewritten as:

$$\frac{d}{dt} \int_B \rho s dV \geq - \int_{\partial B} \frac{1}{\theta} \bar{\mathbf{q}} \cdot \hat{\mathbf{n}} dS + \int_B \rho \frac{r}{\theta} dV \quad (3.38)$$

where  $s$  is the specific entropy and  $\rho \frac{r}{\theta}$  corresponds to internal thermal sources of entropy. In local form, equation (3.38) can be written as:

$$\rho \dot{s} + \nabla \cdot \frac{\bar{\mathbf{q}}}{\theta} - \rho \frac{r}{\theta} \geq 0 \quad (3.39)$$

It is important to note that expression (3.39) is applicable only to those materials for which the entropy supply is given by  $\rho \frac{r}{\theta}$  and entropy flux by  $\frac{\bar{\mathbf{q}}}{\theta}$ . Next, eliminating  $r$  between equations (3.35) and (3.39) and introducing the Helmholtz free energy density as the Legendre transformation of  $u$  with respect to  $s$  as  $\psi = u - \theta s$ , we obtain:

$$-\rho(\dot{\psi} + s\dot{\theta}) + \bar{\boldsymbol{\sigma}} : \dot{\bar{\boldsymbol{\epsilon}}}^m - \frac{1}{\theta}(\bar{\mathbf{q}} \cdot \nabla \theta) \geq 0 \quad (3.40)$$

Inequality (3.40) is the Clausius-Duhem inequality for the thermo-elastic-plastic problem (Acharya and Shawki, 1996; Kratochvil and Dillon, 1969).

### 3.7 Free energy density and constitutive relationships

Let us assume that  $\psi = \hat{\psi}(\bar{\boldsymbol{\epsilon}}^e, \theta, \mathbf{a})$ , where  $\mathbf{a}$  is a set of all other possible dependent variables. Then, we have:

$$\dot{\psi} = \frac{\partial \psi}{\partial \bar{\boldsymbol{\epsilon}}^e} : \dot{\bar{\boldsymbol{\epsilon}}}^e + \frac{\partial \psi}{\partial \theta} : \dot{\theta} + \frac{\partial \psi}{\partial \mathbf{a}} \cdot \dot{\mathbf{a}} \quad (3.41)$$

where the dot in  $\frac{\partial \psi}{\partial \mathbf{a}} \cdot \dot{\mathbf{a}}$  represents appropriate number of inner products corresponding to the tensorial order of  $\mathbf{a}$ . Substituting equation (3.41) in (3.40) and rearranging terms gives:

$$-\left(\rho \frac{\partial \psi}{\partial \bar{\boldsymbol{\epsilon}}^e} - \bar{\boldsymbol{\sigma}}\right) : \dot{\bar{\boldsymbol{\epsilon}}}^e - \rho \left(\frac{\partial \psi}{\partial \theta} + s\right) : \dot{\theta} - \rho \frac{\partial \psi}{\partial \mathbf{a}} \cdot \dot{\mathbf{a}} + \bar{\boldsymbol{\sigma}} : \dot{\bar{\boldsymbol{\epsilon}}}^p - \frac{1}{\theta}(\bar{\mathbf{q}} \cdot \nabla \theta) \geq 0 \quad (3.42)$$

Equation (3.42) is linear in  $\dot{\bar{\boldsymbol{\epsilon}}}^e$ ,  $\dot{\theta}$  and  $\dot{\mathbf{a}}$ . Furthermore, since there exist body forces and energy supplies that ensure that the balance equations of momentum and energy are identically satisfied, these laws do not impose any constraints on  $\dot{\bar{\boldsymbol{\epsilon}}}^e$ ,  $\dot{\theta}$  and  $\dot{\mathbf{a}}$ . Hence, they can take arbitrarily prescribed values. Therefore, in order that the Clausius-Duhem inequality holds identically, it is necessary and sufficient that the coefficients of each of  $\dot{\bar{\boldsymbol{\epsilon}}}^e$ ,  $\dot{\theta}$  and  $\dot{\mathbf{a}}$  vanish individually. Consequently, we have:

$$\bar{\boldsymbol{\sigma}} = \rho \frac{\partial \psi}{\partial \bar{\boldsymbol{\epsilon}}^e} \quad (3.43)$$

$$s = -\frac{\partial \psi}{\partial \theta} \quad (3.44)$$

$$\frac{\partial \psi}{\partial \mathbf{a}} = 0 \quad (3.45)$$

From equation (3.45), we conclude that  $\psi$  is independent of  $\mathbf{a}$ , i.e.  $\psi = \hat{\psi}(\bar{\boldsymbol{\epsilon}}^e, \theta)$ . Now, from the definition of  $\bar{\boldsymbol{\epsilon}}^e = \bar{\boldsymbol{\epsilon}} - \bar{\boldsymbol{\epsilon}}^p - \bar{\boldsymbol{\epsilon}}^\theta$  from equation (3.7), we know that  $\bar{\boldsymbol{\epsilon}}^e$  also accounts for the contribution of  $\theta$ . Therefore, we can write  $\psi = \hat{\psi}(\bar{\boldsymbol{\epsilon}}^e(\theta))$ . This expression is physically appropriate since useful work can only be extracted from the stored elastic energy. Using the axiom of equipresence, we have  $\bar{\boldsymbol{\sigma}} = \hat{\boldsymbol{\sigma}}(\bar{\boldsymbol{\epsilon}}^e(\theta))$  and  $s = \hat{s}(\bar{\boldsymbol{\epsilon}}^e(\theta))$ .

$\psi$  must be equal to zero in the reference or undeformed state and positive in the deformed state. Furthermore, it should be independent of rigid body displacements. The simplest expression of  $\psi$  that satisfies these conditions is:

$$\psi = \frac{1}{2\rho} \bar{\bar{\bar{c}}}: \bar{\bar{\bar{c}}}: \bar{\bar{\bar{e}}}^e = \frac{1}{2\rho} (\bar{\bar{\bar{e}}} - \bar{\bar{\bar{e}}}^p): \bar{\bar{\bar{c}}}: (\bar{\bar{\bar{e}}} - \bar{\bar{\bar{e}}}^p) - \frac{\Delta\theta}{\rho} \bar{\bar{\beta}}: (\bar{\bar{\bar{e}}} - \bar{\bar{\bar{e}}}^p) + \frac{(\Delta\theta)^2}{2\rho} \bar{\bar{\beta}}: \bar{\bar{\gamma}} \quad (3.46)$$

where  $\bar{\bar{\bar{c}}}$  is the fourth order elastic stiffness tensor and  $\bar{\bar{\beta}} = \bar{\bar{\bar{c}}}: \bar{\bar{\gamma}}$  is the second order thermal moduli tensor. Note that all the material and kinematic variables are dependent on  $\theta$ . Next, from equations (3.43) and (3.44), we have the following constitutive laws

$$\bar{\bar{\sigma}} = \bar{\bar{\bar{c}}}: \bar{\bar{\bar{e}}}^e = \bar{\bar{\bar{c}}}: (\bar{\bar{\bar{e}}} - \bar{\bar{\bar{e}}}^p) - \bar{\bar{\beta}} \Delta\theta \quad (3.47)$$

$$s = \frac{1}{\rho} \bar{\bar{\beta}}: \bar{\bar{\bar{e}}}^e = \frac{1}{\rho} (\bar{\bar{\bar{e}}} - \bar{\bar{\bar{e}}}^p): \bar{\bar{\beta}} - \frac{\Delta\theta}{\rho} \bar{\bar{\beta}}: \bar{\bar{\gamma}} \quad (3.48)$$

Equation (3.47) is the well-known Neumann-Duhamel's equation in thermoelasticity which reduces to the 3D Hooke's law under isothermal conditions at the reference temperature. Note here that unlike conventional thermoelasticity, however,  $\bar{\bar{\bar{e}}}^e$  contains contributions of  $\bar{\bar{\bar{e}}}^{e\perp}$  (from within the dislocation core) in addition to  $\bar{\bar{\bar{e}}}^{e\parallel}$ .

Note that while equations (3.46) – (3.48) satisfy the constraints on the free energy density and Clausius-Duhem inequality, they are not unique. Furthermore,  $\bar{\bar{\beta}}(\theta)$  and  $c$  should be such that equation (3.48) satisfies the local form of the Clausius-Kelvin-Planck inequality (3.39) at each time step everywhere in  $\mathcal{B}$ .

Now, using equations (3.43) – (3.45), inequality (3.42) reduces to the local dissipation inequality:

$$d = \bar{\bar{\sigma}}: \dot{\bar{\bar{\bar{e}}}}^p - \frac{1}{\theta} (\bar{\bar{q}} \cdot \nabla \bar{\theta}) \geq 0 \quad (3.49)$$

which gives the global thermo-mechanical dissipation rate  $D$ :

$$D = \int_B \bar{\bar{\sigma}}: \dot{\bar{\bar{\bar{e}}}}^p dV - \int_B \frac{1}{\theta} (\bar{\bar{q}} \cdot \nabla \bar{\theta}) dV \geq 0 \quad (3.50)$$

In order to derive the driving forces for dislocations, similar to the work of (Acharya, 2003), we shall work with the *global* thermo-mechanical dissipation. While the Clausius-Duhem inequality imposes that  $\bar{\bar{\sigma}}$ , through  $\psi$ , is independent of any other variables besides  $\bar{\bar{\bar{e}}}^e$  and  $\theta$ , it does not impose this on  $\dot{\bar{\bar{\bar{e}}}}^p$  and  $\bar{\bar{q}}$ . The only constraint that this inequality imposes on  $\dot{\bar{\bar{\bar{e}}}}^p$  and  $\bar{\bar{q}}$  is that they require to independently satisfy  $\int_B \bar{\bar{\sigma}}: \dot{\bar{\bar{\bar{e}}}}^p dV \geq 0$  and  $\int_B \frac{1}{\theta} (\bar{\bar{q}} \cdot \nabla \bar{\theta}) dV \leq 0$ , everywhere in the domain at any given instant in time. There are infinite possible expressions for  $\dot{\bar{\bar{\bar{e}}}}^p$  and  $\bar{\bar{q}}$  that can respectively satisfy  $\int_B \bar{\bar{\sigma}}: \dot{\bar{\bar{\bar{e}}}}^p dV \geq 0$  and  $\int_B \frac{1}{\theta} (\bar{\bar{q}} \cdot \nabla \bar{\theta}) dV \leq 0$ . For simplicity, we shall assume that  $\dot{\bar{\bar{\bar{e}}}}^p = \widehat{\dot{\bar{\bar{\bar{e}}}}^p}(\bar{\bar{\sigma}}, \theta)$  and  $\bar{\bar{q}} = \widehat{\bar{q}}(\bar{\bar{\bar{e}}}^e, \theta, \nabla \bar{\theta})$ .

Focusing on the first part of the dissipation inequality (3.50), it is well-known that  $\dot{\bar{\bar{\bar{e}}}}^p$  is non-linearly dependent on  $\bar{\bar{\sigma}}$  and  $\theta$ . While the Clausius-Duhem inequality would allow dependence on additional variables, for the present purposes, the dependence on  $\bar{\bar{\sigma}}$  and  $\theta$  is sufficient. In section 4, however, while discussing the possibility of up-scaling the T-FDM model, the importance and justification of considering additional dependent terms for  $\dot{\bar{\bar{\bar{e}}}}^p$  is presented.

Note that due to the symmetry of the Cauchy stress tensor, we have  $\int_B \bar{\bar{\sigma}}: \dot{\bar{\bar{\bar{e}}}}^p dV = \int_B \bar{\bar{\sigma}}: \dot{\bar{\bar{U}}}^p dV \geq 0$ , which needs to be respected at every material point. If we neglect the dislocation source term, then after some manipulation using the relationships presented in section 2 and using equation (3.27), we have:

$$\int_B \bar{\bar{\sigma}}: \dot{\bar{\bar{U}}}^p dV = \int_B \bar{\bar{\sigma}}: \dot{\bar{\bar{U}}}^p dV = \int_B \sum_{\beta} (\bar{\bar{\sigma}} \cdot \bar{\bar{\alpha}}^{\beta}): \bar{\bar{X}} \cdot \bar{\bar{V}}^{\beta} dV = \int_B \sum_{\beta} \bar{\bar{F}}^{\beta} \cdot \bar{\bar{V}}^{\beta} dV \geq 0 \quad (3.51)$$

where  $\bar{\bar{F}}^{\beta} = (\bar{\bar{\sigma}} \cdot \bar{\bar{\alpha}}^{\beta}): \bar{\bar{X}}$  is the driving force for motion of dislocation(s) on slip system  $\beta$ . Note that the relationship  $\int_B \bar{\bar{\sigma}}: \dot{\bar{\bar{U}}}^p dV = \int_B \bar{\bar{\sigma}}: \dot{\bar{\bar{U}}}^p dV$  uses equations (2.2) and (2.3), which require working with the

global dissipation inequality (3.50) and not the local dissipation inequality (3.49). Recalling that  $\bar{\alpha}^\beta = \bar{\mathbf{b}}^\beta \otimes \bar{\mathbf{l}}^\beta$ , we can rewrite  $\bar{\mathbf{F}}^\beta$  as:

$$\bar{\mathbf{F}}^\beta = \widehat{\bar{\mathbf{F}}}^\beta(\bar{\boldsymbol{\sigma}}, \theta) = (\bar{\boldsymbol{\sigma}} \cdot \bar{\mathbf{b}}^\beta) \times \bar{\mathbf{l}}^\beta \quad (3.52)$$

Equation (3.52) is the well-known Peach-Koehler force used in dislocation dynamics simulations as the driving force for dislocation motion.  $\bar{\boldsymbol{\sigma}}$  includes the stress contribution of not only the dislocation self-stress as well as contributions coming from boundary conditions and other dislocations and/or defects, but also the contribution of thermal stresses. In order to ensure that inequality (3.50) is respected under all circumstances, it is necessary that  $\bar{\mathbf{F}}^\beta \cdot \bar{\mathbf{V}}^\beta \geq 0$  for each slip system  $\beta$  at every material point. The simplest way to ensure this is to assume a linear relationship between  $\bar{\mathbf{F}}^\beta$  and  $\bar{\mathbf{V}}^\beta$ :

$$\bar{\mathbf{V}}^\beta = \frac{1}{B^\beta} \bar{\mathbf{F}}^\beta \quad (3.53)$$

where  $B^\beta > 0$  is a material parameter which also depends on  $\bar{\boldsymbol{\sigma}}$  and  $\theta$  (Olmsted et al., 2005).

If  $\hat{\mathbf{n}}^\beta$  is the unit normal to the slip plane of the slip system  $\beta$ , then the glide  $F_g^\beta$ , climb  $F_c^\beta$  and the normal to glide and climb  $F_n^\beta$  components of  $\bar{\mathbf{F}}^\beta$  are:

$$F_g^\beta(\bar{\boldsymbol{\sigma}}, \theta) = \bar{\mathbf{F}}^\beta(\bar{\boldsymbol{\sigma}}, \theta) \cdot \frac{(\hat{\mathbf{n}}^\beta \times \bar{\mathbf{l}}^\beta)}{|\hat{\mathbf{n}}^\beta \times \bar{\mathbf{l}}^\beta|} \quad (3.54a)$$

$$F_c^\beta(\bar{\boldsymbol{\sigma}}, \theta) = \bar{\mathbf{F}}^\beta(\bar{\boldsymbol{\sigma}}, \theta) \cdot \hat{\mathbf{n}}^\beta \quad (3.54b)$$

$$F_n^\beta(\bar{\boldsymbol{\sigma}}, \theta) = \bar{\mathbf{F}}^\beta(\bar{\boldsymbol{\sigma}}, \theta) \cdot \frac{\bar{\mathbf{l}}^\beta}{|\bar{\mathbf{l}}^\beta|} \quad (3.54c)$$

Note that equations (3.54a), (3.54b) and (3.54c) account for both edge and screw dislocations.

Focusing now on the second part of the dissipation inequality (3.50), i.e.  $-\int_B \frac{1}{\theta} (\bar{\mathbf{q}} \cdot \nabla \theta) dV \geq 0$ , the simplest relationship between  $\bar{\mathbf{q}}$  and  $\nabla \theta$  that satisfies this inequality over the entire volume as well as each material point individually is the generalized Fourier law for heat conduction:

$$\bar{\mathbf{q}}(\theta, \nabla \theta, \bar{\boldsymbol{\varepsilon}}^e) = -\bar{\mathbf{K}}(\theta, \bar{\boldsymbol{\varepsilon}}^e) \cdot \nabla \theta \quad (3.55)$$

with the condition that the symmetric part of  $\bar{\mathbf{K}}$  is a positive definite tensor. Note that in the generalized Fourier law,  $\bar{\mathbf{K}}$  is dependent on both  $\theta$  and elastic strain  $\bar{\boldsymbol{\varepsilon}}^e$ .

Finally, from equations (3.55) and (3.36), we have:

$$\rho c_v \dot{\theta} = \nabla \cdot (\bar{\mathbf{K}}(\theta, \bar{\boldsymbol{\varepsilon}}^e) \cdot \nabla \theta) + \bar{\boldsymbol{\sigma}} : \dot{\bar{\boldsymbol{\varepsilon}}^e} + \bar{\boldsymbol{\sigma}} : \dot{\bar{\mathbf{U}}^p} + \rho r \quad (3.56)$$

Note here that equation (3.56) is expressed in the local form and hence the term  $\bar{\boldsymbol{\sigma}} : \dot{\bar{\mathbf{U}}^p}$  does not simply reduce to  $\sum_\beta \bar{\mathbf{F}}^\beta \cdot \bar{\mathbf{V}}^\beta$ .

### 3.8 Equation set for the geometrically linear T-FDM model

The final set of field equations of the geometrically linear T-FDM problem are:

$$\begin{aligned} -\nabla \times \bar{\mathbf{U}}^p &= \bar{\boldsymbol{\alpha}} \\ \bar{\mathbf{U}}^{p\parallel} &= \bar{\mathbf{U}}^{p\parallel} \\ \dot{\bar{\boldsymbol{\alpha}}}^\beta &= -\nabla \times (\bar{\boldsymbol{\alpha}}^\beta \times \bar{\mathbf{V}}^\beta) + \bar{\mathbf{s}}^\beta \quad \text{and} \quad \bar{\boldsymbol{\alpha}} = \sum_\beta \bar{\boldsymbol{\alpha}}^\beta \end{aligned}$$

$$\begin{aligned}
\dot{\bar{\mathbf{U}}}^p &= \sum_{\beta} (\bar{\boldsymbol{\alpha}}^{\beta} \times \bar{\mathbf{V}}^{\beta}) \\
\bar{\boldsymbol{\varepsilon}}^e &= \text{sym}(\bar{\mathbf{U}}^e) = \text{sym}(\bar{\mathbf{U}} - \bar{\mathbf{U}}^{in}) = \text{sym}(\bar{\mathbf{U}} - \bar{\mathbf{U}}^p) - \bar{\boldsymbol{\varepsilon}}^{\theta} \\
\bar{\boldsymbol{\varepsilon}}^{\theta} &= \bar{\boldsymbol{\gamma}} \Delta \theta \\
\bar{\boldsymbol{\sigma}} &= \bar{\mathbf{c}} : \bar{\boldsymbol{\varepsilon}}^e = \bar{\mathbf{c}} : (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) - \bar{\boldsymbol{\beta}} \Delta \theta \\
\bar{\mathbf{q}} &= -\bar{\mathbf{K}} \cdot \nabla \theta \\
\bar{\mathbf{V}}^{\beta} &= \frac{1}{B^{\beta}} \bar{\mathbf{F}}^{\beta} = \frac{1}{B^{\beta}} (\bar{\boldsymbol{\sigma}} \cdot \bar{\mathbf{b}}^{\beta}) \times \bar{\mathbf{l}}^{\beta} \\
\rho \ddot{\mathbf{u}} &= \nabla \cdot \bar{\boldsymbol{\sigma}} + \rho \bar{\mathbf{f}} \\
\rho c_v \dot{\theta} &= \nabla \cdot (\bar{\mathbf{K}} \cdot \nabla \theta) + \bar{\boldsymbol{\sigma}} : \dot{\bar{\boldsymbol{\varepsilon}}}^e + \bar{\boldsymbol{\sigma}} : \dot{\bar{\mathbf{U}}}^p + \rho r
\end{aligned} \tag{3.57}$$

### 3.9 Special cases of the T-FDM model

#### 3.9.1 FDM at reference temperature

In the case of an isothermal and adiabatic system at reference temperature, equation set (3.57) reduces to those of the geometrically linear FDM model.

$$\begin{aligned}
-\nabla \times \bar{\mathbf{U}}^p &= \bar{\boldsymbol{\alpha}} \\
\bar{\mathbf{U}}^{p\parallel} &= \bar{\mathbf{U}}^{p\parallel} \\
\dot{\bar{\boldsymbol{\alpha}}}^{\beta} &= -\nabla \times (\bar{\boldsymbol{\alpha}}^{\beta} \times \bar{\mathbf{V}}^{\beta}) + \bar{\mathbf{s}}^{\beta} \quad \text{and} \quad \bar{\boldsymbol{\alpha}} = \sum_{\beta} \bar{\boldsymbol{\alpha}}^{\beta} \\
\dot{\bar{\mathbf{U}}}^p &= \sum_{\beta} (\bar{\boldsymbol{\alpha}}^{\beta} \times \bar{\mathbf{V}}^{\beta}) \\
\bar{\boldsymbol{\varepsilon}}^e &= \text{sym}(\bar{\mathbf{U}}^e) = \text{sym}(\bar{\mathbf{U}} - \bar{\mathbf{U}}^{in}) = \text{sym}(\bar{\mathbf{U}} - \bar{\mathbf{U}}^p) \\
\bar{\boldsymbol{\sigma}} &= \bar{\mathbf{c}} : \bar{\boldsymbol{\varepsilon}}^e = \bar{\mathbf{c}} : (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) \\
\bar{\mathbf{V}}^{\beta} &= \frac{1}{B^{\beta}} \bar{\mathbf{F}}^{\beta} = \frac{1}{B^{\beta}} (\bar{\boldsymbol{\sigma}} \cdot \bar{\mathbf{b}}^{\beta}) \times \bar{\mathbf{l}}^{\beta} \\
\nabla \cdot \bar{\boldsymbol{\sigma}} + \rho \bar{\mathbf{f}} &= \rho \ddot{\mathbf{u}}
\end{aligned} \tag{3.58}$$

#### 3.9.2 FDM with thermoelasticity

In the case of an isothermal and adiabatic system at an arbitrary temperature, equation set (3.57) reduces to those of the geometrically linear FDM model with a thermoelastic.

$$\begin{aligned}
-\nabla \times \bar{\mathbf{U}}^p &= \bar{\boldsymbol{\alpha}} \\
\bar{\mathbf{U}}^{p\parallel} &= \bar{\mathbf{U}}^{p\parallel} \\
\dot{\bar{\boldsymbol{\alpha}}}^{\beta} &= -\nabla \times (\bar{\boldsymbol{\alpha}}^{\beta} \times \bar{\mathbf{V}}^{\beta}) + \bar{\mathbf{s}}^{\beta} \quad \text{and} \quad \bar{\boldsymbol{\alpha}} = \sum_{\beta} \bar{\boldsymbol{\alpha}}^{\beta} \\
\dot{\bar{\mathbf{U}}}^p &= \sum_{\beta} (\bar{\boldsymbol{\alpha}}^{\beta} \times \bar{\mathbf{V}}^{\beta}) \\
\bar{\boldsymbol{\varepsilon}}^e &= \text{sym}(\bar{\mathbf{U}}^e) = \text{sym}(\bar{\mathbf{U}} - \bar{\mathbf{U}}^{in}) = \text{sym}(\bar{\mathbf{U}} - \bar{\mathbf{U}}^p) - \bar{\boldsymbol{\varepsilon}}^{\theta} \\
\bar{\boldsymbol{\varepsilon}}^{\theta} &= \bar{\boldsymbol{\gamma}} \Delta \theta \\
\bar{\boldsymbol{\sigma}} &= \bar{\mathbf{c}} : \bar{\boldsymbol{\varepsilon}}^e = \bar{\mathbf{c}} : (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) - \bar{\boldsymbol{\beta}} \Delta \theta \\
\bar{\mathbf{V}}^{\beta} &= \frac{1}{B^{\beta}} \bar{\mathbf{F}}^{\beta} = \frac{1}{B^{\beta}} (\bar{\boldsymbol{\sigma}} \cdot \bar{\mathbf{b}}^{\beta}) \times \bar{\mathbf{l}}^{\beta} \\
\nabla \cdot \bar{\boldsymbol{\sigma}} + \rho \bar{\mathbf{f}} &= \rho \ddot{\mathbf{u}}
\end{aligned} \tag{3.59}$$

#### 3.9.3 Thermoelasticity: no dislocations

In case of a system without dislocations, equation set (3.57) reduces to the problem of thermoelasticity:

$$\begin{aligned}
\bar{\boldsymbol{\varepsilon}}^{e\parallel} &= \text{sym}(\bar{\mathbf{U}}^{e\parallel}) = \text{sym}(\bar{\mathbf{U}}) - \bar{\boldsymbol{\varepsilon}}^\theta \\
\bar{\boldsymbol{\varepsilon}}^\theta &= \bar{\boldsymbol{\gamma}}\Delta\theta \\
\bar{\boldsymbol{\sigma}} &= \bar{\mathbb{c}}:\bar{\boldsymbol{\varepsilon}}^{e\parallel} = \bar{\mathbb{c}}:\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\beta}}\Delta\theta \\
\boldsymbol{\nabla} \cdot \bar{\boldsymbol{\sigma}} + \rho\bar{\mathbf{f}} &= \rho\bar{\ddot{\mathbf{u}}} \\
\bar{\mathbf{q}} &= -\bar{\mathbf{K}} \cdot \bar{\boldsymbol{\nabla}}\theta \\
\rho c_v \dot{\theta} &= \boldsymbol{\nabla} \cdot (\bar{\mathbf{K}} \cdot \bar{\boldsymbol{\nabla}}\theta) + \bar{\boldsymbol{\sigma}}:\bar{\boldsymbol{\varepsilon}}^{e\parallel} + \rho r
\end{aligned} \tag{3.60}$$

#### 3.9.4 Stationary T-FDM

In case of a stationary system with steady-state heat conduction, equation set (3.57) reduces to:

$$\begin{aligned}
-\boldsymbol{\nabla} \times \bar{\mathbf{U}}^p &= \bar{\boldsymbol{\alpha}} \\
\bar{\mathbf{U}}^{p\parallel} &= \bar{\mathbf{U}}^{p\parallel} \\
\bar{\boldsymbol{\varepsilon}}^e &= \text{sym}(\bar{\mathbf{U}}^e) = \text{sym}(\bar{\mathbf{U}} - \bar{\mathbf{U}}^{in}) = \text{sym}(\bar{\mathbf{U}} - \bar{\mathbf{U}}^p) - \bar{\boldsymbol{\varepsilon}}^\theta \\
\bar{\boldsymbol{\varepsilon}}^\theta &= \bar{\boldsymbol{\gamma}}\Delta\theta \\
\bar{\boldsymbol{\sigma}} &= \bar{\mathbb{c}}:\bar{\boldsymbol{\varepsilon}}^e = \bar{\mathbb{c}}:(\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) - \bar{\boldsymbol{\beta}}\Delta\theta \\
\bar{\mathbf{q}} &= -\bar{\mathbf{K}} \cdot \bar{\boldsymbol{\nabla}}\theta \\
\boldsymbol{\nabla} \cdot \bar{\boldsymbol{\sigma}} + \rho\bar{\mathbf{f}} &= 0 \\
\rho c_v \dot{\theta} &= \boldsymbol{\nabla} \cdot (\bar{\mathbf{K}} \cdot \bar{\boldsymbol{\nabla}}\theta)
\end{aligned} \tag{3.61}$$

## 4. Discussion

### 4.1 Implications of the adopted thermodynamics framework

#### 4.1.1 Local thermodynamic equilibrium and the Clausius-Kelvin-Planck inequality under large thermal gradients

Similar to many continuum-based dislocation mechanics models, thermodynamic considerations in the T-FDM model are based on the principles of rational thermodynamics (RT), which is the most commonly used non-equilibrium thermodynamics framework in continuum mechanics. RT is based on the principles of rational mechanics, which itself derives motivation from classical irreversible thermodynamics (Lebon et al., 2008).

At the core of all RT based models is the assumption of local thermodynamic equilibrium. Since the T-FDM model is designed to study dislocation dynamics under large transient temperature gradients, such as those occurring due to solid-state thermal cycling during additive manufacturing, it is crucial to verify that local thermodynamic equilibrium is always respected under such conditions. Typically, the highest temperature rates occurring at a material point in a heat affected solid during an additive manufacturing process are of the order of  $10^6 \text{ K/s}$ , i.e.  $10^{-6} \text{ K/picosecond}$ . Atomic fluctuations that accommodate thermal changes typically do so in timespans of  $10^{-2} - 1 \text{ picoseconds}$ . Therefore, we can safely assume that even for the highest temperature rates occurring during additive manufacturing, thermal changes are instantaneously accommodated via atomic fluctuations in comparison to the timespan in which boundary conditions change. In other words, thermal equilibrium can be assumed to exist at each material point in the system at any given instant in time. Furthermore, the thermal stresses generated (if any) due to the temperature gradients are also equilibrated rapidly resulting in a mechanical equilibrium at each material point. For current purposes, we assume that under such large temperature changes, a material point does not have sufficient time to change its chemical configuration, thus maintaining chemical equilibrium;



chemical changes due to temperature changes shall be addressed in a future work. The combined effect of these considerations is that for a system subjected to  $10^6$  K/s temperature rates, local thermodynamic equilibrium can be assumed everywhere in the system at any given instant in time.

The second important governing principle in RT based models is the Clausius-Kelvin-Planck formulation of the second law of thermodynamics as described via inequality (3.37), which leads to the Clausius-Duhem inequality (3.40). The Clausius-Kelvin-Planck inequality and the local thermodynamic equilibrium conditions impose an upper limit on the magnitudes of transient temperature gradients that can be induced under the action of temperature and heat flux boundary conditions. In order that local thermodynamic equilibrium holds, each material point in the system should be able to adjust to the induced thermal and mechanical changes in a timespan that is negligibly small in comparison to the timespan over which the boundary conditions evolve. Indeed, this will be the case when T-FDM is applied to study dislocation dynamics due to solid-state thermal cycling during additive manufacturing.

However, there is a drawback in using the classical Clausius-Kelvin-Planck inequality. The inherent assumption associated with this inequality is that during an irreversible process, the *entire* system changes from an *equilibrium state* A to another *equilibrium state* B resulting in a non-negative entropy change. In our case, at any given time step, the entire system is neither in thermal equilibrium nor mechanical equilibrium. Nevertheless, this inequality is used for the convenience of straightforwardly deriving dislocation driving forces using the properties of the Stokes-Helmholtz decomposition from equations (2.2) and (2.3); note that in the original FDM model (Acharya, 2003), this inequality was also applied at the level of the entire system.

#### 4.1.2 Definition of temperature

As noted by Lebon et al. (Lebon et al., 2008), in most RT based dislocation mechanics models, entropy and temperature are taken as primitive undefined entities whose physical meaning is often unclear. In fact, during the development of the T-FDM model, an empirical temperature scale was not defined but it was assumed to exist. While an undefined temperature is not a significant cause for concern under isothermal and adiabatic conditions, it can no longer be ignored when considering significant temperature changes.

In section 4.1.1, we argued that local thermodynamic equilibrium was admissible for the range of problems that will be tackled by the T-FDM model. Based on this assumption, we can use the equilibrium definition of absolute temperature. This requires redefining the dependent variables for entropy  $s$ . From equations (3.43), (3.44) and (3.45), we can construct the following differential expression for  $\psi$

$$d\psi = -sd\theta + \frac{1}{\rho} \bar{\sigma} : d\bar{\epsilon}^e \quad (4.1)$$

Using its Legendre transform  $\psi = u - \theta s$ , equation (4.1) can also be written as

$$ds = \frac{1}{\theta} du - \frac{1}{\rho\theta} \bar{\sigma} : d\bar{\epsilon}^e \quad (4.2)$$

Equation (4.2) is the Gibbs equation for our thermo-elasto-plastic problem, which also implies that  $s = \hat{s}(\bar{\epsilon}^e, u)$ . Then, we get the following definition of  $\theta$ :

$$\frac{1}{\theta} = \left. \frac{\partial s}{\partial u} \right|_{\bar{\epsilon}^e} = \text{constant} \quad (4.3)$$

In order for the above definition of temperature to be valid in thermal equilibrium, it is necessary to augment the above equation as follows:

$$\frac{1}{\theta} = \left. \frac{\partial s}{\partial u} \right|_{\bar{\epsilon}^e = \text{constant}, \bar{q}=0} = \frac{1}{T} \quad (4.4)$$

where  $T$  is the equilibrium measure of  $\theta$ .

Next, we test its validity for the range of applications of the T-FDM model. At the beginning of section 4.1.1, we also argued that when local thermodynamic equilibrium prevails, the temperature distribution is uniform within a subdomain volume represented by a material point of our system. In other words, there are no temperature gradients present within the subdomain even though there may be strong temperature gradients present in the entire system. Then, from the Fourier law of heat conduction equation (3.55), we can straightforwardly assume that  $\bar{\mathbf{q}} = 0$  at each material point. Therefore, we can use the equilibrium definition of temperature equation (4.2) for the range of applicability of the T-FDM model.

#### 4.1.3 Additional contributions to entropy

While the existence of entropy as a state function has been proven (Coleman et al., 1981; Coleman and Owen, 1974; Serrin, 1979), however, there is no consensus on its unambiguous definition. An expression for entropy is often obtained from an assumed expression for the free energy potential; for example, see expression (3.48) and its derivation. However, any such expression for entropy is non-unique. In fact, there are infinite different expressions of entropy that can satisfy the Clausius-Duhem inequality (Coleman et al., 1981; Meixner, 1973). This can also be viewed as an advantage in the sense that we can account for additional contributions to entropy that are overlooked in the classical formulation.

The classical formulation of entropy change is related to the heat exchanged between the system and its surroundings. However, there exist entropic contributions that do not necessarily require adhering to the classical definition. One such example is the configurational entropy associated with dislocation structures. In statistical mechanics, configurational entropy is the portion of a system's entropy related to the number of ways in which the constituents of a system can spatially arrange themselves. Until recently, its contribution to dislocation mechanics had been neglected with the argument that compared to other contributions to a system's entropy, the contribution of the configurational entropy of dislocations is negligible (Cottrell, 1953). However, Langar et al. (Langer et al., 2010) argued that the contribution of configurational entropy of dislocations is small with respect to the total entropy of a large system, it nevertheless forms an essential ingredient in a theory of dislocation-mediated deformation. Its inclusion should be in such a way that the equations of motion for a system that contains millions of "irregularly" moving dislocations must take the system towards states of higher probability. Then, in cases when ordinary thermal fluctuations are irrelevant, configurational entropy of dislocations must be a non-decreasing function of time.

At the length scales where dislocation dynamics models operate, configurational entropy of dislocations should have a significant contribution to the overall entropy of the system. Furthermore, under isothermal and adiabatic conditions, the configurational entropy of dislocations will also be a non-decreasing function of time. Interestingly, in the presence of a heat flux, the configurational entropy of dislocations may be a decreasing function of time, however, the combined dislocation and thermal entropies must be a non-decreasing function of time.

In its current form, the proposed RT based formulation of the T-FDM model is unable to account for the configurational entropy of dislocations. The main reason behind this inability is the use of the classical Clausius-Kelvin-Planck inequality (3.37). To highlight this shortcoming, consider the rate form of the Gibbs equation (4.2) and substitute  $\dot{u}$  from equation (3.35):

$$\dot{s} = -\frac{1}{\rho} \nabla \cdot \frac{\bar{\mathbf{q}}}{\theta} + \frac{1}{\rho\theta} \bar{\boldsymbol{\sigma}} : \dot{\bar{\boldsymbol{\epsilon}}}^p + \frac{r}{\theta} \quad (4.5)$$

From equation (4.5), it is clear that the dislocation configurational entropy change appears neither in the first two terms on the right-hand side nor in the term  $\frac{r}{\theta}$ , which is related to entropic changes due to internal heat losses.

In order to account for configurational entropy of dislocations, we need to augment the list of dependent variables for entropy with internal variables that provide an appropriate measure for dislocation configuration. However, since we know that entropy is a state variable, care must be taken that the new internal variable is also a state quantity. Bearing these constraints in mind, we can use the areal dislocation density tensor  $\bar{\alpha}^\beta$ , which is a measure of geometrically necessary dislocations, as a dependent variable for  $s$  such that  $s = \hat{s}(\bar{\epsilon}^e, u, \bar{\alpha}^\beta)$ . However, the Clausius-Duhem inequality imposes that  $s = -\frac{\partial\psi}{\partial\theta}$  and the only way to ensure that  $s = -\frac{\partial\psi}{\partial\theta}$  is respected is to use the axiom of equipresence and introduce  $\bar{\alpha}^\beta$  as a dependent variable of  $\psi$  such that  $\psi = \hat{\psi}(\bar{\epsilon}^e, \theta, \bar{\alpha}^\beta)$ . However, from equation (3.45), we know that  $\psi$  is independent of all other variables except  $\bar{\epsilon}^e$  and  $\theta$ . If, however, we were to insist on a dependence of  $\psi$  on  $\bar{\alpha}^\beta$ , then we would require introducing a term involving  $\bar{\alpha}^\beta$  and its work-conjugate in the rate of change of local internal energy equation (3.35). This additional term would then require to be introduced as additional work done on the boundaries of the system, which in turn would require prescribing auxiliary boundary conditions involving  $\bar{\alpha}^\beta$  and its work conjugate. Such non-conventional boundary conditions often appear in strain gradient plasticity models, for example, in the work of Gurtin (Gurtin, 2002, 2000).

Forest and Amestoy (Forest and Amestoy, 2008) explored an interesting approach to account for higher order gradients of essential thermodynamic variables within an RT based framework. They introduced entropy and its gradient as internal state variables in their constitutive formulation and proposed quadratic expressions for the internal energy density as a function of entropy and its gradient. Then, from the resulting Clausius-Duhem inequality, they showed that the free energy density was also dependent on the gradient of entropy. Meanwhile, Acharya (Acharya, 2011) derived an expression for entropy from a statistical mechanics standpoint and correlated it to the continuum measure of entropy formulated within an RT based framework.

#### 4.1.4 Constitutive relationships from dissipative formulation

We were able to derive two temperature dependent constitutive relationships from the Clausius-Duhem inequality (3.50): (i) a linear relationship (3.53) between dislocation driving forces and velocity, and (ii) the generalized Fourier law for heat conduction equation (3.55).

Although equation (3.53) respects the dissipation condition that  $\bar{\mathbf{F}}^\beta \cdot \bar{\mathbf{V}}^\beta \geq 0$ , it does not account for lattice resistance to dislocation motion. Consequently, with this expression of the dislocation velocity, mobile dislocations would begin to move under any arbitrarily small applied force. However, even under isothermal conditions, dislocation motion is restricted by local strength of the material, which can arise from factors such as energetic barriers due to crystallography (for instance, climb at low temperatures), solid solute particles, precipitates, etc. Bearing these conditions in mind, it is important to develop more advanced relationships for  $\bar{\mathbf{V}}^\beta$  while ensuring that  $\bar{\mathbf{F}}^\beta \cdot \bar{\mathbf{V}}^\beta \geq 0$  is respected. To that end, we first split the dislocation velocity into components along the glide, climb and normal to the glide and climb directions, such that  $\bar{\mathbf{V}}^\beta = V_g^\beta \hat{e}_g + V_c^\beta \hat{e}_c + V_n^\beta \hat{e}_n$ . Then, we introduce the lattice resistances along each of these directions  $\chi_g^\beta > 0$ ,  $\chi_c^\beta > 0$  and  $\chi_n^\beta > 0$ , such that we can construct the lattice resistance vector  $\bar{\chi}^\beta = \chi_g^\beta \hat{e}_g + \chi_c^\beta \hat{e}_c + \chi_n^\beta \hat{e}_n$ ;  $\hat{e}_g = \frac{(\hat{n}^\beta \times \bar{\mathbf{l}}^\beta)}{|\hat{n}^\beta \times \bar{\mathbf{l}}^\beta|}$ ,  $\hat{e}_c = \hat{n}^\beta$  and  $\hat{e}_n = \frac{\bar{\mathbf{l}}^\beta}{|\bar{\mathbf{l}}^\beta|}$ . We will continue to assume a linear relationship between  $\bar{\mathbf{F}}^\beta$  and  $\bar{\mathbf{V}}^\beta$ . Then, while respecting  $\bar{\mathbf{F}}^\beta \cdot \bar{\mathbf{V}}^\beta \geq 0$ , we can write the following expression for the velocity:

$$V_i^\beta = \frac{1}{B^\beta} \left( |F_i^\beta| - X_i^\beta \right) H \left( |F_i^\beta| - X_i^\beta \right) \text{sgn} \left( F_i^\beta \right) \hat{e}_i, \quad i = g, c \text{ or } n \quad (4.6)$$

where  $H(x)$  is the Heaviside step function and  $\hat{e}_i$  is a unit vector along direction  $i$ . Note that relationship (4.6) is obtained from dissipation considerations. It does not explicitly include inertial terms related to dislocation motion but these will play a role on dislocation velocity through its dependence on  $\bar{\sigma}$  (via  $\bar{F}^\beta$ ), which is governed by the momentum balance equation (3.34).

In the generalized Fourier law of heat conduction equation (3.55), heat conductivity  $\bar{K}$  has a dependence on  $\bar{\epsilon}^e$ . Note that dependence or independence of  $\bar{K}$  on  $\bar{\epsilon}^e$  are both permitted by the Clausius-Duhem inequality as long as  $-\frac{1}{\theta}(\bar{q} \cdot \nabla\theta) \geq 0$  is satisfied. We need to identify which is physically justified for the desired application of the T-FDM model, i.e. to study dislocation dynamics during additive manufacturing.

Let us consider a cube-shaped perfect single crystal being subjected to a temperature  $T_H$  on a face with normal  $\hat{n}$  and  $T_L (< T_H)$  on the face with normal  $-\hat{n}$ . For the purposes of this exercise, we shall assume that the faces whose normal vectors are perpendicular to  $\hat{n}$  are subjected to zero heat flux boundary condition. For simplicity, we shall assume that the cube is mechanically unconstrained on its boundaries and body forces are negligible. Next, we suppose that a half plane of atoms is suddenly removed from our perfect single crystal. We let the system relax until a steady-state temperature distribution has been re-attained under the action of original temperature boundary conditions. Then, how does the temperature distribution in a perfect single crystal under a steady-state compare with the temperature distribution in the presence of a dislocation after steady-state has been re-attained, under the action of the same boundary conditions? It is reasonable to expect that based on the thermodynamic considerations of the T-FDM model, whether the distributions are the same or not depends on whether  $\bar{K}$  is independent or dependent on  $\bar{\epsilon}^e$ .

The dependence of  $\bar{K}$  on strains has been observed experimentally (Murphy et al., 2014; Zou et al., 2002). In-situ Raman piezothermography experiments performed by Murphy et al. (Murphy et al., 2014) revealed that spatially uniform tensile strain affects phonon behavior, which in turn affects the heat capacity. Experiments performed by Zou et al. (Zou et al., 2002) on GaN films showed that higher dislocation number densities ( $> 10^{14}/m^2$ ) reduces the room temperature thermal conductivity. Dislocation densities greater than  $10^{14}/m^2$  are rather easily obtained in additively manufactured materials, and it may be important to consider the role of  $\bar{\epsilon}^e$  on  $\bar{K}$  to account for the role of dislocations on temperature distribution in the body.

## 4.2 Future work

### 4.2.1 Extension to a finite strain framework

Finite strain formulations for both the FDM approach (Acharya, 2004, 2001) and the thermo-elastic-plastic problem (Simo and Miehe, 1992) have already been proposed. The logical approach to develop a finite strain T-FDM model would be to combine the existing finite strain formulations of the two approaches.

### 4.2.2 Numerical implementation and application

The interdependence of  $\bar{\sigma}$ ,  $\bar{U}^p$  and  $\theta$  makes it a practical necessity to solve the T-FDM problem using a numerical approach. Stable variational formulations have been developed for both the thermo-elastic-plastic (Yang et al., 2006) and the FDM approaches (Roy and Acharya, 2005). Furthermore, the FDM model was numerically implemented via a combined Galerkin-Least squares approach to solve the dislocation transport equation and a least square finite element approach to solve the remaining equations of the FDM problem (Roy and Acharya, 2005; Varadhan et al., 2006). These developments can guide the creation of a stable T-FDM variational model and its finite element implementation.

More recently, a fast Fourier transform approach was used by Berbenni and co-workers (Berbenni et al., 2014; Djaka et al., 2017, 2015) to solve the static and dynamic FDM problem. The widely used

Radix-2 FFT algorithm, originally proposed by (Cooley and Tukey, 1965), has a computational cost of  $O(N \log_2 N)$ , which is much lower than the computational cost of an optimized finite element approach  $O(N^2)$ ;  $N$  is the number of material points. Furthermore, the FFT approach uses a structured grid without meshing, which can take microstructure input directly from electron and x-ray synchrotron experiments. However, a drawback of the conventional FFT approach is that it requires applying periodic and non-standard boundary conditions.

#### 4.2.3 Up-scaling the T-FDM model

An important motivation for developing a thermo-mechanical dislocation dynamics model based on the FDM theory was to exploit the straightforward scalability of the FDM model while respecting the thermodynamic considerations that were used to formulate the governing equations (Acharya and Roy, 2006). Acharya and Roy have shown that the governing equations of FDM remain nearly the same after performing a spatial and temporal up-scaling from the microscale, i.e. at the level of individual dislocations, to the meso-scale, at the level where crystal plasticity models operate. The mesoscale FDM model is known as the PhenoMenological FDM (PMFDM) model (Acharya and Roy, 2006; Roy and Acharya, 2006). An important difference between the FDM and the PMFDM models is that the dislocation transport equation in the latter model accounts for the contribution of statistical ensemble dislocations that have a net zero areal dislocation density ( $\bar{\alpha} = 0$ ) but a non-zero dislocation number density. This consideration allows a direct connection with the plastic distortion rate  $\bar{L}^p$  in conventional crystal plasticity approaches. Performing a similar spatial and temporal averaging of the T-FDM governing equations, however, is not as straightforward as in the case of the FDM model.

Acharya and Roy (Acharya and Roy, 2006) employed a weighted, spatial and temporal, running average to compute the up-scaled measures of microscale fields. If  $\mathbf{f}(\bar{\mathbf{x}}, t)$  is any microscale tensorial field, then its mesoscopic space-time-averaged field  $\underline{\mathbf{f}}(\bar{\mathbf{x}}, t)$  is given as follows:

$$\underline{\mathbf{f}}(\bar{\mathbf{x}}, t) = \frac{1}{\int_{I(t)} \int_{\Omega(\bar{\mathbf{x}})} w(\bar{\mathbf{x}} - \bar{\mathbf{x}}', t - t') d\bar{\mathbf{x}}' dt'} \int_t \int_{\mathcal{B}} w(\bar{\mathbf{x}} - \bar{\mathbf{x}}', t - t') \mathbf{f}(\bar{\mathbf{x}}', t') d\bar{\mathbf{x}}' dt' \quad (4.7)$$

where  $\mathcal{B}$  is our considered system,  $\mathcal{t}$  is some sufficiently large time interval,  $\Omega(\bar{\mathbf{x}})$  is a boundary region within  $\mathcal{B}$  around the point  $\bar{\mathbf{x}}$  with linear dimension of the order of the spatial resolution of the desired mesoscale model, and  $I(t)$  is a bounded interval in  $\mathcal{t}$  containing  $t$ . The weighting function  $w$  is non-dimensional, smooth in  $\bar{\mathbf{x}}$ ,  $\bar{\mathbf{x}}'$ ,  $t$  and  $t'$ , and for fixed  $\bar{\mathbf{x}}$  and  $t$ , they are non-zero only in  $\Omega(\bar{\mathbf{x}}) \times I(t)$  when viewed as a function of  $(\bar{\mathbf{x}}', t')$ . Acharya and Roy applied (4.7) to each side of all equations in the set (3.58) with a crucial assumption that the elastic moduli are spatially uniform and noted, as discussed above, that most equations retained their form in the PMFDM framework.

In T-FDM, we allow for strong temperature rates and gradients in a microscopic body  $\mathcal{B}$  that is represented by a material point at the mesoscale. Within the domains  $\Omega(\bar{\mathbf{x}})$  and  $\mathcal{B}$  we deal with a heterogeneous distribution of  $\theta$ , which evolves heterogeneously in the intervals  $\mathcal{t}$  and  $I(t)$ . Consequently, we have spatial and temporal variations in material properties, including the elastic moduli, as well as kinematic quantities, which makes it impossible to apply equation (4.7) to these quantities and recover them in the same form at the mesoscale. From a mesoscale perspective, at a material point, the application of local thermodynamic equilibrium and the definition of temperature as an equilibrium measure in equation (4.3) becomes questionable. Furthermore, at the mesoscale, a weighted running average of the temperature over  $\mathcal{B}$  and  $\mathcal{t}$  may not be sufficient to understand the evolution of different quantities; we will have to consider the entire distribution of  $\theta(\bar{\mathbf{x}}', t')$ . In other words, a rigorous treatment of the thermo-mechanical problem will require considering non-local and memory effects on the evolution of meso-scale thermodynamic quantities. In RT based approaches, this is typically done by accounting for gradients of

essential thermodynamic variables and their temporal evolutions; for example,  $\overline{\nabla\theta}$  and its time derivative can be used in the constitutive framework. However, as discussed in section 3.7, the Clausius-Duhem inequality imposes that  $\psi$ , and hence,  $\overline{\sigma}$  and  $\overline{\epsilon}^e$  are independent of  $\overline{\nabla\theta}$ , but the mesoscale  $\overline{\sigma}$  and  $\overline{\epsilon}^e$  may depend on  $\overline{\nabla\theta}$  simply because the microscale  $\overline{\epsilon}$  and  $\overline{\epsilon}^e$  depends on local temperature. Interestingly, as remarked in section 3.7, the Clausius-Duhem inequality does not impose that  $\overline{\epsilon}^p$  is independent of  $\overline{\nabla\theta}$ . For a mesoscale material point representing a microscale domain having non-negligible temperature gradients, it is physically justified to have  $\overline{\epsilon}^p$  depend on  $\overline{\nabla\theta}$ . Nevertheless, since an RT based framework doesn't allow  $\overline{\sigma}$  to depend on  $\overline{\nabla\theta}$ , it may become necessary to adopt a different thermodynamics framework.

#### 4.2.4 Restructuring T-FDM in an internal variable thermodynamics (IVT) framework

In section 4.1.1, we noted that the main shortcoming of the proposed thermodynamic framework is the use of the classical Clausius-Kelvin-Planck form of the second law on a body that clearly transitions from one non-equilibrium state to another. In section 4.1.3, we noted that within an RT based framework, accounting for additional contributions to entropy requires imposing auxiliary boundary conditions. For example, accounting for the configurational entropy of dislocations requires imposing auxiliary boundary conditions involving  $\overline{\alpha}^\beta$  and its work conjugate. In most practical loading scenarios, except perhaps nanoindentation and similar nano-scale loadings, it is difficult to justify using a dislocation density boundary condition along with traction/displacement boundary conditions. In section 4.2.3, we noted that up-scaling of the T-FDM model would introduce a dependence of  $\overline{\nabla\theta}$  on spatially averaged  $\overline{\sigma}$  and  $\overline{\epsilon}^e$ . However, such a dependence is not allowed by the Clausius-Duhem inequality (3.40).

It may be possible to overcome these shortcomings by reconstructing the model within an IVT framework (Coleman and Gurtin, 1967; Mandel, 1978; Maugin, 1999; Rice, 1971). In IVT, the local equilibrium hypothesis is replaced by the accompanying state axiom (Lebon et al., 2008). According to this axiom, each non-equilibrium state has a corresponding accompanying equilibrium state, and every irreversible process has an accompanying reversible process. The accompanying equilibrium state is a fictitious one whose state space is formed by the union of the independent spaces of standard equilibrium variables and internal variables. The entire set of accompanying state variables can be obtained via the Gedanken approach where a body in a non-equilibrium state is assumed to be suddenly surrounded an adiabatic rigid enclosure that does not allow exchanging heat or work with the surroundings. The body is then assumed to relax to an equilibrium state. Due to the adiabatic rigid enclosure, the internal energy of the body remains the same. It is also assumed that the kinematic quantities and internal variables remain unchanged. An accompanying reversible process takes the relaxed system from one equilibrium state to another. However, in contrast to a true reversible process occurring at infinitesimal velocity, the accompanying reversible process occurs at finite velocity and results in a non-zero entropy production (Lebon et al., 2008). The main difference between the local equilibrium hypothesis and the accompanying state axiom is that in the former case non-equilibrium entropy and temperature are assumed to be the same as their equilibrium counterparts, whereas in the latter case non-equilibrium entropy and temperature are different from their equilibrium counterparts.

The term ‘‘internal variable’’ encompasses those quantities that are measurable but not controllable via externally applied forces. Consequently, they do not participate in mechanical work and therefore they do not appear explicitly in the balance equations of mass, momentum and energy; this avoids using auxiliary boundary conditions such as  $\overline{\alpha}^\beta$  and its work conjugate. However, internal variables appear in the entropy and free energy formulations. Typically, internal variables evolve locally with time via their own evolution equations. With respect to the theory of field dislocations,  $\overline{\alpha}^\beta$  qualifies as an internal variable; it evolves via the transport equation (3.26).

In IVT, instead of the Clausius-Kelvin-Planck formulation, the starting point for the second law formulation is the Gibbs equation in the accompanying equilibrium state (Lebon et al., 2008). If we assume  $s$  to depend on  $\bar{\mathbf{e}}^e, u$  and  $\bar{\boldsymbol{\alpha}}^\beta$  such that  $s = \hat{s}(\bar{\mathbf{e}}^e, u, \bar{\boldsymbol{\alpha}}^\beta)$ , then the rate form of the Gibbs equation can be written as:

$$\dot{s} = \frac{1}{\theta} \dot{u} - \frac{1}{\rho\theta} \bar{\boldsymbol{\sigma}}' : \dot{\bar{\mathbf{e}}}^e + \frac{1}{\rho\theta} \sum_{\beta} \bar{\boldsymbol{\xi}}^\beta : \dot{\bar{\boldsymbol{\alpha}}}^\beta \quad (4.8)$$

where  $\frac{1}{\theta} = \frac{\partial s}{\partial u}$ ,  $\frac{\bar{\boldsymbol{\sigma}}'}{\rho\theta} = -\frac{\partial s}{\partial \bar{\mathbf{e}}^e}$ , and  $\frac{\bar{\boldsymbol{\xi}}^\beta}{\rho\theta} = \frac{\partial s}{\partial \bar{\boldsymbol{\alpha}}^\beta}$ . In general,  $\bar{\boldsymbol{\sigma}}' = -\theta\rho \frac{\partial s}{\partial \bar{\mathbf{e}}^e}$  is the stress tensor in the accompanying equilibrium state and it is different from  $\bar{\boldsymbol{\sigma}} = \rho \frac{\partial \psi}{\partial \bar{\mathbf{e}}^e}$ , which is the stress tensor in the original non-equilibrium state. If, however, the process is sufficiently slow such that equilibrium is rapidly achieved at any given instant in time, then we may assume  $\bar{\boldsymbol{\sigma}}' = \bar{\boldsymbol{\sigma}}$  (Kestin and Bataille, 1980; Lebon et al., 2008). If we make this assumption and keep equation (3.35) for  $\dot{u}$  without the term  $\rho r$ , then after eliminating  $\dot{u}$  from this equation and using equation (3.51) we have:

$$\dot{s} + \frac{1}{\rho} \bar{\boldsymbol{\nabla}} \cdot \left( \frac{\bar{\mathbf{q}}}{\theta} \right) = \bar{\mathbf{q}} \cdot \bar{\boldsymbol{\nabla}} \theta^{-1} + \frac{1}{\rho\theta} \bar{\boldsymbol{\sigma}} : \dot{\bar{\mathbf{e}}}^p + \frac{1}{\rho\theta} \sum_{\beta} \bar{\boldsymbol{\xi}}^\beta : \dot{\bar{\boldsymbol{\alpha}}}^\beta \quad (4.9)$$

The right-hand side of equation (4.9) can be defined as the entropy production rate  $\sigma^s$ , which has to satisfy the condition:

$$\sigma^s = \bar{\mathbf{q}} \cdot \bar{\boldsymbol{\nabla}} \theta^{-1} + \frac{1}{\rho\theta} \bar{\boldsymbol{\sigma}} : \dot{\bar{\mathbf{e}}}^p + \frac{1}{\rho\theta} \sum_{\beta} \bar{\boldsymbol{\xi}}^\beta : \dot{\bar{\boldsymbol{\alpha}}}^\beta \geq 0 \quad (4.10)$$

Now, recalling the definition of the Helmholtz free energy density as  $\psi = u - \theta s$ , we can obtain the following expression from equations (3.35) without  $\rho r$  and (4.8):

$$\dot{\psi} = -s\dot{\theta} + \frac{1}{\rho} \bar{\boldsymbol{\sigma}} : \dot{\bar{\mathbf{e}}}^e - \frac{1}{\rho} \sum_{\beta} \bar{\boldsymbol{\xi}}^\beta : \dot{\bar{\boldsymbol{\alpha}}}^\beta \quad (4.11)$$

Equation (4.10) shows that  $\psi = \hat{\psi}(\bar{\mathbf{e}}^e, \theta, \bar{\boldsymbol{\alpha}}^\beta)$  is not an assumption but a derivation based on the rate form of the Gibbs equation (4.9) and the rate of change of internal energy density (3.35). From this equation, we can deduce that similar to equations (3.43) and (3.44),  $\bar{\boldsymbol{\sigma}} = \rho \frac{\partial \psi}{\partial \bar{\mathbf{e}}^e}$  and  $s = -\frac{\partial \psi}{\partial \theta}$ . In addition, and importantly, we have  $\bar{\boldsymbol{\xi}}^\beta = -\rho \frac{\partial \psi}{\partial \bar{\boldsymbol{\alpha}}^\beta} = \rho\theta \frac{\partial s}{\partial \bar{\boldsymbol{\alpha}}^\beta}$ . Using these definitions, we can formulate an expression for the free energy density functional similar to expression (3.46), however, with additional terms involving  $\bar{\boldsymbol{\alpha}}^\beta$  and without the need to introduce additional boundary conditions. Note that from equations (4.8) – (4.11) and (3.35), we obtain the Clausius-Duhem inequality of equation (3.40), albeit with a sign change on the last term:

$$-\rho(\dot{\psi} + s\dot{\theta}) + \bar{\boldsymbol{\sigma}} : \dot{\bar{\mathbf{e}}}^m + \frac{1}{\theta} (\bar{\mathbf{q}} \cdot \bar{\boldsymbol{\nabla}} \theta) \geq 0 \quad (4.12)$$

Adopting IVT is also advantageous for developing theoretical frameworks of a variety of physio-chemical models, for instance, when coupling T-FDM with a phase-field approach for evolution of chemical heterogeneities. Finally, since we are interested in deriving the dislocation driving forces straightforwardly from thermodynamic considerations, it could be interesting to use the properties of the Stokes-Helmholtz decomposition on the accompanying equilibrium state to avoid using the classical Clausius-Kelvin-Planck inequality on a body that transitions irreversibly from one non-equilibrium state to another. These developments will be undertaken in a future work.

## 5. Summary and conclusions

In this work, a strong coupling between the field dislocations mechanics (FDM) model (Acharya, 2003, 2001) and the heat conduction problem is proposed to obtain the T-FDM (thermal-FDM) model. The proposed model operates at the length scale where we can isolate individual dislocations. The main motivation for developing this model was to study dislocation interactions with other defects and dislocation structure evolution in heat-affected crystalline solids during an additive manufacturing process. However, the T-FDM model is applicable to study the dynamics of individual dislocations and/or their ensemble under any permissible combination of displacement, traction, temperature and heat flux boundary conditions.

Similar to most continuum-based dislocation mechanics models, the T-FDM modeling framework is based on the main governing principles of RT (rational thermodynamics): local thermodynamic equilibrium and the classical Clausius-Kelvin-Planck formulation of the second law of thermodynamics applied on the entire system. Kinematic relationships are inherited from the FDM model, which uses the Stokes-Helmholtz decomposition into compatible and incompatible fields to uniquely obtain the elastic/plastic distortion from a prescribed areal dislocation density tensor. At the length scale at which the T-FDM model operates, all kinematic quantities are dependent on local temperature. Temperature dependent constitutive relationships are derived from the global dissipation and local free energy considerations. Exploiting the properties of the Stokes-Helmholtz decomposition within the global dissipation formulation naturally lead us to obtain temperature dependent crystallographic dislocation driving forces. The global dissipation also imposes restrictions on the free energy formulation, which gives us constitutive relationships for Cauchy stress and entropy as a function of elastic strains and temperature that are similar to those obtained in thermoelastic problems.

The consequences of the thermodynamic modeling framework are critically analyzed. The assumption of local thermodynamic equilibrium is found to be respected even during very high temperature rates such as those occurring during an additive manufacturing process; the equilibrium definition of temperature is sufficient for such applications. Attempts to account for the contributions of additional state variables to entropy, such as the configurational entropy of dislocations, suggests that the proposed model should be restructured within a thermodynamic framework that is different from RT; the analysis strongly suggests adopting the internal variable thermodynamics (IVT) framework.

## 6. References

- Acharya, A., 2011. Microcanonical Entropy and Mesoscale Dislocation Mechanics and Plasticity. *J Elast* 104, 23–44. <https://doi.org/10.1007/s10659-011-9328-3>
- Acharya, A., 2004. Constitutive analysis of finite deformation field dislocation mechanics. *Journal of the Mechanics and Physics of Solids* 52, 301–316. [https://doi.org/10.1016/S0022-5096\(03\)00093-0](https://doi.org/10.1016/S0022-5096(03)00093-0)
- Acharya, A., 2003. Driving forces and boundary conditions in continuum dislocation mechanics. *Proceedings of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences* 459, 1343–1363. <https://doi.org/10.1098/rspa.2002.1095>
- Acharya, A., 2001. A model of crystal plasticity based on the theory of continuously distributed dislocations. *Journal of the Mechanics and Physics of Solids* 49, 761–784. [https://doi.org/10.1016/S0022-5096\(00\)00060-0](https://doi.org/10.1016/S0022-5096(00)00060-0)
- Acharya, A., Roy, A., 2006. Size Effects and Idealized Dislocation Microstructure at Small Scales: Predictions of a Phenomenological Model of Mesoscopic Field Dislocation Mechanics: Part I. *Journal of the Physics and Mechanics of Solids* 54, 1687–1710. <https://doi.org/10.1016/j.jmps.2006.01.009>
- Acharya, A., Shawki, T.G., 1996. The Clausius-Duhem Inequality and the structure of rate-independent plasticity. *International Journal of Plasticity* 12, 229–238. [https://doi.org/10.1016/S0749-6419\(96\)00005-8](https://doi.org/10.1016/S0749-6419(96)00005-8)



- Berbenni, S., Taupin, V., Djaka, K.S., Fressengeas, C., 2014. A Numerical Spectral Approach for Solving Elasto-Static Field Dislocation and G-Disclination Mechanics. *International Journal of Solids and Structures*.
- Bilby, B.A., Bullough, R., Smith, E., 1955. Continuous Distributions of Dislocations: A new Application of the Methods of Non-Riemannian Geometry. *Proceedings of the Royal Society of London: Series A, Mathematical and physical sciences* 231, 263–273.
- Coleman, B.D., 1964. Thermodynamics of materials with memory. *Arch. Rational Mech. Anal.* 17, 1–46. <https://doi.org/10.1007/BF00283864>
- Coleman, B.D., Gurtin, M.E., 1967. Thermodynamics with Internal State Variables. *J. Chem. Phys.* 47, 597–613. <https://doi.org/10.1063/1.1711937>
- Coleman, B.D., Noll, W., 1960. An approximation theorem for functionals, with applications in continuum mechanics. *Arch. Rational Mech. Anal.* 6, 355–370. <https://doi.org/10.1007/BF00276168>
- Coleman, B.D., Owen, D.R., 1975. On thermodynamics and elastic-plastic materials. *Arch. Rational Mech. Anal.* 59, 25–51. <https://doi.org/10.1007/BF00281515>
- Coleman, B.D., Owen, D.R., 1974. A mathematical foundation for thermodynamics. *Arch. Rational Mech. Anal.* 54, 1–104. <https://doi.org/10.1007/BF00251256>
- Coleman, B.D., Owen, D.R., Serrin, J., 1981. The second law of thermodynamics for systems with approximate cycles. *Arch. Rational Mech. Anal.* 77, 103–142. <https://doi.org/10.1007/BF00250620>
- Cooley, J.W., Tukey, J.W., 1965. An algorithm for the machine calculation of complex Fourier series. *Math. Comp.* 19, 297–301. <https://doi.org/10.1090/S0025-5718-1965-0178586-1>
- Cottrell, A.H., 1953. *Dislocations and plastic flow in crystals*. Oxford University Press, New York.
- Djaka, K.S., Taupin, V., Berbenni, S., Fressengeas, C., 2015. A numerical spectral approach to solve the dislocation density transport equation. *Modelling Simul. Mater. Sci. Eng.* 23, 065008. <https://doi.org/10.1088/0965-0393/23/6/065008>
- Djaka, K.S., Villani, A., Taupin, V., Capolungo, L., Berbenni, S., 2017. Field Dislocation Mechanics for heterogeneous elastic materials: A numerical spectral approach. *Computer Methods in Applied Mechanics and Engineering* 315, 921–942. <https://doi.org/10.1016/j.cma.2016.11.036>
- Eshelby, J.D., Peierls, R.E., 1957. The determination of the elastic field of an ellipsoidal inclusion, and related problems. *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences* 241, 376–396. <https://doi.org/10.1098/rspa.1957.0133>
- Forest, S., 2008. Some links between Cosserat, strain gradient crystal plasticity and the statistical theory of dislocations. *Philosophical Magazine* 88, 3549–3563.
- Forest, S., Amestoy, M., 2008. Hypertemperature in thermoelastic solids. *Comptes Rendus Mécanique* 336, 347–353. <https://doi.org/10.1016/j.crme.2008.01.007>
- Fox, N., 1966. A Continuum Theory of Dislocations for Single Crystals. *IMA J Appl Math* 2, 285–298. <https://doi.org/10.1093/imamat/2.4.285>
- Ghoniem, N.M., Tong, S.-H., Sun, L.Z., 2000. Parametric dislocation dynamics: A thermodynamics-based approach to investigations of mesoscopic plastic deformation. *Phys. Rev. B* 61, 913–927. <https://doi.org/10.1103/PhysRevB.61.913>
- Gurtin, M.E., 2002. A gradient theory of single-crystal viscoplasticity that accounts for geometrically necessary dislocations. *Journal of the Mechanics and Physics of Solids* 50, 5–32. [https://doi.org/10.1016/S0022-5096\(01\)00104-1](https://doi.org/10.1016/S0022-5096(01)00104-1)
- Gurtin, M.E., 2000. On the plasticity of single crystals: free energy, microforces, plastic-strain gradients. *Journal of the Mechanics and Physics of Solids* 48, 989–1036. [https://doi.org/10.1016/S0022-5096\(99\)00059-9](https://doi.org/10.1016/S0022-5096(99)00059-9)
- Gurtin, M.E., 1968. On the thermodynamics of materials with memory. *Arch. Rational Mech. Anal.* 28, 40–50. <https://doi.org/10.1007/BF00281562>

- Jiang, B., 1998. *The Least-Squares Finite Element Method: Theory and Applications in Computational Fluid Dynamics and Electromagnetics*, Scientific Computation. Springer-Verlag, Berlin Heidelberg. <https://doi.org/10.1007/978-3-662-03740-9>
- Kestin, J., Bataille, J., 1980. Thermodynamics of solids, in: *Proc. 3rd International Symposium on Continuum Models of Discrete Systems (Freudenstadt)*, (Edited by E. Kroner and K. H. Anthony). University of Waterloo press, Ontario, pp. 99–147.
- Kosevich, A.M., 1979. Crystal dislocations and the theory of elasticity, in: *Dislocations in Solids*, Nabarro, F. R. N. (Editor). North Holland Publishing Company, Amsterdam, pp. 33–141.
- Kratochvil, J., Dillon, O.W., 1969. Thermodynamics of Elastic-Plastic Materials as a Theory with Internal State Variables. *Journal of Applied Physics* 40, 3207–3218. <https://doi.org/10.1063/1.1658167>
- Kröner, E., 1981. Continuum theory of defects, in: *Physics of Defects*. North-Holland Publ. Co., Amsterdam, pp. 217–315.
- Kröner, E., 1958. Kontinuumstheorie der versetzungen und eigenspannungen. *Ergebnisse der Angewandten Mathematik* 5, 1–179.
- Langer, J.S., Bouchbinder, E., Lookman, T., 2010. Thermodynamic theory of dislocation-mediated plasticity. *Acta Materialia* 58, 3718–3732. <https://doi.org/10.1016/j.actamat.2010.03.009>
- Lebon, G., Jou, D., Casas-Vázquez, J., 2008. *Understanding Non-equilibrium Thermodynamics: Foundations, Applications, Frontiers*. Springer-Verlag, Berlin Heidelberg. <https://doi.org/10.1007/978-3-540-74252-4>
- Mandel, J., 1978. *Propriétés mécaniques des matériaux: rhéologie, plasticité*. Eyrolles, Paris.
- Maugin, G.A., 1999. *The Thermomechanics of Nonlinear Irreversible Behaviors: An Introduction*, World Scientific Series on Nonlinear Science Series A. World Scientific Publishing Co. Pte. Ltd., Singapore.
- Meixner, J., 1973. The entropy problem in thermodynamics of processes. *Rheol Acta* 12, 465–467. <https://doi.org/10.1007/BF01503000>
- Mura, T., 1963. Continuous Distribution of Moving Dislocations. *Philosophical Magazine* 8, 843–857.
- Murphy, K.F., Piccione, B., Zanjani, M.B., Lukes, J.R., Gianola, D.S., 2014. Strain- and Defect-Mediated Thermal Conductivity in Silicon Nanowires. *Nano Lett.* 14, 3785–3792. <https://doi.org/10.1021/nl500840d>
- Nye, J.F., 1953. Some geometrical relations in dislocated crystals. *Acta Metallurgica* 1, 153–162. [https://doi.org/10.1016/0001-6160\(53\)90054-6](https://doi.org/10.1016/0001-6160(53)90054-6)
- Olmsted, D.L., Hector Jr, L.G., Curtin, W.A., Clifton, R.J., 2005. Atomistic simulations of dislocation mobility in Al, Ni and Al/Mg alloys. *Modelling Simul. Mater. Sci. Eng.* 13, 371–388. <https://doi.org/10.1088/0965-0393/13/3/007>
- Rice, J.R., 1971. Inelastic constitutive relations for solids: An internal-variable theory and its application to metal plasticity. *Journal of the Mechanics and Physics of Solids* 19, 433–455. [https://doi.org/10.1016/0022-5096\(71\)90010-X](https://doi.org/10.1016/0022-5096(71)90010-X)
- Roy, A., Acharya, A., 2006. Size Effects and Idealized Dislocation Microstructure at Small Scales: Predictions of a Phenomenological Model of Mesoscopic Field Dislocation Mechanics: Part II. *Journal of the Physics and Mechanics of Solids* 54, 1711–1743. <https://doi.org/10.1016/j.jmps.2006.01.012>
- Roy, A., Acharya, A., 2005. Finite Element Approximation of Field Dislocation Mechanics. *Journal of the Mechanics and Physics of Solids* 53, 143–170.
- Salençon, J., 2001. *Handbook of Continuum Mechanics: General Concepts Thermoelasticity*. Springer-Verlag, Berlin Heidelberg. <https://doi.org/10.1007/978-3-642-56542-7>
- Serrin, J., 1979. Conceptual analysis of the classical second laws of thermodynamics. *Arch. Rational Mech. Anal.* 70, 355–371. <https://doi.org/10.1007/BF00281160>
- Simo, J.C., Miehe, C., 1992. Associative coupled thermoplasticity at finite strains: Formulation, numerical analysis and implementation. *Computer Methods in Applied Mechanics and Engineering* 98, 41–104. [https://doi.org/10.1016/0045-7825\(92\)90170-O](https://doi.org/10.1016/0045-7825(92)90170-O)

- Truesdell, C., 1984. Rational Thermodynamics, 2nd ed. Springer-Verlag, New York.  
<https://doi.org/10.1007/978-1-4612-5206-1>
- Truesdell, C., 1968. Thermodynamics for Beginners, in: Parkus, H., Sedov, L.I. (Eds.), Irreversible Aspects of Continuum Mechanics and Transfer of Physical Characteristics in Moving Fluids, IUTAM Symposia. Springer, Vienna, pp. 373–389. [https://doi.org/10.1007/978-3-7091-5581-3\\_26](https://doi.org/10.1007/978-3-7091-5581-3_26)
- Truesdell, C., Noll, W., 2004. The Non-Linear Field Theories of Mechanics, 3rd ed. Springer-Verlag, Berlin Heidelberg. <https://doi.org/10.1007/978-3-662-10388-3>
- Varadhan, S.N., Beaudoin, A.J., Acharya, A., Fressengeas, C., 2006. Dislocation Transport using an Explicit Galerkin/Least-Squares Formulation. Modelling and Simulation in Materials Science and Engineering 14, 1245–1270. <https://iopscience.iop.org/article/10.1088/0965-0393/14/7/011>
- Weyl, H., 1940. The method of orthogonal projection in potential theory. Duke Math. J. 7, 411–444. <https://doi.org/10.1215/S0012-7094-40-00725-6>
- Willis, J.R., 1967. Second-order effects of dislocations in anisotropic crystals. International Journal of Engineering Science 5, 171–190. [https://doi.org/10.1016/0020-7225\(67\)90003-1](https://doi.org/10.1016/0020-7225(67)90003-1)
- Yang, Q., Stainier, L., Ortiz, M., 2006. A variational formulation of the coupled thermo-mechanical boundary-value problem for general dissipative solids. Journal of the Mechanics and Physics of Solids 54, 401–424. <https://doi.org/10.1016/j.jmps.2005.08.010>
- Zou, J., Kotchetkov, D., Balandin, A.A., Florescu, D.I., Pollak, F.H., 2002. Thermal conductivity of GaN films: Effects of impurities and dislocations. Journal of Applied Physics 92, 2534–2539. <https://doi.org/10.1063/1.1497704>