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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. Thermal strains are uniquely separated into compatible and incompatible components via the Stokes-Helmholtz decomposition and the curl of the incompatible part of thermal strains is directly related to the areal dislocation density tensor. A dislocation density evolution (including transport) law is developed and shown to be related to the evolution of the curl of incompatible thermal strains. This relationship demonstrates that dislocation generation, annihilation, motion and/or interactions with other defects can be triggered due to transient temperature changes, and conversely an evolving dislocation density induces temperature changes. The model development is completed with constitutive laws derived from energetic and dissipative considerations. The advantages and consequences of the assumptions of the T-FDM model under rapidly changing temperatures, both spatially and temporally, are discussed. The T-FDM model is designed to operate at the length scale of individual dislocations and at this level, 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. Some illustrative examples are presented to demonstrate the applicability of the model and to better understand some of the novel concepts proposed in this work.

Highlights

- Strong temperature gradients during 3D-printing can trigger dislocation dynamics
- A novel fully-coupled dislocation dynamics and heat conduction model is proposed
- The model predicts dislocation dynamics due to temperature changes and vice versa
- 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 mechanics, at the length scale where individual dislocations can be characterized, 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 enable the study of 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 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.

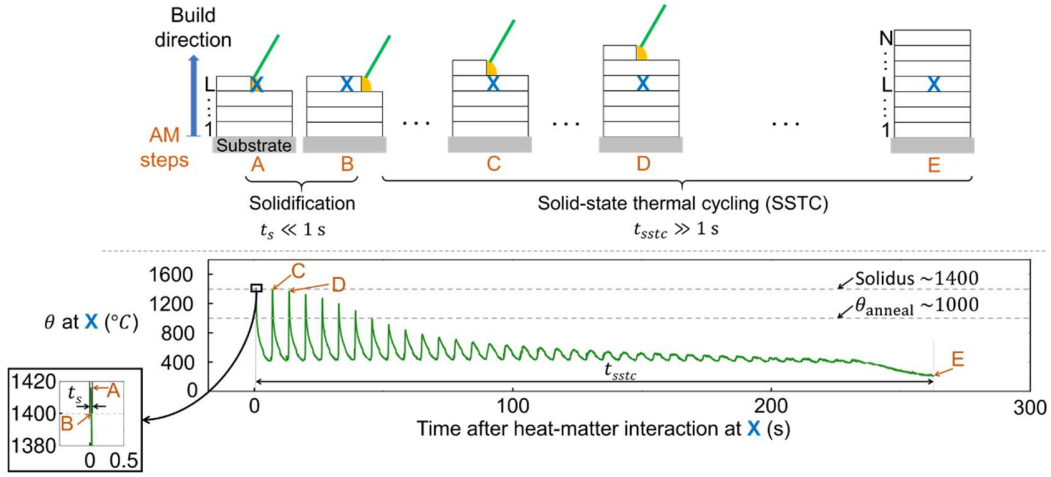


Figure 1: An illustration of temperature (θ) vs time (t) evolution at a material point X during additive manufacturing of a wall. $t = 0$ corresponds to the moment the heat-matter interactions occur at X in a layer $L < N$, where N is the total number of layers.

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

The idea of dislocations being generated from strong temperature gradients was put forth by Kröner (Kröner, 1959, 1958). Kröner noted that in a continuous medium experiencing a heterogeneous temperature field, it is possible to eliminate elastic distortions by introducing dislocations of a density proportional to the curl of thermal strains. An extract from the translated version of (Kröner, 1958) reads, “*Certainly, this process is important when large thermal stresses occur as they do during the cooling of cast iron. Since in this case it is easy to calculate the necessary dislocation arrangement, this is an impressive example of the practical use of the concept that thermal stress is considered as being caused by dislocations.*” This observation by Kröner is also applicable to dislocations formed due to large temperature changes occurring due to solid-state thermal cycling during an additive manufacturing process.

Kröner (Kröner, 1958) argued that a uniform increase in temperature for an unconstrained body results in an increase in the displacement without introducing restoring forces, which is also characteristic of plastic deformation. Based on this postulation, the concept of a quasi-plastic distortion, which does not result in repulsive forces, was introduced. Then, similar to the relationship between an incompatible plastic distortion field and the Nye’s tensor (Nye, 1953) in the theory of dislocations, the curl of an incompatible thermal strain field can be associated with an areal density tensor, which was called the “quasi-dislocation”

density tensor (Kröner, 1958). Quasi-dislocations can be induced due to incompatibility in any form of inelastic distortion fields, for example, due to heterogeneous temperatures, magnetic fields, etc. (Kröner, 1958). In this work, the term “thermal quasi-dislocations” is adopted to specifically refer to quasi-dislocations due to incompatible thermal strains. Unlike dislocations, thermal quasi-dislocations do not manifest as line crystal defects in materials; the emphasis is on the mathematical relationship correlating incompatible thermal strains to the areal dislocation density. In (Kröner, 1958), a static theory was proposed for any kind of quasi-dislocations, however, a dynamics model was not developed.

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 (Kratochvil and Dillon, 1969) as well as between heat conduction and dislocation mechanics theory (Acharya, 2011; Acharya and Roy, 2006; Ghoniem et al., 2000; Roy and Acharya, 2006). To the author’s knowledge, however, none of the existing dislocation dynamics models account for incompatible thermal strains due to heterogeneous temperature fields, the relationship between thermal quasi-dislocations and dislocations, or dislocation driving forces generated due to transient temperature gradients. For example, 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 thermo-mechanical developments, however, temperature effects were neglected when deriving dislocation driving forces. In (Acharya and Roy, 2006), the role of uniform temperature changes on the mechanical response was considered and in (Roy and Acharya, 2006), the thermal cycling response of a thin-film was studied by simulating uniform temperature changes. Modeling the role of transient temperature gradients on driving dislocation dynamics and vice versa, however, was neither the focus of these works nor was it undertaken there. In (Acharya, 2011), heat conduction was considered in the energetic and dissipation formulations to impose restrictions on the shape of the constitutive relationships for a dislocation mechanics model. The focus of that work was to correlate the specific entropy field as defined in continuum mechanics and the statistical mechanics understanding of entropy, which was then applied to a dislocation mechanics model; an explicit relationship between dislocation density evolution and transient temperature changes was not developed.

Meanwhile, temperature changes induced due to dislocation slip have been studied in a few works. In the earliest works on this topic (Eshelby and Pratt, 1956; Freudenthal and Weiner, 1956), analytical expressions for temperature rise at the level of a slip plane due to the motion of an ensemble of dislocations were proposed. It was concluded that under *normal* slip conditions the temperature rise would correspond to a few degrees to a few tens of degrees; a significant rise in temperature could be achieved due to a sudden release of very closely packed dislocations or at very high loading rates. Dislocation dynamics simulations were performed in (De Hosson et al., 2001) and the simulated temperature changes were compared with analytical solutions for different metals. In all these works, a one way coupling between dislocation dynamics and temperature changes had been proposed, which does not account for dislocation generation, annihilation, motion or interactions with other defects induced by temperature changes.

In this work, a thermodynamically rigorous strongly coupled thermo-elasto-plastic dislocation dynamics model is proposed in a small displacement, small strain and large temperature change framework based on the fundamental idea of thermal quasi-dislocations introduced by Kröner (Kröner, 1959, 1958) and the field dislocation mechanics (FDM) model developed by Acharya (Acharya, 2004, 2003, 2001).

FDM (Acharya, 2004, 2003, 2001) 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, 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. The curl of the incompatible part of the elastic/plastic distortion is related to the areal dislocation density field, which makes FDM a non-local model. Nevertheless, it does not require using higher-order stresses/higher-order traction boundary conditions, which are typical in gradient plasticity models (for example (Forest, 2008)) or micro-stress/micro-traction conditions (for example, (Gurtin, 2002, 2000)). For any (mechanical) initial boundary value problem, FDM allows to uniquely determine the elastic and plastic distortion fields by prescribing the areal dislocation density and volume/boundary conditions involving the plastic distortion field (Acharya et al., 2019). In addition, the thermodynamic considerations in FDM straightforwardly result in dislocation driving forces that are crystallographic in nature. Therefore, FDM is the most appropriate approach for the desired strong coupling with heat conduction.

This paper is structured as follows. The notations and tensorial operations used in this work are presented in section 2. 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 and thermomechanics of the coupled FDM, thermal quasi-dislocations and heat conduction problem. In the discussion section 4, some consequences of the thermodynamic considerations of the T-FDM model are presented. In addition, some illustrative problems are analytically solved to demonstrate the applicability of the model and better understand the concept of thermal quasi-dislocations and their relationship with dislocations. Concluding remarks 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 ∇ 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 first 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:

$$\begin{aligned}
(\bar{\mathbf{a}} \times \bar{\mathbf{b}})_i &= e_{ijk} a_j b_k \hat{\mathbf{e}}_i \\
(\bar{\bar{\mathbf{A}}} \times \bar{\mathbf{b}})_{ij} &= e_{jkl} A_{ik} b_l \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j \\
(\bar{\mathbf{a}} \times \bar{\bar{\mathbf{B}}})_{ij} &= e_{ikl} a_k B_{lj} \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j
\end{aligned}$$

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

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

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

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). The proposed coupling will also be performed in the 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 will allow us to develop the thermodynamic aspects of the T-FDM model, and its implications will be discussed in section 4.

3.1 Deformation fields in presence of continuously represented stationary dislocations within a steady-state 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 at any instance in time, \mathcal{B} has a heterogeneous temperature distribution due to some combination of steady-state heat-flux and/or temperature boundary conditions as well as some *a priori* unknown and arbitrarily located 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 θ_0 to denote the reference temperature.

It is clear that \mathcal{B} is not in a global thermal equilibrium. However, we shall adopt the local thermodynamic equilibrium hypothesis, which is the first 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. We will also assume that \mathcal{B} is a single crystal. A material point in \mathcal{B} is assumed to represent an ensemble of atoms with a resolution that is coarse enough

that we cannot observe the atomic order but fine enough that we can distinguish the distortion fields generated by individual dislocations. In addition, θ is assumed to be constant across the underlying ensemble of atoms in coherence with the local thermodynamic equilibrium hypothesis.

Let \mathcal{B} contain an arbitrary distribution of continuously represented stationary dislocations. We aim to determine the deformation fields of stationary dislocations within \mathcal{B} far from the boundary $\partial\mathcal{B}$ at an arbitrary instant in time.

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 θ 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 η either on local θ or on $\mathcal{T}(\theta)$. Note that the usage of these notations does not imply that a variable η is solely dependent on θ or $\mathcal{T}(\theta)$.

We will restrict ourselves to the case of small displacements and small strains but allow large temperature differences.

We shall assume 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 $\bar{\bar{\mathbf{U}}}(\theta)$, defined as the gradient of total displacement:

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

is a compatible (curl-free) field and satisfies

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

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

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

is also compatible and it satisfies:

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

everywhere in \mathcal{B} , at any instant in time.

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

$$\bar{\bar{\mathbf{U}}}(\theta) = \bar{\bar{\mathbf{U}}}^e(\theta) + \bar{\bar{\mathbf{U}}}^{in}(\theta), \quad (3.5)$$

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

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

with $\bar{\bar{\boldsymbol{\epsilon}}}^e = \text{sym}(\bar{\bar{\mathbf{U}}}^e)$, $\bar{\bar{\boldsymbol{\epsilon}}}^{in} = \text{sym}(\bar{\bar{\mathbf{U}}}^{in})$.

$\bar{\bar{\mathbf{U}}}^{in}(\theta)$ has contributions coming from plastic distortion $\bar{\bar{\mathbf{U}}}^p(\theta)$ induced by the presence of dislocations and thermal distortion due to the presence of a temperature field $\theta(\bar{\mathbf{x}})$. It is well established that thermal distortion is a symmetric tensor and hence, a pure strain $\bar{\bar{\boldsymbol{\epsilon}}}^{\theta}(\theta)$. Kröner (Kröner, 1958) noted that $\bar{\bar{\boldsymbol{\epsilon}}}^{\theta}(\theta)$ does not result in any repulsive forces, and called it a quasi-plastic distortion field.

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

$$\bar{\mathbf{U}}^{in}(\theta) = \bar{\mathbf{\epsilon}}^\theta(\theta) + \bar{\mathbf{U}}^p(\theta), \quad (3.7)$$

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

where $\bar{\mathbf{\epsilon}}^p(\theta)$ is the plastic strain tensor.

The presence of dislocations induces incompatibility in $\bar{\mathbf{U}}^p(\theta)$. The presence of a heterogeneous temperature field under thermal loading and arbitrary local heat sources can induce an incompatibility in $\bar{\mathbf{\epsilon}}^\theta(\theta)$. Together, dislocations and a heterogeneous temperature field induce an incompatibility in the elastic distortion $\bar{\mathbf{U}}^e(\theta)$.

For $\bar{\mathbf{U}}^e(\theta)$ and $\bar{\mathbf{U}}^p(\theta)$, following (Acharya and Roy, 2006), we invoke the Stokes-Helmholtz decomposition to uniquely decompose them into their respective compatible (curl-free and denoted via the superscript “||”) and incompatible (divergence-free and denoted via the superscript “⊥”) components:

$$\bar{\mathbf{U}}^i(\theta) = \bar{\mathbf{U}}^{i||}(\theta) + \bar{\mathbf{U}}^{i\perp}(\theta) = \nabla \bar{\mathbf{w}}^i(\theta) + \bar{\mathbf{\chi}}^i(\theta); i = e, p \quad (3.9)$$

where $\bar{\mathbf{w}}^i$ and $\bar{\mathbf{\chi}}^i$ are *a priori* unknown vector and second order tensor fields, respectively. $\bar{\mathbf{w}}^i$ is such that $\nabla \times \bar{\mathbf{U}}^{i||}(\theta) = \mathbf{0}$ but $\nabla \bar{\mathbf{w}}^i$ does not have to be zero. $\bar{\mathbf{\chi}}^i(\theta)$ is such that $\nabla \times \bar{\mathbf{\chi}}^i(\theta) \neq \mathbf{0}$ but $\nabla \cdot \bar{\mathbf{\chi}}^i(\theta) = \mathbf{0}$.

Due to the symmetry of $\bar{\mathbf{\epsilon}}^\theta(\theta)$, its Stokes-Helmholtz decomposition needs a careful consideration, which is carried out in the appendix. In the general case, using equation (A.6), we can decompose $\bar{\mathbf{\epsilon}}^\theta$ into compatible and incompatible asymmetric tensors, say $\bar{\mathbf{U}}^{\theta||}$ and $\bar{\mathbf{U}}^{\theta\perp}$, respectively, such that:

$$\bar{\mathbf{\epsilon}}^\theta(\theta) = \bar{\mathbf{U}}^{\theta||}(\theta) + \bar{\mathbf{U}}^{\theta\perp}(\theta) = \left[\frac{1}{2} \left(\nabla \nabla \Phi + \nabla \Phi \nabla + \nabla (\nabla \times \bar{\mathbf{b}}') \right) \right] + \left[\frac{1}{2} (\nabla \times \bar{\mathbf{b}}') \nabla + \nabla \times \bar{\mathbf{\zeta}} \times \nabla \right] \quad (3.10a)$$

where Φ , $\bar{\mathbf{b}}'$ and $\bar{\mathbf{\zeta}}$ are any scalar, vector and second-order tensor functions, respectively, that are at least thrice differentiable. $\bar{\mathbf{U}}^{\theta||}(\theta)$ and $\bar{\mathbf{U}}^{\theta\perp}(\theta)$ correspond to the first and second set of terms within the square brackets in equation (3.10a).

While (3.10a) demonstrates the most general form of the Stokes-Helmholtz decomposition for $\bar{\mathbf{\epsilon}}^\theta(\theta)$, it nevertheless involves three unknowns Φ , $\bar{\mathbf{b}}'$ and $\bar{\mathbf{\zeta}}$. However, it may not be necessary to determine them because we can use the well-established empirical form of $\bar{\mathbf{\epsilon}}^\theta(\theta)$:

$$\bar{\mathbf{\epsilon}}^\theta(\theta) = \bar{\boldsymbol{\gamma}}(\theta) \Delta \theta \quad (3.10b)$$

where $\bar{\boldsymbol{\gamma}}(\theta)$ is the local thermal expansion coefficient tensor, which is symmetric, and $\Delta \theta = \theta - \theta_0$. As will be demonstrated in section 4.2, prior to performing any tensorial operation using equation (3.10b), it is imperative to determine whether $\bar{\mathbf{\epsilon}}^\theta$ is compatible or incompatible using equation (3.10a).

In (Kröner, 1958), $\bar{\mathbf{\epsilon}}^\theta(\theta)$ was assumed to be a spherically symmetric tensor $\gamma(\theta) \Delta \theta \bar{\mathbb{I}}$; where $\bar{\mathbb{I}} = \delta_{ij}$ and $\gamma(\theta) > 0$. This assumption restricts the usage of equation (3.10b) to materials with cubic symmetry. In this work, we allow $\bar{\boldsymbol{\gamma}}(\theta)$ to be any symmetric positive definite tensor. Note that in (Kröner, 1958), $\gamma(\theta) \Delta \theta$ was assumed to be equal to $\Delta \Phi = \partial^2 \Phi / \partial x_i^2$ and $\bar{\mathbf{\epsilon}}^\theta(\theta)$ was expressed as $\bar{\mathbf{\epsilon}}^\theta(\theta) = \nabla \nabla \Phi + \nabla \times (\Phi \bar{\mathbb{I}}) \times \nabla$; the contribution of $\nabla (\nabla \times \bar{\mathbf{b}}')$ was neglected in that work.

Equations (3.6), (3.8), (3.10a) and (3.10b) imply that

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

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

Consider an arbitrary material surface S inside \mathcal{B} and let an ensemble of dislocations and thermal quasi-dislocations thread this surface. In the general case, the presence of dislocations and thermal quasi-dislocations precludes a unique definition of the elastic displacement field. If we were to draw an arbitrary circuit C on the surface S surrounding dislocations and thermal quasi-dislocations, 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 C such that:

$$\bar{\mathbf{b}} = \llbracket \bar{\mathbf{u}}^e \rrbracket = \int_C \bar{\mathbf{U}}^e(\theta) \cdot d\bar{\mathbf{L}}(\theta) = \int_C \bar{\mathbf{U}}^{e\perp}(\theta) \cdot d\bar{\mathbf{L}}(\theta) = - \int_C \left(\bar{\mathbf{U}}^{p\perp}(\theta) + \bar{\mathbf{U}}^{\theta\perp}(\theta) \right) \cdot d\bar{\mathbf{L}}(\theta) \quad (3.12)$$

where $d\bar{\mathbf{L}}$ is the local tangent to C . C is referred to as the Burgers circuit and $\bar{\mathbf{b}}$ is referred to as the Burgers vector of the ensemble of the defect. In an isothermal case when $\bar{\mathbf{U}}^{e\perp}(\theta) = -\bar{\mathbf{U}}^{p\perp}(\theta)$, $\bar{\mathbf{b}}$ is solely induced by dislocations; this contribution will be denoted by $\bar{\mathbf{b}}^p$.

When determining $\bar{\mathbf{b}}$ for an ensemble of dislocations under strong temperature gradients, special 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 θ , i.e. $\bar{\mathbf{b}} = \bar{\mathbf{b}}(\theta)$ or on the temperature distribution in the neighborhood within S (delimited by C), i.e. $\bar{\mathbf{b}} = \bar{\mathbf{b}}(\mathcal{T}(\theta))$. Indeed, this is because while $\bar{\mathbf{U}}^{p\perp}(\theta)$ may vanish in the immediate neighborhood of a material point, however $\bar{\mathbf{U}}^{\theta\perp}(\theta)$ may not vanish in this neighborhood in the presence of large temperature gradients. In this work, we shall concern ourselves with the case where $\bar{\mathbf{b}} = \bar{\mathbf{b}}(\theta)$. This implies that the size of S cannot be larger than the largest possible surface in the underlying ensemble of atoms at a material point in \mathcal{B} . Consequently, in most cases considered in this model only one dislocation may traverse S at a given point in time. Occasionally, a few dislocations, each on a different slip system, may traverse S . Rarely, more than one dislocation on a slip system would traverse S .

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 $\bar{\bar{\alpha}}(\theta)$ as

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

we get

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

$\bar{\bar{\alpha}}(\theta)$ is a continuous areal density field better known as the Nye's tensor (Nye, 1953). In conventional dislocation mechanics, $\bar{\bar{\alpha}}(\theta)$ is also known as the dislocation density tensor. However, based on its definition according to equation (3.14), it also contains the contribution of thermal quasi-dislocations, and henceforth it shall be only referred to as the Nye's tensor.

When it comes to determining $\bar{\mathbf{U}}^{e\perp}$ from $\bar{\bar{\alpha}}(\theta)$, equation (3.14) is insufficient because it does not ensure that $\bar{\mathbf{U}}^{e\perp}$ is equal to zero in the absence of $\bar{\bar{\alpha}}(\theta)$, which should be the case. Following (Acharya and Roy, 2006), equation (3.14) needs to be augmented with additional conditions that can be derived from equation (3.9),

$$\nabla \cdot \bar{\mathbf{U}}^{e\perp}(\theta) = 0 \text{ in } \mathcal{B} \quad (3.16a)$$

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

In equation set (3.16), the latter condition is imposed to ensure that its solution does not contain a gradient term. Taking curl of equation (3.14) we get

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

Using equation set (3.16) we get,

$$\nabla \cdot \nabla \bar{\mathbf{U}}^{e\perp}(\theta) = -\nabla \times \bar{\boldsymbol{\alpha}}(\theta) \text{ in } \mathcal{B} \quad (3.18a)$$

$$\bar{\mathbf{U}}^{e\perp}(\theta) \cdot \hat{\mathbf{n}} = 0 \text{ on } \partial\mathcal{B} \quad (3.18b)$$

The left-hand side of equation (3.18a) is a Poisson type equation whose solution for $\bar{\mathbf{U}}^{e\perp}(\theta)$ under the given boundary condition vanishes when $\bar{\boldsymbol{\alpha}}(\theta) = 0$.

Now, using relationships (3.7) and (3.11), equation (3.14) can be reformulated as

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

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

Equation (3.19a) reveals two distinct contributions to the Nye's tensor. The first contribution comes from the presence of dislocations whose areal density is given by the dislocation density tensor $\bar{\boldsymbol{\alpha}}^p(\theta) = -\nabla \times \bar{\mathbf{U}}^{p\perp}(\theta)$. While $\bar{\boldsymbol{\alpha}}^p(\theta)$ is not associated with the incompatible thermal strains, it is nevertheless affected by the local temperature, which affects the Burgers and line vectors. The second contribution comes from thermal quasi-dislocations whose areal density is given by $\bar{\boldsymbol{\alpha}}^\theta(\theta) = -\nabla \times \bar{\boldsymbol{\varepsilon}}^\theta(\theta) = -\nabla \times \bar{\mathbf{U}}^{\theta\perp}(\theta)$. Note that $\bar{\boldsymbol{\alpha}}^\theta(\theta)$ arises purely from an incompatibility in $\bar{\boldsymbol{\varepsilon}}^\theta$.

From equations (3.9), (3.10a) and (3.18), we can deduce that:

$$\nabla \cdot \nabla \bar{\mathbf{U}}^{p\perp}(\theta) + \nabla \cdot \nabla \bar{\mathbf{U}}^{\theta\perp}(\theta) = \nabla \times \bar{\boldsymbol{\alpha}}(\theta) \text{ in } \mathcal{B}, \quad (3.20a)$$

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

which, similar to equation (3.16a), also implies that $\nabla \cdot \bar{\mathbf{U}}^{p\perp}(\theta) = \mathbf{0}$ and $\nabla \cdot \bar{\mathbf{U}}^{\theta\perp}(\theta) = \mathbf{0}$.

From (3.14) and (3.19), we obtain the following continuity conditions,

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

We are also interested in connecting the above developments with the crystallography of the material. This requires associating dislocations with a slip system based on their slip plane and direction. Let $\bar{\boldsymbol{\alpha}}^{p,\beta}(\theta)$ define the field density of a single dislocation on a slip system β . If this dislocation crosses a surface S , then from equation (3.15) we get the Burgers vector of this dislocation as $\bar{\mathbf{b}}^{p,\beta}(\theta) = \int_S \bar{\boldsymbol{\alpha}}^{p,\beta}(\theta) \cdot \hat{\mathbf{n}} dS$. If $\bar{\mathbf{l}}^{p,\beta}(\theta)$ is the local tangent to this dislocation line, then $\bar{\boldsymbol{\alpha}}^{p,\beta}(\theta)$ can be written as:

$$\bar{\boldsymbol{\alpha}}^{p,\beta}(\theta) = \frac{1}{V} \left(\bar{\mathbf{b}}^{p,\beta}(\theta) \otimes \bar{\mathbf{l}}^{p,\beta}(\theta) \right) \quad (3.22)$$

where V is a reference volume that should be chosen such that variations in θ within this volume are negligible. Similar to the case of S in equation (3.13), the maximum value of V would correspond to the volume of the underlying ensemble of atoms at a material point in \mathcal{B} . This dislocation together with thermal quasi-dislocations within the volume V would contribute to the Nye's tensor and Burgers vector as follows:

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

$$\bar{\mathbf{b}}(\theta) = \bar{\mathbf{b}}^{p,\beta}(\theta) + \bar{\mathbf{b}}^\theta(\theta) \quad (3.23b)$$

where $\bar{\mathbf{b}}^\theta(\theta) = \int_S \bar{\boldsymbol{\alpha}}^\theta(\theta) \cdot \hat{\mathbf{n}} dS$. Note that the manner in which the model is constructed, it allows us to characterize thermal quasi-dislocations via an "equivalent to a Burgers vector". However, attributing a line direction to this defect is not allowed because thermal quasi-dislocations do not manifest as line crystal defects.

If there are multiple dislocations on the same slip system β that traverse S , then $\bar{\mathbf{b}}^{p,\beta}(\theta)$ and $\bar{\bar{\mathbf{a}}}^{p,\beta}(\theta)$ in equation set (3.23) determine the net Burgers vector and density tensor, respectively, of the ensemble of these dislocations.

If multiple dislocations from different slip systems traverse S , then their net local Burgers vector $\bar{\mathbf{b}}^p(\theta) = \sum_{i=1}^{N_\beta} \bar{\mathbf{b}}^{p,\beta_i}(\theta) = \sum_{i=1}^{N_\beta} \int_S \bar{\bar{\mathbf{a}}}^{p,\beta_i}(\theta) \cdot \hat{\mathbf{n}} dS = \int_S \left(\sum_{i=1}^{N_\beta} \bar{\bar{\mathbf{a}}}^{p,\beta_i}(\theta) \right) \cdot \hat{\mathbf{n}} dS = \int_S \bar{\bar{\mathbf{a}}}^p(\theta) \cdot \hat{\mathbf{n}} dS$; N_β is the total number of slip systems at a given material point. For this configuration, the Nye's tensor $\bar{\bar{\mathbf{a}}}(\theta)$ and Burgers vector $\bar{\mathbf{b}}(\theta)$ are:

$$\bar{\bar{\mathbf{a}}}(\theta) = \bar{\bar{\mathbf{a}}}^p(\theta) + \bar{\bar{\mathbf{a}}}^\theta(\theta) = \frac{1}{V} \sum_{i=1}^{N_\beta} \left(\bar{\mathbf{b}}^{p,\beta_i}(\theta) \otimes \bar{\mathbf{l}}^{p,\beta_i}(\theta) \right) + \bar{\bar{\mathbf{a}}}^\theta(\theta) \quad (3.24a)$$

$$\bar{\mathbf{b}}(\theta) = \sum_{i=1}^{N_\beta} \bar{\mathbf{b}}^{p,\beta_i}(\theta) + \int_S \bar{\bar{\mathbf{a}}}^\theta(\theta) \cdot \hat{\mathbf{n}} dS \quad (3.24b)$$

Note here that relationships (3.23b) and (3.24b) are only valid for small S ; for S encompassing regions of multiple material points, a dependence on $\mathcal{T}(\theta)$ must be considered.

Finally, we note that under steady-state heat conduction, the temperature field $\theta(\bar{\mathbf{x}})$ doesn't evolve with time. Consequently, in the absence of mechanical loading, immobile dislocations will continue to remain immobile and no new dislocations will be generated. In this case, the condition $\frac{d}{dt} \int_S \bar{\bar{\mathbf{a}}}(\theta) \cdot \hat{\mathbf{n}} dS = 0$ needs to be satisfied for all surfaces S in \mathcal{B} .

The material derivative operator $\frac{d}{dt}$ can be rewritten as $\frac{d}{dt} = \frac{\partial}{\partial t} + (\dot{\bar{\mathbf{u}}} \cdot \nabla)$, where $\frac{\partial}{\partial t}$ is the Eulerian derivative and $\dot{\bar{\mathbf{u}}} \cdot \nabla$ is the convective derivative. Under a small strain and small displacement assumption, we can neglect the latter and only use $\frac{\partial}{\partial t}$. For simplicity, in the remainder of the article we shall denote $\frac{\partial}{\partial t}$ with an overhead dot.

3.2 Kinematics of continuously represented stationary dislocations in a transient heterogeneous temperature field

Let us now assume that the heat flux and/or temperature boundary conditions evolve with time but the dislocations in \mathcal{B} remain immobile. An evolving temperature field naturally entails an evolving $\bar{\bar{\mathbf{e}}}^\theta(\theta)$. Consequently, the thermal quasi-dislocations will also evolve with time via $\dot{\bar{\bar{\mathbf{a}}}^\theta}(\theta) = -\nabla \times \dot{\bar{\bar{\mathbf{e}}}^\theta}(\theta) = -\nabla \times \bar{\bar{\mathbf{u}}}^{\theta\perp}(\theta)$. Since we have assumed $\bar{\bar{\mathbf{e}}}^\theta$ has the relationship (3.9), we obtain $\dot{\bar{\bar{\mathbf{a}}}^\theta}(\theta) = \frac{\partial}{\partial t} [\nabla \times (\bar{\bar{\mathbf{y}}} \Delta \theta)] = (\nabla \times \dot{\bar{\bar{\mathbf{y}}}}) \Delta \theta + (\nabla \times \bar{\bar{\mathbf{y}}}) \dot{\theta} - \dot{\bar{\bar{\mathbf{y}}}} \cdot [\nabla(\Delta \theta) \cdot \bar{\bar{\mathbf{X}}}] - \bar{\bar{\mathbf{y}}} \cdot [\nabla(\Delta \theta) \cdot \bar{\bar{\mathbf{X}}}]$. If we assume that $\bar{\bar{\mathbf{y}}}$ does not evolve in space and time, then $\dot{\bar{\bar{\mathbf{a}}}^\theta}(\theta) = -\bar{\bar{\mathbf{y}}} \cdot [\nabla(\Delta \theta) \cdot \bar{\bar{\mathbf{X}}}]$.

The local dislocation density $\bar{\bar{\mathbf{a}}}^{p,\beta}(\theta)$ evolves in its magnitude and spread because of the dependence of the Burgers and line vectors on the evolving local temperature (equation (3.22)). A change in the magnitude of the dislocation density can be thought of as the local generation/annihilation of dislocations without their motion. This can be represented via a local dislocation source/sink term that also evolves the density of existing dislocations, say $\bar{\bar{\mathbf{s}}}^{p,\beta_i}(\theta)$; if no dislocations exist in the body and no dislocations are generated, then $\bar{\bar{\mathbf{s}}}^{p,\beta_i}(\theta) = \mathbf{0}$ for all slip systems everywhere in the body. For multiple dislocations on different slip systems, we can combine their source terms to have $\bar{\bar{\mathbf{s}}}^p(\theta) = \sum_{i=1}^{N_\beta} \bar{\bar{\mathbf{s}}}^{p,\beta_i}$. In the case of existing dislocations, we will assume that only the magnitude of their Burgers and line vectors

would evolve with time and let $\bar{\mathbf{s}}^{p,\beta_i}(\theta) = [\hat{\mathbf{b}}^{p,\beta_i}(\theta) \otimes \hat{\mathbf{l}}^{p,\beta_i}(\theta)] \frac{\partial}{\partial t} \left(\frac{|\bar{\mathbf{b}}^{p,\beta_i}| |\hat{\mathbf{l}}^{p,\beta_i}|}{v} \right)$, where $\hat{\mathbf{b}}^{p,\beta_i}$ and $\hat{\mathbf{l}}^{p,\beta_i}$ are unit Burgers and line vectors, respectively. Note that an evolving dislocation density entails an evolving $\bar{\mathbf{U}}^{p\perp}$, however, it does not imply an evolving $\bar{\mathbf{U}}^{p\parallel}$ because $\bar{\mathbf{U}}^{p\parallel}$ is associated with the history of dislocation motion (Acharya, 2001), which in this case remains unchanged.

The incompatible elastic distortions $\bar{\mathbf{U}}^{e\perp}$ may or may not evolve with time. The former case would imply that the stress field associated with dislocations evolves in time; an expression for the stress field is given later in section 3.8. In the latter case, $\bar{\mathbf{s}}^p(\theta) = -\dot{\bar{\boldsymbol{\alpha}}}^\theta(\theta)$ implies that dislocations are being generated, annihilated or their densities are evolving due to temperature changes, however, there will be no dislocation motion.

Based on the above considerations and equations (3.10), (3.11), (3.14) and (3.19) we can deduce the following relationships for the case of transient heat conduction in a body containing stationary dislocations:

$$\left. \begin{aligned} \dot{\bar{\boldsymbol{\alpha}}}^p &= -\nabla \times \dot{\bar{\mathbf{U}}}^{p\perp} = \bar{\mathbf{s}}^p(\theta) = \sum_{i=1}^{N_\beta} \dot{\bar{\boldsymbol{\alpha}}}^{p,\beta} = \sum_{i=1}^{N_\beta} \bar{\mathbf{s}}^{p,\beta} \\ \dot{\bar{\boldsymbol{\alpha}}}(\theta) &= \nabla \times \dot{\bar{\mathbf{U}}}^{e\perp}(\theta) = \dot{\bar{\boldsymbol{\alpha}}}^p + \dot{\bar{\boldsymbol{\alpha}}}^\theta(\theta) = \sum_{i=1}^{N_\beta} \bar{\mathbf{s}}^{p,\beta} - \dot{\bar{\boldsymbol{\alpha}}}^\theta(\theta) \\ \dot{\bar{\boldsymbol{\alpha}}}^\theta(\theta) &= (\nabla \times \dot{\bar{\boldsymbol{\gamma}}})\Delta\theta + (\nabla \times \bar{\boldsymbol{\gamma}})\dot{\theta} - \dot{\bar{\boldsymbol{\gamma}}} \cdot [\nabla(\Delta\theta) \cdot \bar{\mathbf{X}}] - \bar{\boldsymbol{\gamma}} \cdot [\nabla(\Delta\theta) \cdot \bar{\mathbf{X}}] \\ \dot{\bar{\mathbf{U}}}^{p\parallel}(\theta) &= \mathbf{0} \end{aligned} \right\} \quad (3.25)$$

3.3 Kinematics of continuously represented mobile dislocations in a transient heterogeneous temperature field

Let us now assume that \mathcal{B} is subjected to a thermo-elastic-plastic deformation under the action of some transient traction and/or displacement as well as heat flux and/or temperature boundary conditions. We are now considering the case of mobile dislocations.

We adopt the approach of (Acharya, 2011) to derive the dynamic equation of dislocation motion. We follow the temporal evolution of the Burgers vector content within a circuit $\mathcal{C}(t)$ bounding an arbitrary curved area patch $S(t)$ in \mathcal{B} , which is sufficiently small to have a uniform θ within the region bounded by this surface. We will assume that $S(t)$ is traversed by a dislocation on a slip system β at a velocity $\bar{\mathbf{V}}^\beta$ with respect to the material. We will also account for $\bar{\mathbf{s}}^{p,\beta}(\theta)$ (seen in section 3.2) arising from local temperature changes. The associated equation for the dynamics of dislocations is:

$$\begin{aligned} \frac{\partial}{\partial t} \int_{S(t)} \bar{\boldsymbol{\alpha}}^{p,\beta}(\theta) \cdot \hat{\mathbf{n}} dS &= - \int_{\mathcal{C}(t)} \left(\bar{\boldsymbol{\alpha}}^{p,\beta}(\theta) \times \bar{\mathbf{V}}^\beta(\theta) \right) \cdot d\bar{\mathbf{x}} + \int_{S(t)} \bar{\mathbf{s}}^{p,\beta}(\theta) \cdot \hat{\mathbf{n}} dS \\ &= - \int_{S(t)} \left[\nabla \times \left(\bar{\boldsymbol{\alpha}}^{p,\beta}(\theta) \times \bar{\mathbf{V}}^\beta(\theta) \right) + \bar{\mathbf{s}}^{p,\beta}(\theta) \right] \cdot \hat{\mathbf{n}} dS \end{aligned} \quad (3.26)$$

Equation (3.26) is similar to the expression proposed in (Acharya, 2011, 2001); a detailed explanation for the origin of the right hand side of this equation can be found in these references.

In the local form, equation (3.26) reads:

$$\dot{\bar{\boldsymbol{\alpha}}}^{p,\beta}(\theta) = -\nabla \times \left(\bar{\boldsymbol{\alpha}}^{p,\beta}(\theta) \times \bar{\mathbf{V}}^{p,\beta}(\theta) \right) + \bar{\mathbf{s}}^{p,\beta}(\theta) \quad (3.27)$$

Let $\bar{\bar{\mathbf{U}}}^{p,\beta}(\theta)$ be the local slip distortion tensor associated with the motion of a mobile dislocation on slip system β . The rate of change of $\bar{\bar{\mathbf{U}}}^{p,\beta}(\theta)$ with respect to time can be written as:

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

which is unique up to a gradient term. The rate of change of the Nye's tensor can then be obtained from equation (3.27) as:

$$\dot{\bar{\alpha}}(\theta) = \dot{\bar{\alpha}}^{p,\beta}(\theta) + \dot{\bar{\alpha}}^\theta(\theta) = -\nabla \times (\bar{\alpha}^{p,\beta}(\theta) \times \bar{V}^\beta(\theta)) + \bar{s}^{p,\beta}(\theta) + \dot{\bar{\alpha}}^\theta(\theta) \quad (3.29)$$

Equation (3.29) reveals an intimate relationship between dislocation motion, dislocation density generation/annihilation/evolution without motion due to temperature changes, and thermal quasi-dislocation density evolution. It can be best appreciated when $\dot{\bar{\alpha}}(\theta) = \mathbf{0}$. In this case, on one hand, we have $\dot{\bar{\alpha}}^{p,\beta}(\theta) = -\dot{\bar{\alpha}}^\theta(\theta)$. This equation implies that the incompatibility in elastic distortion does not evolve during temperature changes if the change in thermal quasi-dislocation density associated with the temperature change is accommodated through the generation, annihilation and/or motion of dislocations. On the other hand, we can view the same equation as $\dot{\bar{\alpha}}^\theta = \nabla \times (\bar{\alpha}^{p,\beta}(\theta) \times \bar{V}^\beta(\theta)) - \bar{s}^{p,\beta}(\theta)$. This relationship implies that dislocation motion can result in the evolution of thermal quasi-dislocation density and incompatible thermal strains, which would affect the local temperature. However, the appropriate equation for temperature evolution must come from thermodynamic considerations, which is demonstrated later via equation (3.57) in section 3.10.

Equation (3.29) also indicates that since $\dot{\bar{\alpha}}^\theta(\theta)$ is not associated with any particular slip system, its evolution may also result in the evolution of dislocations on different slip systems. Therefore, this equation has to be generalized to the case of multiple dislocations on different slip systems. If multiple dislocations on different slip systems are passing through a material point, then the net slip distortion tensor rate due to all these dislocations is given as:

$$\dot{\bar{U}}^p(\theta) = \sum_{i=1}^{N_\beta} \dot{\bar{U}}^{p,\beta_i}(\theta) = \sum_{i=1}^{N_\beta} (\bar{\alpha}^{p,\beta_i}(\theta) \times \bar{V}^{p,\beta_i}(\theta)) \quad (3.30)$$

For this case, the rate of change of the Nye's tensor is given by:

$$\dot{\bar{\alpha}}(\theta) = \sum_{i=1}^{N_\beta} (\dot{\bar{\alpha}}^{p,\beta_i}(\theta)) + \dot{\bar{\alpha}}^\theta = -\sum_{i=1}^{N_\beta} [\nabla \times (\bar{\alpha}^{p,\beta_i}(\theta) \times \bar{V}^{p,\beta_i}(\theta)) - \bar{s}^{p,\beta_i}(\theta)] + \dot{\bar{\alpha}}^\theta \quad (3.31)$$

Equation (3.31) is the most general form for the relationship between the evolutions of dislocation and thermal quasi-dislocation densities. In addition to the observations that can be made from equation (3.29), equation (3.31) indicates that dislocation motion on any slip system can result in the evolution of the thermal quasi-dislocation density. Whereas the evolution of thermal quasi-dislocations can result in the motion of dislocations on other slip systems, including on those that are “inactive” based on restrictions imposed by crystallography and local stress conditions. Furthermore, if $\bar{V}^{p,\beta}(\theta)$ has an out-of-slip-plane component, then cross-slip, climb and non-Schmid mechanisms could also occur (Acharya, 2003).

In a more general case, dislocation motion, generation and annihilation along with the evolution of thermal quasi-dislocations would also be accompanied by the evolution of $\bar{U}^{e\perp}$ via a non-zero $\dot{\bar{\alpha}}(\theta)$. It is through this possibility that equations (3.29) and (3.31) could allow the presence of stationary dislocations in a field of evolving thermal quasi-dislocations.

Finally, note that while we have $\bar{U}^{p,\beta}(\theta) = \bar{\bar{U}}^{p,\beta}(\theta)$ for a slip system β , typically $\bar{U}^p(\theta) \neq \bar{\bar{U}}^p(\theta)$ in the case where multiple dislocations on different slip systems are involved. However, we can assume that (Acharya, 2001):

$$\bar{U}^{p\parallel}(\theta) = \bar{\bar{U}}^{p\parallel}(\theta) \quad (3.32)$$

3.4 Boundary conditions for thermomechanical loadings

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

Let \mathcal{B} undergo the aforementioned thermo-elastic-plastic deformation under the action of evolving traction $\bar{\mathbf{T}}$ on surface $\partial\mathcal{B}_T$, displacement $\bar{\mathbf{u}}_d$ on surface $\partial\mathcal{B}_d$, heat flux $\bar{\mathbf{q}}_h$ on surface $\partial\mathcal{B}_q$ and temperature θ' on surface $\partial\mathcal{B}_\theta$.

$$\bar{\mathbf{T}} = \bar{\boldsymbol{\sigma}} \cdot \hat{\mathbf{n}}, \forall \bar{\mathbf{x}} \in \partial\mathcal{B}_T \quad (3.33a)$$

$$\bar{\mathbf{u}} = \bar{\mathbf{u}}_d, \forall \bar{\mathbf{x}} \in \partial\mathcal{B}_d \quad (3.33b)$$

$$\bar{\mathbf{q}} = \bar{\mathbf{q}}_h, \forall \bar{\mathbf{x}} \in \partial\mathcal{B}_q \quad (3.33c)$$

$$\theta = \theta', \forall \bar{\mathbf{x}} \in \partial\mathcal{B}_\theta \quad (3.33d)$$

$\bar{\boldsymbol{\sigma}}$ 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.

We allow the existence of large but finite temperature and/or stress gradients under the action of the boundary conditions listed in equation set (3.33). Furthermore, these gradients may evolve with time. However, we impose that the time required for every material point in \mathcal{B} to adjust to any thermal and/or mechanical changes occurring under the action of boundary conditions (3.33a-d) is negligibly small in comparison to the timespan during which the boundary conditions evolve. In other words, the changes to the mechanical and thermal fields induced by the boundary conditions are instantaneously accommodated at each material point so that local thermodynamic equilibrium is respected at any given instant in time.

The following condition, which follows from equations (3.18b) and (3.20), has to be satisfied everywhere on $\partial\mathcal{B}$:

$$\bar{\mathbf{U}}^{e\perp} \cdot \hat{\mathbf{n}} = \bar{\mathbf{U}}^{p\perp} \cdot \hat{\mathbf{n}} = \bar{\mathbf{U}}^{\theta\perp} \cdot \hat{\mathbf{n}} = 0 \text{ on } \partial\mathcal{B} \quad (3.33e)$$

In addition, one must satisfy the condition $\bar{\mathbf{U}}^{p,\beta_i} \cdot \hat{\mathbf{n}}$ for all slip systems β_i on $\partial\mathcal{B}$, which yields:

$$(\nabla \dot{\mathbf{z}}^{p,\beta_i} - \bar{\boldsymbol{\alpha}}^{p,\beta_i} \times \bar{\mathbf{V}}^{p,\beta_i}) \cdot \hat{\mathbf{n}} = 0, \forall \bar{\mathbf{x}} \in \partial\mathcal{B} \quad (3.33f)$$

where $\nabla \dot{\mathbf{z}}^{p,\beta_i} = \bar{\mathbf{U}}^{p,\beta_i\parallel}$ and $\dot{\mathbf{z}}^{p,\beta_i}$ need to be prescribed in at least one point in \mathcal{B} (Acharya and Roy, 2006).

In order to obtain a unique solution to equation (3.27) for each slip system, Acharya (Acharya, 2003) proposed the following condition for the flux of dislocation density on $\partial\mathcal{B}$:

$$\bar{\mathbf{f}}^\beta = \bar{\boldsymbol{\alpha}}^{p,\beta} (\bar{\mathbf{V}}^\beta \cdot \hat{\mathbf{n}}), \forall \bar{\mathbf{x}} \in \partial\mathcal{B} \quad (3.33g)$$

with $\bar{\mathbf{V}}^\beta \cdot \hat{\mathbf{n}} \leq 0$ to ensure that there is not outflux of dislocations from \mathcal{B} to the surroundings. This condition can also be applied to equations (3.29) and (3.31) because the term associated with dislocation flux remains the same as in equation (3.27).

Finally, note that since there is no motion of thermal quasi-dislocations, conditions akin to equations (3.33f) and (3.33g) are not required for $\bar{\boldsymbol{\alpha}}^\theta$.

3.5 Balance of linear momentum

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

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

where ρ (local density), $\bar{\mathbf{f}}$ (local body force) and $\bar{\boldsymbol{\sigma}}$ also depend on θ .

3.6 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):

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

where ρr is representative of internal heat sources, losses to the surroundings, etc.

3.7 Thermo-mechanical dissipation

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 $\bar{\mathbf{V}}^\beta$, we perform a dissipation analysis based on the second law of thermodynamics. The second basic tenet of any RT based model is to apply the second law in the form of the classical Clausius-Kelvin-Planck inequality (Truesdell and Toupin, 1960), 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:

$$\Delta S \geq \int_A^B \frac{\delta Q}{\theta} \quad (3.36)$$

where ΔS is the entropy change in \mathcal{B} , and δQ is the path dependent heat exchanged between \mathcal{B} and its surroundings. Since the total quantity of heat δQ results from the exchange with the surroundings through the boundaries and the presence of internal sources, equation (3.36) can be rewritten as:

$$\frac{\partial}{\partial t} \int_{\mathcal{B}} \rho s \, dV \geq - \int_{\partial \mathcal{B}} \frac{1}{\theta} \bar{\mathbf{q}} \cdot \hat{\mathbf{n}} \, dS + \int_{\mathcal{B}} \rho \frac{r}{\theta} \, dV \quad (3.37)$$

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

$$\rho \dot{s} + \nabla \cdot \frac{\bar{\mathbf{q}}}{\theta} - \rho \frac{r}{\theta} \geq 0 \quad (3.38)$$

Next, eliminating r between equations (3.35) and (3.38) and introducing the Helmholtz free energy density ψ as the Legendre transformation of u with respect to s , i.e. $\psi = u - \theta s$, we obtain the local dissipation inequality:

$$-\rho(\dot{\psi} + s\dot{\theta}) + \bar{\boldsymbol{\sigma}} : \dot{\bar{\boldsymbol{\varepsilon}}} - \frac{1}{\theta} (\bar{\mathbf{q}} \cdot \nabla \theta) \geq 0 \quad (3.39)$$

Inequality (3.39) is known as the Clausius-Duhem inequality.

3.8 Free energy density and energetic constitutive relationships

The free energy density ψ can be taken as a function of the elastic strain and \mathbf{a} , the set of internal variables, such that $\psi = \hat{\psi}(\bar{\boldsymbol{\varepsilon}}^e, \mathbf{a})$. Following (Coleman and Mizel, 1963), we know that ψ is independent of $\nabla \theta$ and higher gradients of θ , i.e. $\nabla^n \theta, n \geq 2$.

Recalling from equation (3.7) that $\bar{\boldsymbol{\varepsilon}}^e = \bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p - \bar{\boldsymbol{\varepsilon}}^\theta$, we have $\psi \equiv \hat{\psi}(\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p - \bar{\boldsymbol{\varepsilon}}^\theta, \mathbf{a}) \equiv \hat{\psi}(\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p, \theta, \mathbf{a})$. The time derivative of ψ can be defined as:

$$\dot{\psi} = \frac{\partial \psi}{\partial (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p)} : (\dot{\bar{\boldsymbol{\varepsilon}}} - \dot{\bar{\boldsymbol{\varepsilon}}^p}) + \frac{\partial \psi}{\partial \theta} \dot{\theta} + \frac{\partial \psi}{\partial \mathbf{a}} \cdot \dot{\mathbf{a}} \quad (3.40)$$

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 (3.40) in (3.39), adding and subtracting $\bar{\boldsymbol{\sigma}} : \dot{\bar{\boldsymbol{\varepsilon}}^p}$, and rearranging terms gives:

$$-\left(\rho \frac{\partial \psi}{\partial(\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p)} - \bar{\boldsymbol{\sigma}}\right) : (\dot{\bar{\boldsymbol{\varepsilon}}} - \dot{\bar{\boldsymbol{\varepsilon}}}^p) - \rho \left(\frac{\partial \psi}{\partial \theta} + s\right) \dot{\theta} - \rho \frac{\partial \psi}{\partial \mathbf{a}} \cdot \dot{\mathbf{a}} + \bar{\boldsymbol{\sigma}} : \dot{\bar{\boldsymbol{\varepsilon}}}^p - \frac{1}{\theta} (\bar{\mathbf{q}} \cdot \nabla \theta) \geq 0 \quad (3.41)$$

For the inequality (3.41) to hold, the following conditions need to be satisfied (Coleman and Gurtin, 1967):

$$\bar{\boldsymbol{\sigma}} = \frac{\partial(\rho \psi)}{\partial(\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p)} \quad (3.42)$$

$$s = -\frac{1}{\rho} \frac{\partial(\rho \psi)}{\partial \theta} \quad (3.43)$$

Note that the term $-\rho \frac{\partial \psi}{\partial \mathbf{a}} \cdot \dot{\mathbf{a}}$ is known as internal dissipation and in the general case:

$$\frac{\partial \psi}{\partial \mathbf{a}} \neq 0 \quad (3.44)$$

In this work, we shall restrict ourselves to the case where ψ is independent of \mathbf{a} , i.e. $\psi = \hat{\psi}(\bar{\boldsymbol{\varepsilon}}^e(\theta)) = \hat{\psi}(\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p, \theta)$; note that dependence on internal variables can also be considered (Acharya, 2010), however, it is not necessary for present purposes. Using the axiom of equipresence (Truesdell and Toupin, 1960), we have $\bar{\boldsymbol{\sigma}} = \hat{\bar{\boldsymbol{\sigma}}}(\bar{\boldsymbol{\varepsilon}}^e(\theta)) = \hat{\bar{\boldsymbol{\sigma}}}(\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p, \theta)$ and $s = \hat{s}(\bar{\boldsymbol{\varepsilon}}^e(\theta)) = \hat{s}(\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p, \theta)$.

Let us assume that the initial state of \mathcal{B} is characterized by $\bar{\boldsymbol{\alpha}}_0(\bar{\mathbf{x}}) \neq \mathbf{0}$, $\bar{\boldsymbol{\varepsilon}}_0^p(\bar{\mathbf{x}}) \neq \mathbf{0}$, $\bar{\boldsymbol{\sigma}}_0(\bar{\mathbf{x}}) \neq \mathbf{0}$ and $s_0(\bar{\mathbf{x}}) \neq 0 \exists \bar{\mathbf{x}} \in V$, and $\bar{\boldsymbol{\varepsilon}}_0(\bar{\mathbf{x}}) = \mathbf{0}$ and $\theta(\bar{\mathbf{x}}) = \theta_0 \neq 0, \forall \bar{\mathbf{x}} \in V$. In this initial/reference state as well as any subsequent states, ψ must be positive. In the absence of dislocations and at zero deformation, we assume $\psi = \psi_0 = 0$. ψ should be independent of rigid body displacements. Recalling that we are in the case of small strains but large variations in θ are allowed, a simple expression for ψ that fulfills all these conditions is (Maitournam, 2017):

$$\rho \psi = \bar{\boldsymbol{\sigma}}_0 : (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) - \rho s_0 \Delta \theta + \frac{1}{2} (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) : \bar{\bar{\mathbf{c}}} : (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) - \Delta \theta \bar{\bar{\boldsymbol{\beta}}} : (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) - \rho c_\varepsilon \theta \left(\ln \frac{\theta}{\theta_0} - 1 + \frac{\theta_0}{\theta} \right) \quad (3.45)$$

where $\bar{\bar{\mathbf{c}}}$ is the fourth order elastic stiffness tensor, $\bar{\bar{\boldsymbol{\beta}}} = \bar{\bar{\mathbf{c}}} : \bar{\bar{\boldsymbol{\gamma}}}$ is the second order thermal moduli tensor, c_ε is the specific heat capacity at constant strain, $\bar{\boldsymbol{\sigma}}_0 = -\bar{\bar{\mathbf{c}}} : \bar{\boldsymbol{\varepsilon}}_0^p$ is the initial local stress in our body containing dislocations and $\Delta \theta = \theta - \theta_0$. While deriving expression (3.45), it has been assumed that variations in $\bar{\bar{\mathbf{c}}}$, $\bar{\bar{\boldsymbol{\gamma}}}$, ρ and c_ε with respect to θ are negligible and these values are evaluated at $\bar{\boldsymbol{\varepsilon}}_0(\bar{\mathbf{x}}) = \mathbf{0}$ and θ_0 . From equations (3.42) and (3.43), we have the following constitutive laws:

$$\bar{\boldsymbol{\sigma}} = \bar{\boldsymbol{\sigma}}_0 + \bar{\bar{\mathbf{c}}} : (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) - \bar{\bar{\boldsymbol{\beta}}} \Delta \theta \quad (3.46)$$

$$s = s_0 + \frac{1}{\rho} (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) : \bar{\bar{\boldsymbol{\beta}}} + c_\varepsilon \ln \frac{\theta}{\theta_0} \quad (3.47)$$

Equation (3.46) 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 that $\bar{\boldsymbol{\varepsilon}}^p$ contains contributions from both $\bar{\boldsymbol{\varepsilon}}^{p\parallel}$ and $\bar{\boldsymbol{\varepsilon}}^{p\perp}$ and we have bypassed the Stokes-Helmholtz decomposition (3.10a) for $\bar{\boldsymbol{\varepsilon}}^\theta$ by directly using the relationship (3.10b). Furthermore, we have also not attempted to obtain an expression for s_0 ; it is more convenient to follow the evolution of $\Delta s = s - s_0 = \frac{1}{\rho} (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) : \bar{\bar{\boldsymbol{\beta}}} + c_\varepsilon \ln \frac{\theta}{\theta_0}$.

3.9 Dissipative constitutive relationships

Now, using equations (3.42) – (3.43) and neglecting $-\rho \frac{\partial \psi}{\partial \mathbf{a}} \cdot \dot{\mathbf{a}}$, inequality (3.41) reduces to the local dissipation inequality:

$$d = \bar{\sigma} : \dot{\bar{\epsilon}}^p - \frac{1}{\theta} (\bar{q} \cdot \nabla \theta) \geq 0 \quad (3.48)$$

which gives the global thermo-mechanical dissipation rate D :

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

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. For the inequality (3.49) to be always satisfied, $\int_B \bar{\sigma} : \dot{\bar{\epsilon}}^p dV \geq 0$ and $\int_B \frac{1}{\theta} (\bar{q} \cdot \nabla \theta) dV \leq 0$ should be independently satisfied at any given instant in time. There are infinite possible expressions for $\dot{\bar{\epsilon}}^p$ and \bar{q} that can respectively satisfy these conditions. For simplicity, we shall assume that $\dot{\bar{\epsilon}}^p = \widehat{\dot{\bar{\epsilon}}^p}(\bar{\sigma}, \theta)$ and $\bar{q} = \widehat{\bar{q}}(\theta, \nabla \theta, (\bar{\epsilon} - \bar{\epsilon}^p))$.

Focusing on the first part of the dissipation inequality (3.49), it is well-known that $\dot{\bar{\epsilon}}^p$ is non-linearly dependent on $\bar{\sigma}$ and θ . While the Clausius-Duhem inequality would allow dependence on additional variables, for the present purposes, only the dependence on $\bar{\sigma}$ and θ is considered. Note that due to the symmetry of the Cauchy stress tensor, we have $\int_B \bar{\sigma} : \dot{\bar{\epsilon}}^p dV = \int_B \bar{\sigma} : \dot{\bar{U}}^p dV \geq 0$. Following (Acharya, 2003; Acharya and Roy, 2006), it can be shown that

$$\int_B \bar{\sigma} : \dot{\bar{U}}^p dV = \int_B \bar{\sigma} : \dot{\bar{U}}^p dV - \int_B \bar{W}_\sigma : \bar{s}^p dV \quad (3.50a)$$

where \bar{W}_σ is such that it satisfies $\nabla \times \bar{W}_\sigma = \bar{\sigma}^\perp$ with $\bar{\sigma}^\perp$ being the incompatible part of the Cauchy stress tensor. Using equation (3.30) we get:

$$\begin{aligned} \int_B \bar{\sigma} : \dot{\bar{U}}^p dV &= \int_B \sum_{i=1}^{N_\beta} (\bar{\sigma} \cdot \bar{\alpha}^{p,\beta_i}) : \bar{X} \cdot \bar{V}^{p,\beta_i} dV - \int_B \bar{W}_\sigma : \bar{s}^p dV \\ &= \int_B \sum_{i=1}^{N_\beta} \bar{F}^{p,\beta_i} \cdot \bar{V}^{p,\beta_i} dV - \int_B \bar{W}_\sigma : \bar{s}^p dV \end{aligned} \quad (3.50b)$$

where $\bar{F}^{p,\beta_i} = (\bar{\sigma} \cdot \bar{\alpha}^{p,\beta_i}) : \bar{X}$.

Focusing first on the second term on the right hand side of equation (3.50b), since we have to satisfy the condition (3.21), i.e. $\nabla \cdot \bar{\alpha}^p = \mathbf{0}$, we can deduce that \bar{s}^p has to satisfy the constraint $\nabla \cdot \bar{s}^p = \mathbf{0}$, which allows to define $\bar{s}^p = \sum_{i=1}^{N_\beta} \bar{s}^{p,\beta_i} = \nabla \times \bar{\Omega}$, for a given $\bar{\Omega}$ (Acharya, 2003). Substituting this constraint in equation (3.50b) gives:

$$\int_B \bar{\sigma} : \dot{\bar{U}}^p dV = \int_B \sum_{i=1}^{N_\beta} \bar{F}^{p,\beta_i} \cdot \bar{V}^{p,\beta_i} dV - \int_B \bar{\sigma}^\perp : \bar{\Omega} dV \quad (3.50c)$$

$\bar{\Omega}$ is interpreted as a nucleation rate (Acharya, 2004, 2003). Focusing now on the first term on the right-hand side of equation (3.50c) and substituting equation (3.22) in the expression for \bar{F}^{p,β_i} we have:

$$\bar{F}^{p,\beta_i} = \frac{1}{V} (\bar{\sigma} \cdot \bar{b}^{p,\beta_i}) \times \bar{l}^{p,\beta_i} \quad (3.51)$$

Equation (3.51) is the well-known Peach-Koehler (PK) force used in dislocation dynamics simulations as the mechanical driving force for dislocation motion. Note that \bar{F}^{p,β_i} is also a function of θ through its dependence on $\bar{\sigma}$, \bar{b}^{p,β_i} and \bar{l}^{p,β_i} . To ensure that inequality (3.50) is respected under all circumstances (including presence/absence of \bar{s}^p), it is necessary that $\bar{F}^{p,\beta_i} \cdot \bar{V}^{p,\beta_i} \geq 0$ for each slip system β at every material point. The simplest way to ensure this is to assume the following linear relationship:

$$\bar{V}^{p,\beta_i} = \frac{1}{B^{p,\beta_i}} \bar{F}^{p,\beta_i} \quad (3.52)$$

where $B^{p,\beta_i} > 0$ is a material parameter, which is the inverse of the dislocation mobility and also depends on $\bar{\sigma}$ and θ (Olmsted et al., 2005). Equations (3.51) and (3.52) also include out-of-slip-plane components of the dislocation driving force and velocity, which are necessary to allow climb and cross-slip mechanisms as well as account for non-Schmid effects (Acharya, 2003).

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

$$F_g^\beta(\bar{\sigma}, \theta) = \bar{\mathbf{F}}^\beta(\bar{\sigma}, \theta) \cdot \frac{(\hat{\mathbf{n}}^\beta \times \bar{\mathbf{l}}^\beta)}{|\hat{\mathbf{n}}^\beta \times \bar{\mathbf{l}}^\beta|} \quad (3.53a)$$

$$F_c^\beta(\bar{\sigma}, \theta) = \bar{\mathbf{F}}^\beta(\bar{\sigma}, \theta) \cdot \hat{\mathbf{n}}^\beta \quad (3.53b)$$

$$F_n^\beta(\bar{\sigma}, \theta) = \bar{\mathbf{F}}^\beta(\bar{\sigma}, \theta) \cdot \frac{\bar{\mathbf{l}}^\beta}{|\bar{\mathbf{l}}^\beta|} \quad (3.53c)$$

Equations (3.53a), (3.53b) and (3.53c) account for both edge and screw dislocations. Dislocation velocity $\bar{\mathbf{V}}^\beta$ can also be decomposed into glide $\bar{\mathbf{V}}_g^\beta$, climb $\bar{\mathbf{V}}_c^\beta$ and normal to glide and climb components $\bar{\mathbf{V}}_n^\beta$. Decomposing the velocity into components requires adopting a non-linear crystal elasticity approach in order to represent individual dislocations with compact cores, i.e. to avoid unrealistic spread of the dislocation core, and capture the effects of Peierls stresses (Acharya, 2003; Zhang et al., 2015). Note that more complex relationships for each velocity component may become necessary at different θ ; for example, different $B^\beta(\bar{\sigma}, \theta)$ can be used for the glide and climb velocity components. Furthermore, a distinction between the mobility $(1/B^\beta(\bar{\sigma}, \theta))$ of edge and screw components (Zhu et al., 2013) and their dependence on temperature will also become important.

Focusing now on the second part of the dissipation inequality (3.49), 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 well-known generalized Fourier law for heat conduction:

$$\bar{\mathbf{q}}(\theta, \nabla \theta, (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p)) = -\bar{\mathbf{K}}(\theta, (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p)) \cdot \nabla \theta \quad (3.54)$$

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 θ and $(\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p)$.

Coleman and Mizel (Coleman and Mizel, 1963) noteworthy viewed the Fourier law (3.54) as a limiting approximation, valid only for sufficiently homogeneous temperature fields, to a general nonlinear constitutive assumption for $\bar{\mathbf{q}}$. Noting that $\bar{\mathbf{q}}$ is more sensitive to $\nabla \theta$ than any $\nabla^n \theta$ ($n \geq 2$), they argued that a nonlinear constitutive assumption of $\bar{\mathbf{q}}$ is more appropriate for a heterogeneous temperature distribution and provided corrections to the Fourier law involving a dependence on higher gradients of temperature.

3.10 Temperature rate

In order to obtain the temperature rate $\dot{\theta}$, we shall use equation (3.40) in the rate form of the Legendre transform of the internal energy density $u = \psi + \theta s$ to obtain:

$$\dot{u} = \dot{\psi} + s\dot{\theta} + \theta\dot{s} = \frac{1}{\rho} \bar{\boldsymbol{\sigma}} : (\dot{\bar{\boldsymbol{\varepsilon}}} - \dot{\bar{\boldsymbol{\varepsilon}}}^p) + \theta\dot{s} \quad (3.55)$$

Next, in equation (3.55), we substitute $s = -\partial\psi/\partial\theta$ from equation (3.43), expand $\dot{\psi}$ via equation (3.40) while neglecting internal variables, and rearrange terms to get:

$$\rho \dot{u} = \bar{\sigma} : (\dot{\bar{\epsilon}} - \dot{\bar{\epsilon}}^p) + \theta \bar{\beta} : (\dot{\bar{\epsilon}} - \dot{\bar{\epsilon}}^p) + \rho c_\epsilon \dot{\theta} \quad (3.56)$$

Inserting equation (3.56) into equation (3.35) gives:

$$\rho c_\epsilon \dot{\theta} = \nabla \cdot (\bar{\mathbf{K}} \cdot \nabla \theta) + \bar{\sigma} : \dot{\bar{\epsilon}}^p - \theta \bar{\beta} : (\dot{\bar{\epsilon}} - \dot{\bar{\epsilon}}^p) + \rho r \quad (3.57)$$

Equation (3.57) complements equation (3.29) to show the intimate relationship between dislocation and thermal quasi-dislocation evolutions, and how one can act as a source/sink for the other. Note that due to the symmetry of $\bar{\sigma}$ and $\bar{\beta}$, we have $\bar{\sigma} : \dot{\bar{\epsilon}}^p = \bar{\sigma} : \dot{\bar{\mathbf{U}}}^p$ and $\bar{\beta} : (\dot{\bar{\epsilon}} - \dot{\bar{\epsilon}}^p) = \bar{\beta} : (\dot{\bar{\mathbf{U}}} - \dot{\bar{\mathbf{U}}}^p)$ with $\dot{\bar{\mathbf{U}}}^p$ containing contributions from both $\dot{\bar{\mathbf{U}}}^{p\parallel}$ and $\dot{\bar{\mathbf{U}}}^{p\perp}$. This demonstrates that dislocation generation/annihilation/motion results in local temperature changes. If we consider a steady-state heat conduction situation with non-evolving dislocations, then we have $\dot{\theta} = 0$. However, if a stationary dislocation begins to move, say under an applied mechanical load, then its motion will cause $\dot{\theta} \neq 0$. Consequently, heat conduction would no longer be steady state. In turn, the temperature change would result in the evolution of the thermal quasi-dislocation density through the relationship for $\dot{\bar{\alpha}}^\theta$ presented in equation set (3.25).

Since ρr corresponds to heat losses to the surroundings, it is possible that some part of $\bar{\sigma} : \dot{\bar{\epsilon}}^p$ does not result in an increase in θ but it is dissipated as heat to the surroundings. If we neglect other heat loss terms, then $\bar{\sigma} : \dot{\bar{\epsilon}}^p + \rho r$ could be replaced with a term $\eta \bar{\sigma} : \dot{\bar{\epsilon}}^p$ (with $0 < \eta \leq 1$) such that equation (3.57) becomes $\rho c_\epsilon \dot{\theta} = \nabla \cdot (\bar{\mathbf{K}} \cdot \nabla \theta) + \eta \bar{\sigma} : \dot{\bar{\epsilon}}^p - \theta \bar{\beta} : (\dot{\bar{\epsilon}} - \dot{\bar{\epsilon}}^p)$. η can be thought of as the single crystal level equivalent of the so-called Taylor-Quinney factor (Taylor and Quinney, 1934). For $\eta < 1$, we have some portion of the plastic work rate that is dissipated as heat lost to the surroundings and the remaining part results in a change in the temperature. For $\eta = 1$, all the plastic work rate goes to changing the temperature, which corresponds to the case of “adiabatic shearing” if the heat-flux boundary condition is equal to zero.

Note that in the absence of plastic activity, equation (3.57) reduces to the well-known temperature rate equation in thermoelasticity, i.e. $\rho c_\epsilon \dot{\theta} = \nabla \cdot (\bar{\mathbf{K}} \cdot \nabla \theta) - \theta \bar{\beta} : \dot{\bar{\epsilon}} + \rho r$.

3.11 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} \bar{\mathbf{U}} &= \bar{\mathbf{U}}^e + \bar{\mathbf{U}}^p + \bar{\epsilon}^\theta = \bar{\mathbf{U}}^{e\parallel} + \bar{\mathbf{U}}^{p\parallel} + \bar{\mathbf{U}}^{\theta\parallel} \quad \text{and} \quad \bar{\mathbf{U}}^{e\perp} + \bar{\mathbf{U}}^{p\perp} + \bar{\mathbf{U}}^{\theta\perp} = \mathbf{0} \\ \bar{\epsilon}^\theta &= \left[\frac{1}{2} (\nabla \nabla \Phi + \nabla \Phi \nabla + \nabla (\nabla \times \bar{\mathbf{b}}')) \right] + \left[\frac{1}{2} (\nabla \times \bar{\mathbf{b}}') \nabla + \nabla \times \bar{\xi} \times \nabla \right] = \bar{\gamma} \Delta \theta \\ \bar{\alpha} &= \nabla \times \bar{\mathbf{U}}^{e\perp} = -\nabla \times \bar{\mathbf{U}}^{p\perp} - \nabla \times \bar{\mathbf{U}}^{\theta\perp} = \bar{\alpha}^p + \bar{\alpha}^\theta \\ \dot{\bar{\mathbf{U}}}^p &= \sum_{i=1}^{N_\beta} \dot{\bar{\mathbf{U}}}^{p,\beta_i} = \sum_{i=1}^{N_\beta} \bar{\alpha}^{\beta_i} \times \bar{\mathbf{V}}^{\beta_i} \quad \text{and} \quad \dot{\bar{\mathbf{U}}}^{p\parallel} = \dot{\bar{\mathbf{U}}}^{p\parallel} \\ \dot{\bar{\alpha}}^{p,\beta_i} &= -\nabla \times \dot{\bar{\mathbf{U}}}^{p,\beta_i} + \bar{\mathbf{s}}^{p,\beta_i} = -\nabla \times (\bar{\alpha}^{p,\beta_i} \times \bar{\mathbf{V}}^{p,\beta_i}) + \bar{\mathbf{s}}^{p,\beta_i} \quad \text{and} \quad \bar{\alpha}^p = \sum_{i=1}^{N_\beta} \bar{\alpha}^{p,\beta_i} \\ \dot{\bar{\alpha}}^\theta &= (\nabla \times \dot{\bar{\gamma}}) \Delta \theta + (\nabla \times \bar{\gamma}) \dot{\theta} - \dot{\bar{\gamma}} \cdot [\nabla (\Delta \theta) \cdot \bar{\mathbf{X}}] - \bar{\gamma} \cdot [\nabla (\Delta \theta) \cdot \bar{\mathbf{X}}] \\ \dot{\bar{\alpha}} &= \nabla \times \dot{\bar{\mathbf{U}}}^{e\perp} = \dot{\bar{\alpha}}^p + \dot{\bar{\alpha}}^\theta = -\sum_{i=1}^{N_\beta} [\nabla \times (\bar{\alpha}^{p,\beta_i} \times \bar{\mathbf{V}}^{p,\beta_i}) - \bar{\mathbf{s}}^{p,\beta_i}] + \dot{\bar{\alpha}}^\theta \\ \bar{\sigma} &= \bar{\mathbf{c}} : \bar{\epsilon}^e = \bar{\mathbf{c}} : (\bar{\epsilon} - \bar{\epsilon}^p) - \bar{\beta} \Delta \theta \\ \bar{\mathbf{q}} &= -\bar{\mathbf{K}} \cdot \nabla \theta \\ \bar{\mathbf{V}}^{p,\beta_i} &= \frac{1}{B^{p,\beta_i}} \bar{\mathbf{F}}^{p,\beta_i} = \frac{1}{B^{p,\beta_i}} (\bar{\sigma} \cdot \bar{\mathbf{b}}^{p,\beta_i}) \times \bar{\mathbf{l}}^{p,\beta_i} \\ \rho \ddot{\mathbf{u}} &= \nabla \cdot \bar{\sigma} + \rho \bar{\mathbf{f}} \\ \rho c_\epsilon \dot{\theta} &= \nabla \cdot (\bar{\mathbf{K}} \cdot \nabla \theta) + \bar{\sigma} : \dot{\bar{\epsilon}}^p - \theta \bar{\beta} : (\dot{\bar{\epsilon}} - \dot{\bar{\epsilon}}^p) + \rho r \end{aligned} \quad (3.58)$$

3.12 Special cases of the T-FDM model

From the equation set (3.58) of the T-FDM model, it is possible to straightforwardly recover the equation sets for the conventional FDM, thermoelasticity, etc.

3.12.1 T-FDM with stationary dislocations

For a system subjected to mechanical loading and transient heat-flux/temperature boundary conditions without the motion of dislocations, i.e. $\dot{\bar{\mathbf{U}}}^p = \mathbf{0}$, we have $\dot{\bar{\mathbf{U}}}^{p\parallel} = \mathbf{0}$ but $\dot{\bar{\mathbf{\epsilon}}}^{p\perp} = \text{sym}(\dot{\bar{\mathbf{U}}}^{p\perp}) \neq \mathbf{0}$ (see section 3.2). In this case, equation set (3.58) reduces to:

$$\begin{aligned}
\bar{\mathbf{U}} &= \bar{\mathbf{U}}^e + \bar{\mathbf{U}}^p + \bar{\mathbf{\epsilon}}^\theta = \bar{\mathbf{U}}^{e\parallel} + \bar{\mathbf{U}}^{p\parallel} + \bar{\mathbf{U}}^{\theta\parallel} \quad \text{and} \quad \bar{\mathbf{U}}^{e\perp} + \bar{\mathbf{U}}^{p\perp} + \bar{\mathbf{U}}^{\theta\perp} = \mathbf{0} \\
\bar{\mathbf{\epsilon}}^\theta &= \left[\frac{1}{2} (\nabla \nabla \Phi + \nabla \Phi \nabla + \nabla (\nabla \times \bar{\mathbf{b}}')) \right] + \left[\frac{1}{2} (\nabla \times \bar{\mathbf{b}}') \nabla + \nabla \times \bar{\boldsymbol{\zeta}} \times \nabla \right] = \bar{\boldsymbol{\gamma}} \Delta \theta \\
\bar{\boldsymbol{\alpha}} &= \nabla \times \bar{\mathbf{U}}^{e\perp} = -\nabla \times \bar{\mathbf{U}}^{p\perp} - \nabla \times \bar{\mathbf{U}}^{\theta\perp} = \bar{\boldsymbol{\alpha}}^p + \bar{\boldsymbol{\alpha}}^\theta \\
\dot{\bar{\mathbf{U}}}^p &= \sum_{i=1}^{N_\beta} \dot{\bar{\mathbf{U}}}^{p,\beta_i} = \mathbf{0} \quad \text{and} \quad \bar{\mathbf{U}}^{p\parallel} = \bar{\bar{\mathbf{U}}}^{p\parallel} \\
\dot{\bar{\boldsymbol{\alpha}}}^{p,\beta_i} &= \bar{\bar{\mathbf{s}}}^{p,\beta_i} \quad \text{and} \quad \bar{\boldsymbol{\alpha}}^p = \sum_{i=1}^{N_\beta} \bar{\bar{\boldsymbol{\alpha}}}^{p,\beta_i} \\
\dot{\bar{\boldsymbol{\alpha}}}^\theta &= (\nabla \times \bar{\boldsymbol{\gamma}}) \Delta \theta + (\nabla \times \bar{\boldsymbol{\gamma}}) \dot{\theta} - \dot{\bar{\boldsymbol{\gamma}}} \cdot [\nabla (\Delta \theta) \cdot \bar{\bar{\mathbf{X}}}] - \bar{\boldsymbol{\gamma}} \cdot [\nabla (\Delta \theta) \cdot \bar{\bar{\mathbf{X}}}] \\
\dot{\bar{\boldsymbol{\alpha}}} &= \nabla \times \dot{\bar{\mathbf{U}}}^{e\perp} = \bar{\bar{\mathbf{s}}}^{p,\beta} + \dot{\bar{\boldsymbol{\alpha}}}^\theta \\
\bar{\boldsymbol{\sigma}} &= \bar{\bar{\mathbf{c}}}: \bar{\bar{\boldsymbol{\epsilon}}}^e = \bar{\bar{\mathbf{c}}}: (\bar{\bar{\boldsymbol{\epsilon}}} - \bar{\bar{\boldsymbol{\epsilon}}}^p) - \bar{\bar{\boldsymbol{\beta}}} \Delta \theta \\
\bar{\mathbf{q}} &= -\bar{\bar{\mathbf{K}}} \cdot \nabla \bar{\theta} \\
\rho \ddot{\bar{\mathbf{u}}} &= \nabla \cdot \bar{\bar{\boldsymbol{\sigma}}} + \rho \bar{\mathbf{f}} \\
\rho c_\varepsilon \dot{\theta} &= \nabla \cdot (\bar{\bar{\mathbf{K}}} \cdot \nabla \bar{\theta}) + \bar{\bar{\boldsymbol{\sigma}}}: \dot{\bar{\boldsymbol{\epsilon}}}^{p\perp} - \theta \bar{\bar{\boldsymbol{\beta}}}: (\dot{\bar{\boldsymbol{\epsilon}}} - \dot{\bar{\boldsymbol{\epsilon}}}^{p\perp}) + \rho r
\end{aligned} \tag{3.59}$$

3.12.2 T-FDM with stationary dislocations and steady-state heat conduction

For a system containing dislocations subjected to a steady-state heat-flux/temperature boundary condition without any mechanical loading such that the dislocations remain stationary, equation set (3.58) reduces to:

$$\begin{aligned}
\bar{\mathbf{U}} &= \bar{\mathbf{U}}^e + \bar{\mathbf{U}}^p + \bar{\mathbf{\epsilon}}^\theta = \bar{\mathbf{U}}^{e\parallel} + \bar{\mathbf{U}}^{p\parallel} + \bar{\mathbf{U}}^{\theta\parallel} \quad \text{and} \quad \bar{\mathbf{U}}^{e\perp} + \bar{\mathbf{U}}^{p\perp} + \bar{\mathbf{U}}^{\theta\perp} = \mathbf{0} \\
\bar{\mathbf{\epsilon}}^\theta &= \left[\frac{1}{2} (\nabla \nabla \Phi + \nabla \Phi \nabla + \nabla (\nabla \times \bar{\mathbf{b}}')) \right] + \left[\frac{1}{2} (\nabla \times \bar{\mathbf{b}}') \nabla + \nabla \times \bar{\boldsymbol{\zeta}} \times \nabla \right] = \bar{\boldsymbol{\gamma}} \Delta \theta \\
\bar{\boldsymbol{\alpha}} &= \nabla \times \bar{\mathbf{U}}^{e\perp} = -\nabla \times \bar{\mathbf{U}}^{p\perp} - \nabla \times \bar{\mathbf{U}}^{\theta\perp} = \bar{\boldsymbol{\alpha}}^p + \bar{\boldsymbol{\alpha}}^\theta \\
\dot{\bar{\boldsymbol{\alpha}}} &= \mathbf{0} \quad \text{and} \quad \dot{\bar{\boldsymbol{\alpha}}}^{p,\beta_i} = \mathbf{0} \quad \text{and} \quad \dot{\bar{\boldsymbol{\alpha}}}^\theta = \mathbf{0} \\
\bar{\boldsymbol{\alpha}}^p &= \sum_{i=1}^{N_\beta} \bar{\bar{\boldsymbol{\alpha}}}^{p,\beta_i} \\
\dot{\bar{\mathbf{U}}}^p &= \sum_{i=1}^{N_\beta} \dot{\bar{\mathbf{U}}}^{p,\beta_i} = \mathbf{0} \quad \text{and} \quad \bar{\mathbf{U}}^{p\parallel} = \bar{\bar{\mathbf{U}}}^{p\parallel} \\
\bar{\boldsymbol{\sigma}} &= \bar{\bar{\mathbf{c}}}: \bar{\bar{\boldsymbol{\epsilon}}}^e = \bar{\bar{\mathbf{c}}}: (\bar{\bar{\boldsymbol{\epsilon}}} - \bar{\bar{\boldsymbol{\epsilon}}}^p) - \bar{\bar{\boldsymbol{\beta}}} \Delta \theta \\
\bar{\mathbf{q}} &= -\bar{\bar{\mathbf{K}}} \cdot \nabla \bar{\theta} \\
\mathbf{0} &= \nabla \cdot \bar{\bar{\boldsymbol{\sigma}}} + \rho \bar{\mathbf{f}}
\end{aligned} \tag{3.60}$$

3.12.3 FDM at reference temperature

In the case of an isothermal and adiabatic system at reference temperature, equation set (3.58) reduces to those of the geometrically linear FDM model.

$$\begin{aligned}
\bar{\mathbf{U}} &= \bar{\mathbf{U}}^e + \bar{\mathbf{U}}^p = \bar{\mathbf{U}}^{e\parallel} + \bar{\mathbf{U}}^{p\parallel} \quad \text{and} \quad \bar{\mathbf{U}}^{e\perp} + \bar{\mathbf{U}}^{p\perp} = \mathbf{0} \\
\bar{\boldsymbol{\alpha}} &= \nabla \times \bar{\mathbf{U}}^{e\perp} = -\nabla \times \bar{\mathbf{U}}^{p\perp} = \bar{\boldsymbol{\alpha}}^p \\
\dot{\bar{\boldsymbol{\alpha}}}^{p,\beta_i} &= -\nabla \times \dot{\bar{\mathbf{U}}}^{p,\beta_i} = -\nabla \times (\bar{\boldsymbol{\alpha}}^{p,\beta_i} \times \bar{\mathbf{V}}^{p,\beta_i}) \quad \text{and} \quad \bar{\boldsymbol{\alpha}}^p = \sum_{i=1}^{N_\beta} \bar{\bar{\boldsymbol{\alpha}}}^{p,\beta_i}
\end{aligned}$$

$$\begin{aligned}
\dot{\bar{\mathbf{U}}}^p &= \sum_{i=1}^{N_\beta} \dot{\bar{\mathbf{U}}}^{p,\beta_i} = \sum_{i=1}^{N_\beta} \bar{\boldsymbol{\alpha}}^{p,\beta_i} \times \bar{\mathbf{V}}^{p,\beta_i} \quad \text{and} \quad \bar{\mathbf{U}}^{p\parallel} = \bar{\bar{\mathbf{U}}}^{p\parallel} \\
\bar{\boldsymbol{\alpha}} &= \bar{\bar{\boldsymbol{\alpha}}}^p \\
\bar{\boldsymbol{\sigma}} &= \bar{\bar{\mathbf{c}}}: \bar{\boldsymbol{\varepsilon}}^e = \bar{\bar{\mathbf{c}}}: (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) \\
\bar{\mathbf{V}}^{p,\beta_i} &= \frac{1}{B^{p,\beta_i}} \bar{\mathbf{F}}^{p,\beta_i} = \frac{1}{B^{p,\beta_i}} (\bar{\boldsymbol{\sigma}} \cdot \bar{\mathbf{b}}^{p,\beta_i}) \times \bar{\mathbf{l}}^{p,\beta_i} \\
\rho \ddot{\mathbf{u}} &= \nabla \cdot \bar{\boldsymbol{\sigma}} + \rho \bar{\mathbf{f}}
\end{aligned} \tag{3.61}$$

3.12.4 FDM at arbitrary constant temperature

In the case of an isothermal and adiabatic system at an arbitrary temperature, equation set (3.58) also reduces to those of the geometrically linear FDM model but with the coupling term in equation (3.46).

$$\begin{aligned}
\bar{\mathbf{U}} &= \bar{\mathbf{U}}^e + \bar{\mathbf{U}}^p + \bar{\boldsymbol{\varepsilon}}^\theta = \bar{\mathbf{U}}^{e\parallel} + \bar{\mathbf{U}}^{p\parallel} + \bar{\boldsymbol{\varepsilon}}^{\theta\parallel} \quad \text{and} \quad \bar{\mathbf{U}}^{e\perp} + \bar{\mathbf{U}}^{p\perp} = \mathbf{0} \\
\bar{\boldsymbol{\varepsilon}}^\theta &= \left[\frac{1}{2} (\nabla \nabla \Phi + \nabla \Phi \nabla) \right] = \bar{\bar{\gamma}} \Delta \theta \\
\bar{\boldsymbol{\alpha}} &= \nabla \times \bar{\mathbf{U}}^{e\perp} = -\nabla \times \bar{\mathbf{U}}^{p\perp} = \bar{\boldsymbol{\alpha}}^p \\
\dot{\bar{\boldsymbol{\alpha}}}^{p,\beta_i} &= -\nabla \times \dot{\bar{\mathbf{U}}}^{p,\beta_i} = -\nabla \times (\bar{\boldsymbol{\alpha}}^{p,\beta_i} \times \bar{\mathbf{V}}^{p,\beta_i}) \quad \text{and} \quad \bar{\boldsymbol{\alpha}} = \bar{\boldsymbol{\alpha}}^p = \sum_{i=1}^{N_\beta} \bar{\boldsymbol{\alpha}}^{p,\beta_i} \\
\dot{\bar{\mathbf{U}}}^p &= \sum_{i=1}^{N_\beta} \dot{\bar{\mathbf{U}}}^{p,\beta_i} = \sum_{i=1}^{N_\beta} \bar{\boldsymbol{\alpha}}^{p,\beta_i} \times \bar{\mathbf{V}}^{p,\beta_i} \quad \text{and} \quad \bar{\mathbf{U}}^{p\parallel} = \bar{\bar{\mathbf{U}}}^{p\parallel} \\
\bar{\boldsymbol{\sigma}} &= \bar{\bar{\mathbf{c}}}: \bar{\boldsymbol{\varepsilon}}^e = \bar{\bar{\mathbf{c}}}: (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) - \bar{\bar{\beta}} \Delta \theta \\
\bar{\mathbf{V}}^{p,\beta_i} &= \frac{1}{B^{p,\beta_i}} \bar{\mathbf{F}}^{p,\beta_i} = \frac{1}{B^{p,\beta_i}} (\bar{\boldsymbol{\sigma}} \cdot \bar{\mathbf{b}}^{p,\beta_i}) \times \bar{\mathbf{l}}^{p,\beta_i} \\
\rho \ddot{\mathbf{u}} &= \nabla \cdot \bar{\boldsymbol{\sigma}} + \rho \bar{\mathbf{f}}
\end{aligned} \tag{3.62}$$

3.12.5 Fully-coupled thermoelasticity with thermal quasi-dislocations but no dislocations

In case of a system without dislocations, equation set (3.58) reduces to the following equation set:

$$\begin{aligned}
\bar{\mathbf{U}} &= \bar{\mathbf{U}}^e + \bar{\boldsymbol{\varepsilon}}^\theta = \bar{\mathbf{U}}^{e\parallel} + \bar{\mathbf{U}}^{\theta\parallel} \quad \text{and} \quad \bar{\mathbf{U}}^{e\perp} + \bar{\mathbf{U}}^{\theta\perp} = \mathbf{0} \\
\bar{\boldsymbol{\varepsilon}}^\theta &= \left[\frac{1}{2} (\nabla \nabla \Phi + \nabla \Phi \nabla + \nabla (\nabla \times \bar{\mathbf{b}}')) \right] + \left[\frac{1}{2} (\nabla \times \bar{\mathbf{b}}') \nabla + \nabla \times \bar{\boldsymbol{\zeta}} \times \nabla \right] = \bar{\bar{\gamma}} \Delta \theta \\
\bar{\boldsymbol{\alpha}} &= \nabla \times \bar{\mathbf{U}}^{e\perp} = -\nabla \times \bar{\mathbf{U}}^{\theta\perp} = \bar{\boldsymbol{\alpha}}^\theta \\
\dot{\bar{\boldsymbol{\alpha}}} &= \dot{\bar{\boldsymbol{\alpha}}}^\theta = (\nabla \times \dot{\bar{\gamma}}) \Delta \theta + (\nabla \times \bar{\gamma}) \dot{\theta} - \dot{\bar{\gamma}} \cdot [\nabla (\Delta \theta) \cdot \bar{\mathbf{X}}] - \bar{\gamma} \cdot [\nabla (\Delta \theta) \cdot \bar{\mathbf{X}}] \\
\bar{\boldsymbol{\sigma}} &= \bar{\bar{\mathbf{c}}}: \bar{\boldsymbol{\varepsilon}}^e = \bar{\bar{\mathbf{c}}}: (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^p) - \bar{\bar{\beta}} \Delta \theta \\
\bar{\mathbf{q}} &= -\bar{\bar{\mathbf{K}}} \cdot \nabla \theta \\
\rho \ddot{\mathbf{u}} &= \nabla \cdot \bar{\boldsymbol{\sigma}} + \rho \bar{\mathbf{f}} \\
\rho c_\varepsilon \dot{\theta} &= \nabla \cdot (\bar{\bar{\mathbf{K}}} \cdot \nabla \theta) - \theta \bar{\bar{\beta}}: \dot{\bar{\boldsymbol{\varepsilon}}} + \rho r
\end{aligned} \tag{3.63}$$

4. Discussion and some illustrative examples

4.1 Implications of the adopted thermodynamics framework

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

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 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 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; 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 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.

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 cannot be ignored when considering large 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 (3.42) and (3.43), we can construct the following differential expression for ψ

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

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

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

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

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

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

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

where T is the equilibrium measure of θ .

In this work, by assuming local thermodynamic equilibrium, we have assumed that the temperature distribution is uniform within a subdomain volume represented by a material point in the body. 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. 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 Definition of 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. At the level of continuum mechanics, an expression for entropy is often obtained from an assumed expression for the free energy potential; for example, see expression (3.47) 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).

Acharya (Acharya, 2011) developed an expression for the entropy of an isolated constrained ergodic Hamiltonian system and demonstrated that it is related to the continuum definition of the specific entropy field. The developments were done assuming that the system is a microcanonical ensemble (also known as an N-V-E ensemble, i.e. having constant number of particles N , constant volume V , and constant energy E), which is an isolated system. This allows defining temperature independently of the surroundings; in (Acharya, 2011) it was argued that in continuum mechanics, where a point-wise temperature is required, the definition of temperature should not depend on the temperature of its surroundings. These developments were then applied to a spatially and temporally averaged version of FDM (Acharya, 2011). With respect to the present work, a similar development would require accounting for the fact that the system represented by a continuum material point is no longer isolated and its energy evolves in time. Furthermore, the temperature at a material point will depend on the temperature of its neighboring material points. In this case, a possible solution could be to assume the system is a canonical (an N-V-T) ensemble, which is allowed to exchange heat with the surroundings; this will be explored in a future work.

Statistical mechanics also opens the possibility to account for additional contributions to entropy that are overlooked in the classical formulation where entropy is related to the heat exchanged between the system and its surroundings (see equation (3.38)). However, there exist entropic contributions that do not adhere to the classical definition, such as the configurational entropy associated with dislocation structures (Langer et al., 2010). 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 has been neglected with the argument that compared to other contributions to a system's entropy, its contribution is negligible (Cottrell, 1953). However, Langer et al. (Langer et al., 2010) argued that while the contribution of configurational entropy of dislocations to the total entropy of a large system is small, 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. Under isothermal and adiabatic conditions, the configurational entropy of dislocations will also be a non-decreasing function of time. However, in the presence of a heat flux, the configurational entropy of dislocations may be a decreasing function of time even though the overall entropy is a non-decreasing function of time, which must be respected at any instant in time.

4.2 Some illustrative examples

Let us consider a rectangular parallelepiped domain \mathcal{B} with homogeneous isotropic linear elastic and thermal properties (λ, μ – Lamé constants, γ – coefficient of thermal expansion, k – thermal

conductivity) to be in thermal equilibrium with its surroundings at θ_0 . All material properties are defined at θ_0 and assumed to be constant with respect to temperature and strain rates. Let the body have dimensions $[-H, H]$, $[-L, L]$ and $[-W, W]$ along \hat{e}_1 , \hat{e}_2 and \hat{e}_3 directions, respectively.

4.2.1 Thermal quasi-dislocations due to steady-state heat conduction in an elastic medium without dislocations

Unconstrained system: Traction-free boundary conditions are imposed everywhere on $\partial\mathcal{B}$. The surface normal to $+\hat{e}_2$ is subjected to θ^h ($\theta_{solidus} > \theta^h > \theta_0$) and the surface normal to $-\hat{e}_2$ is kept at θ_0 . Since we are using the Fourier's law of heat conduction (equation (3.54)), a heat-flux $\bar{\mathbf{q}} = -q\hat{e}_2 = -\frac{(\theta^h - \theta_0)}{2L}\hat{e}_2 = -k\theta_{,2}\hat{e}_2$ ($q > 0$) is *instantaneously* generated everywhere in the body resulting in a steady-state heat conduction. This results in the generation of a linear temperature profile through the body, which satisfies equation (3.57). This temperature field induces thermal strains, which are assumed to be spherically symmetric such that $\varepsilon_{11}^\theta = \varepsilon_{22}^\theta = \varepsilon_{33}^\theta = \gamma(\theta(\bar{\mathbf{x}}) - \theta_0)$.

Next, we consider the Beltrami-Mitchell compatibility condition for our traction free boundary condition problem:

$$\sigma_{ij,kk} + \frac{1}{1+\nu}\sigma_{kk,ij} = 0 \quad (4.5)$$

The only statically admissible $\bar{\boldsymbol{\sigma}}$ that satisfies condition (4.5) is $\bar{\boldsymbol{\sigma}} = \bar{\bar{\mathbf{c}}} : \bar{\boldsymbol{\varepsilon}}^e = \bar{\bar{\mathbf{c}}} : (\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^\theta) = \mathbf{0}$. Consequently, we have $\bar{\boldsymbol{\varepsilon}} = \bar{\boldsymbol{\varepsilon}}^\theta = \bar{\bar{\mathbf{U}}}^{\theta\parallel}$. Based on equation (3.10a), this implies that $\bar{\boldsymbol{\varepsilon}}^{\theta\parallel}(\theta) = \text{sym}(\bar{\bar{\mathbf{U}}}^{\theta\parallel}(\theta)) = \nabla\nabla\Phi$ with $\Phi_{,ij} = 0, i \neq j$. In this case, $\bar{\boldsymbol{\alpha}}^\theta = -\nabla \times \bar{\boldsymbol{\varepsilon}}^{\theta\parallel} = \mathbf{0}$.

Therefore, in a stress-free isotropic linear elastic system subjected to a steady-state heat conduction, the thermal strains are compatible, and no thermal quasi-dislocations are generated.

In section 3.1, just after the introduction of the Stokes-Helmholtz decomposition of $\bar{\boldsymbol{\varepsilon}}^\theta$ in equation (3.10b), it was pointed out that it is imperative to determine whether the induced thermal strains are compatible or incompatible prior to performing any tensorial operations using equation (3.10b). The reasoning can be deduced from the above example. If we were to take the curl of equation (3.10b), then components for $\bar{\boldsymbol{\alpha}}^\theta = (\nabla \times \bar{\boldsymbol{\varepsilon}}^\theta)_{,ij} = e_{ijk}\gamma\theta_{,k}$ (assuming $\gamma = \text{constant}$) would be non-zero for the problem at hand. This would imply that the presence of a compatible thermal strain field in a traction-free body results in the formation of stresses, which clearly should not be the case because it would violate static admissibility conditions.

Partially constrained: We now impose $u_1 = u_3 = 0$ on the surfaces normal to $\pm\hat{e}_1$ and $\pm\hat{e}_3$ by placing \mathcal{B} inside a hollow rigid cylinder, which is a perfect insulator, and assume that \mathcal{B} is in perfect frictionless contact with the inside walls of this cylinder. We continue to assume \mathcal{B} is traction-free on the surfaces normal to $\pm\hat{e}_2$. Similar to the previous case, let \mathcal{B} be instantaneously subjected to θ^h on $+\hat{e}_2$ such that a constant heat-flux of $\bar{\mathbf{q}} = -q\hat{e}_2$, a thermal gradient $\theta_{,2} = \frac{q}{k} = \text{constant}$, and spherically symmetric thermal strains $\varepsilon_{11}^\theta = \varepsilon_{22}^\theta = \varepsilon_{33}^\theta = \gamma(\theta(\bar{\mathbf{x}}) - \theta_0)$ are generated. We have $u_2 \neq 0$ and $\varepsilon_{22} = \varepsilon_{22}^\theta$. All other components of $\bar{\mathbf{u}}$ and $\bar{\boldsymbol{\varepsilon}}$ are equal to 0. We now have, $\varepsilon_{11}^e = -\varepsilon_{11}^\theta = \varepsilon_{33}^e = -\varepsilon_{33}^\theta = -\gamma(\theta(\bar{\mathbf{x}}) - \theta_0)$ and the remaining components of $\bar{\boldsymbol{\varepsilon}}^e$ are equal to zero. Based on the above conditions, the only non-zero components of the statically admissible $\bar{\boldsymbol{\sigma}}$ are $\sigma_{11} = \sigma_{33} = -(3\lambda + 2\mu)\gamma(\theta(\bar{\mathbf{x}}) - \theta_0)$, which satisfy the equilibrium equation. We also note that geometrical constraints impose $\bar{\boldsymbol{\omega}} = \bar{\bar{\boldsymbol{\omega}}}^{e\parallel} = \mathbf{0}$ and equation (3.11) imposes $\bar{\bar{\boldsymbol{\omega}}}^{e\perp} = \mathbf{0}$. No dislocations as well as no history of dislocation motion implies $\bar{\bar{\mathbf{U}}}^{p\perp} = \mathbf{0}$ and $\bar{\bar{\mathbf{U}}}^{p\parallel} = \mathbf{0}$, respectively.

Since $\varepsilon_{22} = \varepsilon_{22}^\theta$, therefore ε_{22}^θ is strictly compatible. However, since $\varepsilon_{11} = \varepsilon_{33} = 0$, ε_{11}^θ and ε_{33}^θ are allowed to have contributions from both compatible and incompatible components. Hence, from equation (3.10a), we have $\bar{\alpha}^\theta = -\nabla \times \bar{\varepsilon}^\theta = -\nabla \times \bar{\mathbf{U}}^{\theta\perp} = -\nabla \times \left[\frac{1}{2} (\nabla \times \bar{\mathbf{b}}') \nabla + \nabla \times \bar{\zeta} \times \nabla \right] \neq \mathbf{0}$. If we assume $\bar{\mathbf{b}}' = \mathbf{0}$, then $\bar{\varepsilon}^\theta = \bar{\varepsilon}^{\theta\perp} = \bar{\mathbf{U}}^{\theta\perp}$ and the only non-zero components of $\bar{\alpha}^\theta$ are $\alpha_{13}^\theta = \bar{\varepsilon}_{11,2}^\theta = \gamma \frac{q}{k}$ and $\alpha_{31}^\theta = -\bar{\varepsilon}_{33,2}^\theta = -\gamma \frac{q}{k}$; note here that ε_{22}^θ has not entered in these relationships.

From equation set (3.19), we have $\bar{\alpha} = \nabla \times \bar{\varepsilon}^e = -\nabla \times \bar{\varepsilon}^\theta = \bar{\alpha}^\theta$. The only non-zero components of $\bar{\alpha}$ are $\alpha_{13} = -\bar{\varepsilon}_{11,2}^{e\perp} = \alpha_{13}^\theta = \gamma \frac{q}{k}$ and $\alpha_{31} = \bar{\varepsilon}_{33,2}^{e\perp} = \alpha_{31}^\theta = -\gamma \frac{q}{k}$. From here, we obtain $\bar{\varepsilon}_{11}^{e\perp} = -\gamma \Delta \theta = -\varepsilon_{11}^{\theta\perp}$ and $\bar{\varepsilon}_{33}^{e\perp} = -\gamma \Delta \theta = -\varepsilon_{33}^{\theta\perp}$, which are exact up to a gradient term. Since we also have $\varepsilon_{11}^e = -\varepsilon_{11}^\theta = \varepsilon_{33}^e = -\varepsilon_{33}^\theta$, we could assume that $\varepsilon_{11}^{\theta\parallel} = \varepsilon_{33}^{\theta\parallel} = 0$. Consequently,

$$\sigma_{11} = -(3\lambda + 2\mu)\varepsilon_{11}^{\theta\perp} \quad \text{and} \quad \sigma_{33} = -(3\lambda + 2\mu)\varepsilon_{33}^{\theta\perp} \quad (4.6)$$

These equations imply that for a constrained isotropic linear elastic material subjected to steady-state heat conduction without heat sources, the constraints induce incompatible thermal strains, which result in the generation of incompatible thermal stresses and thermal quasi-dislocations.

Let us now imagine that the body contains dislocations of the kind $\alpha_{13} = \alpha_{13}^p = \gamma \frac{q}{k}$ and $\alpha_{31} = \alpha_{31}^p = -\gamma \frac{q}{k}$ under isothermal conditions at θ_0 . In this case, we have two edge dislocations everywhere in the domain. The first one could have its Burgers and line vectors along directions $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_3$ (or $-\hat{\mathbf{e}}_1$ and $-\hat{\mathbf{e}}_3$), respectively. The second one could have its Burgers and line vectors along directions $-\hat{\mathbf{e}}_3$ and $\hat{\mathbf{e}}_1$ (or $\hat{\mathbf{e}}_3$ and $-\hat{\mathbf{e}}_1$), respectively. Indeed, their presence would be associated with additional components of $\bar{\mathbf{U}}^{e\perp} = -\bar{\mathbf{U}}^{p\perp} \neq \mathbf{0}$ and $\bar{\boldsymbol{\sigma}} \neq \mathbf{0}$. Furthermore, the presence of dislocations also induces incompatible elastic and plastic rotations, which result in the formation of compatible elastic and plastic curvatures $\bar{\boldsymbol{\kappa}}^{e\parallel} = \nabla \bar{\boldsymbol{\omega}}^{e\perp}$ and $\bar{\boldsymbol{\kappa}}^{p\parallel} = \nabla \bar{\boldsymbol{\omega}}^{p\perp} = -\bar{\boldsymbol{\kappa}}^{e\parallel}$, respectively. All these fields will have non-zero gradients. This consideration demonstrates that thermal quasi-dislocations arising from a linear temperature profile under a steady-state condition cannot be transformed into dislocations under these conditions.

4.2.2 A stationary screw dislocation during steady-state heat conduction

Let us consider the case of a straight screw dislocation in an isotropic linear elastic medium at θ_0 . Let the screw dislocation have a Burgers vector $\bar{\mathbf{b}}^p(\theta_0) = b\hat{\mathbf{e}}_3$ and line vector $\bar{\mathbf{l}}^p(\theta_0) = l\hat{\mathbf{e}}_3$. The only non-zero component of $\bar{\alpha}^p$ is $\bar{\alpha}^p(\theta_0) = \alpha_{33}^p(\theta_0)\hat{\mathbf{e}}_3 \otimes \hat{\mathbf{e}}_3$. We shall assume that the body \mathcal{B} is long enough along directions $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$ so that we can impose traction free boundary conditions on the surfaces normal to $\pm\hat{\mathbf{e}}_1$ and $\pm\hat{\mathbf{e}}_2$ without any significant impact on the stress field near the dislocation. We impose periodic boundary conditions along $\hat{\mathbf{e}}_3$ and assume that there is no variation of any field along this direction.

Following (Acharya, 2001), we define

$$\alpha_{33}^p = \begin{cases} \frac{b}{\pi r_0} \left(\frac{1}{r} - \frac{1}{r_0} \right) & ; r < r_0 \\ 0 & ; r \geq r_0 \end{cases} \quad (4.7)$$

where $r = \sqrt{x_1^2 + x_2^2}$ and r_0 defines the limit of the dislocation “core” region. Note that α_{33}^p does not vary along the z -axis. In the presence of this screw dislocation under isothermal conditions at θ_0 , we have $\bar{\mathbf{U}}^{in} = \bar{\mathbf{U}}^{p\perp} = -\bar{\mathbf{U}}^{e\perp}$. The only two non-zero components of $\bar{\mathbf{U}}^{e\perp}$ are $U_{31}^{e\perp}$ and $U_{32}^{e\perp}$. Using the Riemann-Graves integral operator, Acharya (Acharya, 2001) derived the following expressions for $U_{31}^{e\perp}$ and $U_{32}^{e\perp}$:

$$\left. \begin{aligned} U_{31}^{e\perp} &= \begin{cases} -\frac{b}{\pi r_0} \frac{x_2}{r^2} \left(r - \frac{r^2}{2r_0}\right) & ; r < r_0 \\ -\frac{b}{2\pi} \frac{x_2}{r^2} & ; r \geq r_0 \end{cases} \\ U_{32}^{e\perp} &= \begin{cases} \frac{b}{\pi r_0} \frac{x_1}{r^2} \left(r - \frac{r^2}{2r_0}\right) & ; r < r_0 \\ \frac{b}{2\pi} \frac{x_1}{r^2} & ; r \geq r_0 \end{cases} \end{aligned} \right\} \quad (4.8)$$

If we use the following form of the elastic constitutive law $\bar{\sigma} = \bar{\bar{c}}: (\bar{U} - \bar{U}^{in})$ and neglect body forces, then the equilibrium equation $\nabla \cdot \bar{\sigma} = \mathbf{0}$ becomes

$$c_{ijkl} u_{k,lj} = f_i \quad (4.9)$$

where $f_i = c_{imnp} U_{np,m}^{in}$. Following (Berbenni et al., 2014), this equation can be solved in the Fourier space to obtain an expression of the displacement field, and eventually the stress field, as a function of \bar{U}^{in} :

$$\bar{\sigma}(\bar{x}) = \begin{cases} \mathcal{F}^{-1}[(c_{ijkl} \hat{\Gamma}_{klmn}(\bar{\xi}) c_{mnpq} - c_{ijpq}) \hat{U}_{pq}^{in}(\bar{\xi})] & ; \bar{\xi} \neq \mathbf{0} \\ \bar{\bar{\Sigma}} & ; \bar{\xi} = \mathbf{0} \end{cases} \quad (4.10)$$

where an overhead hat implies the Fourier transform of a variable, \mathcal{F}^{-1} is the inverse Fourier transform operator, $\bar{\xi}$ is a vector in Fourier space, $\bar{\bar{\Sigma}} = \langle \bar{\sigma} \rangle$ is the volume averaged stress field that corresponds to the zeroth frequency $\bar{\xi} = \mathbf{0}$ in the Fourier space, $\mathbb{I}_{ijmn} = \delta_{im} \delta_{jn}$, $c_{mnpq} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$ for an isotropic elastic material, and $\hat{\Gamma}_{klmn}(\bar{\xi})$ is the modified Green's operator whose expression for the isotropic linear elastic case is given as:

$$\hat{\Gamma}_{klmn}(\bar{\xi}) = \frac{1}{2\mu \xi^2} (\delta_{km} \xi_n \xi_l + \delta_{kn} \xi_m \xi_l + \delta_{lm} \xi_k \xi_n + \delta_{ln} \xi_k \xi_m) - \frac{\lambda + \mu}{\mu(\lambda + 2\mu)} \frac{\xi_k \xi_l \xi_m \xi_n}{\xi^4} \quad (4.11)$$

Equation (4.10) could have also been used to deduce the relationship (4.6); noting that a multiplication with $\xi_i \xi_j$ in Fourier space corresponds to partial derivatives with respect to x_i and x_j in real space, it is straightforward to obtain equation (4.6) from equation (4.10) for the linearly varying thermal strain components.

For our screw dislocation problem, it can be shown that the only non-zero components of the equilibrated $\bar{\sigma}$ are $\sigma_{31} = \sigma_{13}$ and $\sigma_{32} = \sigma_{23}$, and they are trivially related to $U_{31}^{e\perp} = \mathcal{F}^{-1}[\hat{U}_{31}^{e\perp}]$ and $U_{32}^{e\perp} = \mathcal{F}^{-1}[\hat{U}_{32}^{e\perp}]$, respectively, as

$$\begin{aligned} \sigma_{31} &= \sigma_{13} = \mu U_{31}^{e\perp} \\ \sigma_{32} &= \sigma_{23} = \mu U_{32}^{e\perp} \end{aligned} \quad (4.12)$$

We can deduce from equation (4.8) that $\langle U_{31}^{e\perp} \rangle = \langle U_{32}^{e\perp} \rangle = 0$. Furthermore, the surfaces normal to $\pm \hat{e}_3$ at infinity will experience a non-zero distribution of σ_{13} and σ_{23} whose sum over these surfaces will be zero because $\langle U_{31}^{e\perp} \rangle_S = \langle U_{32}^{e\perp} \rangle_S = 0$; where $\langle \cdot \rangle_S$ represents a sum over a surface.

Next, we impose the same temperature and heat-flux boundary conditions as done in section 4.2.1 to obtain a constant temperature gradient $\theta_{,2} = \frac{q}{k} = \frac{\theta^h - \theta_0}{2L}$ such that the dislocation line experiences the same temperature $\theta^* > \theta_0$ everywhere along the line. This results in an increase in the Burgers vector magnitude $b^* > b$ as well as the line vector magnitude $l^* > l$. The dislocation density α_{33}^p also increases (equation (4.8)) and the dislocation core spreads $r_0^* > r_0$.

Equation (4.12) shows that the body has internal constraints as well as a distribution of σ_{13} and σ_{23} on surfaces normal to $\pm \hat{e}_3$ at infinity due to the presence of the screw dislocation. However, these stresses

do not impede the volume expansion of the body. Hence, similar to the first case in section 4.2, thermal quasi-dislocations will not be generated and the Nye's tensor will be $\bar{\alpha}(\theta) = \alpha_{33}^p(\theta)\hat{e}_3 \otimes \hat{e}_3$

4.2.3 A moving screw dislocation inducing a transient temperature change

Let us reconsider the case of the screw dislocation from section 4.2.2 in a body under isothermal conditions at temperature θ_0 . We assume that the body is periodic along $\pm\hat{e}_3$ and there is no change in any variable along $\pm\hat{e}_3$. Dirichlet boundary conditions $\theta(-H, y, t) = \theta(H, y, t) = \theta(x, -L, t) = \theta(x, L, t) = \theta_0$ are imposed. Traction-free boundary conditions are imposed on surfaces normal to $\pm\hat{e}_1$ and $\pm\hat{e}_2$.

At $t = 0$, we impose a constant shear stress τ along direction $-\hat{e}_3$ on the surface normal to $+\hat{e}_1$ such that we have uniform $\Sigma_{31} = \Sigma_{13} = -\tau$ ($\tau > 0$) everywhere in the domain. This results in a dislocation driving force per unit volume $\bar{\mathbf{F}} = F\hat{e}_2 = \tau b l' \hat{e}_2$, where l' has units m^{-2} . We assume that the dislocation moves with a constant velocity $\bar{\mathbf{V}} = v\hat{e}_2$ ($v > 0$); this is allowed because it satisfies the dissipation condition $\bar{\mathbf{F}} \cdot \bar{\mathbf{V}} > 0$.

Let the time increments be discrete with steps of Δt . During each time step, we assume that the dislocation density, $\alpha_{33} = \bar{\mathbf{b}} \otimes \bar{\mathbf{l}}' = b l' \hat{e}_3 \otimes \hat{e}_3$ and hence $\bar{\mathbf{F}}$, remains constant. Assuming no dislocation sources, equation (3.29) reduces to $\dot{l}' = -v l'_2$ which yields $l' \equiv \hat{l}'(0, x_2 - vt)$ (Acharya, 2001). Then, at the end of each time step, we update b , l' and α_{33} according to the local temperature induced by the moving dislocation.

At the beginning of the first step in time, let the magnitudes of b and l' be b_0 and l'_0 , respectively. During the first step in time Δt , the dislocation moves to the position $(0, v\Delta t)$ and we aim to find the temperature change $\Delta\theta = \theta - \theta_0$ due to this motion. In order to obtain the new temperature distribution, we have to solve the following 2D inhomogeneous heat equation with Dirichlet boundary conditions:

$$\left. \begin{aligned} \rho c_\epsilon \Delta\theta &= k(\Delta\theta_{,11} + \Delta\theta_{,22}) + \frac{\tau v b_0 \hat{l}'_0(x_1, x_2 - vt)}{f_0(x_1, x_2, t)} \\ \Delta\theta(-H, x_2, t) &= \Delta\theta(H, x_2, t) = 0 \\ \Delta\theta(x_1, -L, t) &= \Delta\theta(x_1, L, t) = 0 \\ \Delta\theta(x_1, x_2, 0) &= 0 \end{aligned} \right\} \quad (4.13)$$

The ensuing temperature field, $\theta_1(\bar{\mathbf{x}})$ will not be homogeneous. This temperature field will induce changes to ϵ_{11}^θ , ϵ_{22}^θ and ϵ_{33}^θ . It will introduce incompatibilities in ϵ_{11}^θ and ϵ_{22}^θ , which will result in the generation of stresses σ_{11} and σ_{22} , respectively, which will vary along directions \hat{e}_1 and \hat{e}_2 . The incompatible thermal strains will result in the generation of thermal quasi-dislocations with densities $\alpha_{13}^\theta = U_{11,2}^{\theta\perp}$, $\alpha_{23}^\theta = -U_{22,1}^{\theta\perp}$, $\alpha_{31}^\theta = -U_{33,2}^{\theta\perp}$ and $\alpha_{32}^\theta = -U_{33,1}^{\theta\perp}$. The temperature field $\theta_1(\bar{\mathbf{x}})$ will result in a change in the magnitude of b and l' from b_0 and l'_0 to b_1 and l'_1 , respectively, which has to satisfy equation (3.29). We will assume that this change only occurs at the end of time step Δt .

Now, the presence of ϵ_{11}^θ , ϵ_{22}^θ and ϵ_{33}^θ , and the absence of traction vector components along the normal direction on surfaces normal to $\pm\hat{e}_1$ and $\pm\hat{e}_2$ implies that we would also have a change in ϵ_{11} , ϵ_{22} and ϵ_{33} which will induce $\dot{\epsilon}_{11}$, $\dot{\epsilon}_{22}$ and $\dot{\epsilon}_{33}$. Therefore, for the next time increment Δt , we would have to solve $\rho c_\epsilon \dot{\theta} = k(\theta_{,11} + \theta_{,22}) + \tau v b_1 \hat{l}'_1(x_1, x_2 - 2v\Delta t) + \theta_0(3\lambda + 2\mu)\gamma(\dot{\epsilon}_{11} + \dot{\epsilon}_{22} + \dot{\epsilon}_{33})$ with the same boundary conditions as before, and the initial condition $\theta(\bar{\mathbf{x}}, 0) = \theta_1(\bar{\mathbf{x}})$. Note that for simplicity, we have chosen θ_0 instead of θ in the second term on the right-hand side of the temperature rate equation. The subsequent time steps involve solving the same equation set after updating the variables. By induction, at the $(j + 1)^{th}$ time increment, we need to solve for the following equation set:

$$\left. \begin{aligned} \rho c_\varepsilon \Delta \dot{\theta} &= k(\Delta \theta_{,11} + \Delta \theta_{,22}) + \underbrace{\frac{\tau v b_j \hat{l}_j'(x_1, x_2 - (j+1)v\Delta t) + \theta_0(3\lambda + 2\mu)\gamma(\dot{\varepsilon}_{11} + \dot{\varepsilon}_{22} + \dot{\varepsilon}_{33})}{f_{j+1}(x_1, x_2, t)}}_{f_{j+1}(x_1, x_2, t)} \\ \Delta \theta(-H, x_2, t) &= \Delta \theta(H, x_2, t) = 0 \\ \Delta \theta(x_1, -L, t) &= \Delta \theta(x_1, L, t) = 0 \\ \Delta \theta(x_1, x_2, 0) &= \theta_j(x_1, x_2) - \theta_0 \end{aligned} \right\} \quad (4.14)$$

The solution to (4.14) can be obtained by additively splitting the solution into (i) a part that solves for the initial boundary value problem without $f_{j+1}(x_1, x_2, t)$ and (ii) another part that solves for the inhomogeneous heat equation (i.e. with $f_{j+1}(x_1, x_2, t)$) but with zero initial condition. One of the standard approaches to solve part (i) is to use separation of variables and solving the resulting eigenvalue problem with symmetric boundary conditions using the Fourier series approach (Strauss, 2008). Then the solution to part (ii) follows directly from part (i). For our problem on the intervals $[-H, H]$ along \hat{e}_1 and $[-L, L]$ along \hat{e}_2 , we have the following solution for $\Delta \theta$:

$$\begin{aligned} \Delta \theta_{j+1}(x_1, x_2, t) &= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} A_{mn} \sin\left(\frac{m\pi x_1}{H}\right) \sin\left(\frac{n\pi x_2}{L}\right) \exp\left(-\frac{k}{\rho c_\varepsilon} \left[\frac{m^2 \pi^2}{H^2} + \frac{n^2 \pi^2}{L^2}\right] t\right) + \\ &\int_0^t \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} B_{mn}(\tau) \sin\left(\frac{m\pi x_1}{H}\right) \sin\left(\frac{n\pi x_2}{L}\right) \exp\left(-\frac{k}{\rho c_\varepsilon} \left[\frac{m^2 \pi^2}{H^2} + \frac{n^2 \pi^2}{L^2}\right] (t - \tau)\right) d\tau \end{aligned} \quad (4.15)$$

with

$$A_{mn} = \frac{1}{HL} \int_{-L}^L \int_{-H}^H \sin\left(\frac{m\pi x_1}{H}\right) \sin\left(\frac{n\pi x_2}{L}\right) (\theta_j(x_1, x_2) - \theta_0) dx_1 dx_2$$

and

$$B_{mn}(\tau) = \frac{1}{HL} \int_{-L}^L \int_{-H}^H \sin\left(\frac{m\pi x_1}{H}\right) \sin\left(\frac{n\pi x_2}{L}\right) \frac{f_{j+1}(x_1, x_2, \tau)}{\rho c_\varepsilon} dx_1 dx_2$$

If we set $\theta_j(x_1, x_2) - \theta_0 = 0$, $\forall x_1, x_2 \in \mathcal{B}$, then we obtain the solution to (4.13). Since the moving dislocation acts as a heat source, the highest temperature changes will be localized within the dislocation core. Therefore, the solution (4.15) has to be complemented with the solution to the dislocation transport equation including the source term that updates the dislocation density. The role of temperature rise on the evolution of dislocation density and changes to the dislocation core has not been accounted for in the existing solutions to temperature evolution due to dislocation motion (De Hosson et al., 2001; Eshelby and Pratt, 1956; Freudenthal and Weiner, 1956).

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 main motivation for developing this model is to study dislocation interactions with other defects and dislocation structure evolution in heat-affected crystalline solids experiencing strong rapidly changing temperature gradients such as those occurring during an additive manufacturing process. However, the proposed model could be applied to study the dynamics of individual dislocations and/or their ensembles 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. The T-FDM model operates at the length scale where it is possible to isolate individual dislocations. At this length scale, 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.

Kinematic relationships involving the elastic and plastic distortion are inherited from the FDM model, which uses the Stokes-Helmholtz decomposition to uniquely separate these distortions into their respective compatible and incompatible parts. Importantly, the T-FDM model accounts for incompatible thermal strains and an associated areal density, which is related to the curl of the incompatible thermal strains. The symmetric thermal strain tensor is separated into two asymmetric tensors, one of which is compatible and the other incompatible; this separation is similar to the Stokes-Helmholtz decomposition of elastic and plastic distortions. The introduction of thermal strains involves satisfying an additional set of continuity and boundary conditions.

The kinematic problem is complemented with temperature dependent energetic (Cauchy stress and entropy) and dissipative (dislocation driving forces and heat flux) constitutive relationships derived from the global dissipation and local free energy considerations. Exploitation of the properties of the Stokes-Helmholtz decomposition within the global dissipation formulation naturally leads us to obtain temperature dependent crystallographic dislocation driving forces, which are similar to those obtained in the FDM model.

Analytical solutions to some illustrative problems are used to demonstrate some of the predictive capabilities of the model as well as understand the significance of incompatible thermal strains in generating incompatible stresses. In particular, an analytical solution to the temperature change induced by an infinitely-long moving screw dislocation is computed under Dirichlet temperature boundary conditions. The T-FDM modeling framework allows to account for the change in its dislocation density due to temperature changes induced by its own motion, which is unprecedented.

Prospective work includes numerical implementation of this model to enable the study of dislocation dynamics under transient temperature changes such as those occurring during additive manufacturing, extending the geometrically linear T-FDM model to a finite strain framework and up-scaling the model to the length scale where polycrystalline plasticity models operate.

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6. Appendix: Stokes-Helmholtz type decomposition of a symmetric second order tensor

The developments from equation (A.1) – (A.5b) follow the seminal work of Kröner (Kröner, 1958). A second order tensor field $\bar{\tau}$ that vanishes on boundaries can be uniquely decomposed as follows:

$$\bar{\tau} = \nabla \bar{\alpha} + \nabla \times \bar{\alpha} \quad (\text{A.1})$$

where $\bar{\alpha}$ and $\bar{\alpha}$ are any arbitrary vector and second-order tensor. Now, the following decomposition for an arbitrary tensor $\bar{\alpha}$ is also unique:

$$\bar{\alpha} = \bar{b} \nabla + \bar{\beta} \times \nabla \quad (\text{A.2})$$

Substituting (A.2) into (A.1) and taking $\nabla \times \bar{b} \equiv \bar{c}$, we have

$$\bar{\tau} = \nabla \bar{\alpha} + \bar{c} \nabla + \nabla \times \bar{\beta} \times \nabla \quad (\text{A.3})$$

with the condition that

$$\nabla \cdot \bar{c} = 0 \quad (\text{A.4})$$

Now, if $\bar{\bar{\boldsymbol{\beta}}}$ is a symmetric tensor $\bar{\bar{\boldsymbol{\beta}}}^s$, then $\nabla \times \bar{\bar{\boldsymbol{\beta}}}^s \times \nabla = (\nabla \times \bar{\bar{\boldsymbol{\beta}}} \times \nabla)^s$. Similarly, if $\bar{\bar{\boldsymbol{\beta}}}$ is an anti-symmetric tensor $\bar{\bar{\boldsymbol{\beta}}}^a$, then $\nabla \times \bar{\bar{\boldsymbol{\beta}}}^a \times \nabla = (\nabla \times \bar{\bar{\boldsymbol{\beta}}} \times \nabla)^a$. If we define $\bar{\mathbf{g}} \equiv \bar{\mathbf{a}} + \bar{\mathbf{c}}$ and $\bar{\mathbf{h}} \equiv \bar{\mathbf{a}} - \bar{\mathbf{c}}$, then we get:

$$\bar{\bar{\boldsymbol{\tau}}}^s = \frac{1}{2}(\nabla \bar{\mathbf{g}} + \bar{\mathbf{g}} \nabla) + \nabla \times \bar{\bar{\boldsymbol{\beta}}}^s \times \nabla \quad (\text{A.5a})$$

$$\bar{\bar{\boldsymbol{\tau}}}^a = \frac{1}{2}(\nabla \bar{\mathbf{h}} - \bar{\mathbf{h}} \nabla) + \nabla \times \bar{\bar{\boldsymbol{\beta}}}^a \times \nabla \quad (\text{A.5b})$$

The decompositions shown in equation set (A.5) are unique because they are derived from equations (A.1) and (A.2), which are themselves unique decompositions.

Now, without the loss of generality, we can uniquely decompose $\bar{\mathbf{g}} = \bar{\mathbf{a}} + \bar{\mathbf{c}}$ via the Stokes-Helmholtz decomposition to obtain $\bar{\mathbf{g}} = \nabla \Phi + \nabla \times \bar{\mathbf{b}}'$, where the prime indicates that $\bar{\mathbf{b}}'$ does not have to be equal to $\bar{\mathbf{b}}$ from equation (A.2). With this decomposition, equation (A.5a) can be rewritten after some rearrangements as:

$$\bar{\bar{\boldsymbol{\tau}}}^s = \underbrace{\left[\frac{1}{2}(\nabla \nabla \Phi + \nabla \Phi \nabla + \nabla(\nabla \times \bar{\mathbf{b}}')) \right]}_{\bar{\bar{\mathbf{A}}}^{\parallel}} + \underbrace{\left[\frac{1}{2}(\nabla \times \bar{\mathbf{b}}') \nabla + \nabla \times \bar{\bar{\boldsymbol{\beta}}}^s \times \nabla \right]}_{\bar{\bar{\mathbf{B}}}^{\perp}} \quad (\text{A.6})$$

It is immediately clear that $\bar{\bar{\mathbf{A}}}^{\parallel}$ is curl-free and $\bar{\bar{\mathbf{B}}}^{\perp}$ is divergence-free; however, note that in general $\bar{\bar{\mathbf{A}}}^{\parallel}$ and $\bar{\bar{\mathbf{B}}}^{\perp}$ are asymmetric through the contribution of $\nabla(\nabla \times \bar{\mathbf{b}}')$ and $(\nabla \times \bar{\mathbf{b}}') \nabla$, respectively. Therefore, in the general case, a symmetric tensor $\bar{\bar{\boldsymbol{\tau}}}^s$ could be decomposed via the Stokes-Helmholtz decomposition into two asymmetric tensors as shown in (A.6).

If $\bar{\bar{\boldsymbol{\tau}}}^s$ were to be a diagonal matrix, then $\nabla \bar{\mathbf{g}} = \bar{\mathbf{g}} \nabla$ would have its off-diagonal terms equal to zero. In this case, (A.5a) becomes:

$$\bar{\bar{\boldsymbol{\tau}}}^s = \nabla \bar{\mathbf{g}} + \nabla \times \bar{\bar{\boldsymbol{\beta}}}^s \times \nabla \quad (\text{A.7})$$

It is clear then that $\nabla \bar{\mathbf{g}} = \nabla \nabla \Phi + \nabla(\nabla \times \bar{\mathbf{b}}')$ is curl-free and $\nabla \times \bar{\bar{\boldsymbol{\beta}}}^s \times \nabla$ is divergence-free, making the former entirely compatible and the latter solely incompatible. Note that $\nabla \nabla \Phi$ and $\nabla(\nabla \times \bar{\mathbf{b}}')$ need to satisfy the condition $(\nabla \nabla \Phi)_{ij} + (\nabla(\nabla \times \bar{\mathbf{b}}'))_{ij} = 0$ for $i \neq j$ and $\nabla(\nabla \times \bar{\mathbf{b}}') = (\nabla \times \bar{\mathbf{b}}') \nabla$.

If $\bar{\bar{\boldsymbol{\tau}}}^s$ were to be a spherical symmetric tensor: $\bar{\bar{\boldsymbol{\tau}}}^s = \gamma \delta_{ij}$, then $\nabla \bar{\mathbf{g}} = \bar{\mathbf{g}} \nabla = \gamma_1 \delta_{ij}$ and $\nabla \times \bar{\bar{\boldsymbol{\beta}}}^s \times \nabla = \gamma_2 \delta_{ij}$ such that $\gamma = \gamma_1 + \gamma_2$. The decomposition remains the same as equation (A.7). In (Kröner, 1958), for the specific case of spherically symmetric thermal strains, $\bar{\mathbf{g}}$ was assumed to be $\nabla \Phi$ and $\bar{\bar{\boldsymbol{\beta}}}^s$ was shown to be equal to $\Phi \mathbb{I}$ such that $\Delta \Phi = \gamma \Delta \theta$.

7. References

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