Microcanonical Entropy and Mesoscale Dislocation Mechanics and Plasticity

Amit Acharya[*]
Carnegie Mellon University

Abstract

A methodology is devised to utilize the statistical mechanical entropy of an isolated, constrained atomistic system to define the dissipative driving-force and energetic fields in continuum thermomechanics. A thermodynamic model of dislocation mechanics is discussed. One outcome is a definition for the mesoscale back-stress tensor and the symmetric, polar dislocation density-dependent, Cauchy stress tensor from atomistic ingredients.

Dedication: This paper is dedicated to the memory of Professor Donald E. Carlson, teacher and friend to me. I owe a great debt for all I learned from him, in particular continuum mechanics. Don was a scholar and a gentleman, with a kind heart and a tremendous sense of humor. I miss him.

1. Introduction

This work is an attempt at examining to what extent material-specific atomistic information can be incorporated into defining material response in continuum mechanics at 'slow' time scales ($\geq$ microseconds) with respect to the fast time scale of atomic vibrations (~femtoseconds). We rely on classical equilibrium statistical mechanics of isolated atomistic assemblies as our microscopic theory, e.g. (Berdichevsky 1997); the meso-/macro scale models are intended to be non-standard continuum mechanical models of defects in solids. The bridge is assumed to be the two laws of thermodynamics, as enunciated in the Classical Field Theories of Mechanics (Truesdell and Toupin 1960) in particular, the global form of the Clausius-Duhem Inequality as the embodiment of the Second law of thermodynamics. The essential idea is to give one possible operational form and meaning to the specific internal energy and entropy response functions of continuum thermomechanics, resorting to the atomistic nature of all solids and the equilibrium statistical mechanical microscopic theory of assemblies of such atoms. The nonstandard continuum models of relevant defects have to be developed based on a consideration of fundamental defect kinematics that give rise to balance/conservation laws for geometrically rigorous densities. The notion of 'local thermodynamic equilibrium' also has to be made operational, but this becomes somewhat easier, if only formally, due to a reliance on a microscopic finite dimensional Hamiltonian system for which the existence of a phase-space invariant measure (probability density function) can at least be considered plausible.

We rely on statistical mechanics in the microcanonical ensemble primarily because continuum mechanics requires the notion of a meso/macro point-wise temperature that has to be defined without relying on the fact that it has a surrounding that has the same temperature. For a discussion and comparison of the microcanonical and canonical definitions of the entropy, see

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[*] email: acharyaamit@cmu.edu; Tel. (412) 268 4566; Fax. (412) 268 7813.

(Berdichevsky 1997), and for an independent viewpoint on Berdichevsky's development, (MacKay 1999). Moreover, it seems conceptually natural in the setting of continuum mechanics to have the 'interaction with the bath' of an atomistic subsystem to be handled by the macroscopic partial differential equations (PDEs) of the continuum model.

The main contributions of this work are in 1) making precise how continuum field values at points in space-time can be utilized to describe well-defined local Hamiltonian systems, whose entropy then defines the continuum specific entropy field, and 2) application of the overall scheme to a field description of the mechanics of dislocations. The model makes no restrictions on geometric or material nonlinearities.

The model of dislocation mechanics develops prior work (Acharya; 2001, 2004), (Acharya and Roy, 2006) which in turn builds on the theory of continuously distributed dislocations pioneered by (Kroner 1981), (Mura 1963), (Fox 1966), and (Willis 1967) and extends it to account for dissipative dislocation transport and nonlinearity due to geometric and crystal elasticity effects. Here, the main contribution is a theoretical treatment that produces a completely defined constitutive equation for a (generally non-symmetric) back stress tensor and a symmetric Cauchy stress that includes a dependence on the polar dislocation density tensor. Temperature dependence of the back stress and the Cauchy stress are automatic.

This work does not make any fundamental statement about constitutive kinetic relations beyond uncovering the driving forces for dissipative mechanisms. However, even with the assumption of linear kinetic relations, the governing nonlinear partial differential equations for dislocations coupled to stress are very rich, and it is reasonable to expect them to be capable of predicting complex microstructure. Balance of energy in standard form and the global form of the Clausius-Duhem Inequality are assumed to be valid without question, and this may be construed as a major shortcoming of this work. Given the complexity of the venture as is, this may perhaps be considered acceptable with some justification, see e.g. (Man 1995). There are natural avenues for considering these extremely difficult questions of nonlinear spatio-temporal 'homogenization,' e.g., (Tartar a 2008), (Tartar 2009), (Artstein and Vigodner, 1996), but precise answers for the context at hand, even at a theoretical level, remain elusive despite outstanding work[1], giving a sense of the arduous road ahead on this issue. To give an example of the thorny issues involved, in the conservative approach adopted here (and in all of practical equilibrium statistical mechanics), we declare by *fiat* the existence of a unique invariant measure for time-averaging an atomistic Hamiltonian system. Running time-averages of phase functions can be appended to the original ODE Hamiltonian dynamics to produce a singularly perturbed system (Acharya 2010). The rigorous results of (Arstein and Vigodner, 1996) then clearly indicate possibilities different from averaging based on a unique invariant measure for defining the theory for the dynamics of the time-averages, and it may be expected that such considerations would play a fundamental role in understanding kinetic relations from the ground-up.

This paper is organized as follows: Section 2 defines the specific internal energy field of the continuum theory; Section 3 defines the notion of local thermodynamic equilibrium; Section 4 deals with the definition of the specific entropy field; Section 5 discusses the probabilistic

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[1] Such work is also technically very difficult for the general worker in mechanics (including myself, of course) to comprehend in its entirety. This seems to be an unfortunate barrier for progress, without an easy solution.

interpretation of the microcanonical entropy; Section 6 deals with the mesoscale model of dislocation mechanics. There are three Appendices. In Appendix A, a Helmholtz free energy density is defined from the entropy field, and it is shown how thermodynamic models may be recast in terms of this energy and temperature. Appendix B describes the detailed geometric reasoning behind the conservation law for the dislocation density tensor. Appendix C shows the connections of the dislocation kinematics presented here with that in (Acharya 2004) and Acharya and Roy (2006).

To our knowledge, the approach proposed herein to make a connection between *continuum* and atomistic dynamics is new; there is a connection in spirit, with significantly different details, with the finite-temperature quasicontinuum ideas of Kulkarni et al. (2008). There exists a large literature on thermodynamics for dissipative response of solids at finite strain, beginning with the pioneering works of Coleman and Gurtin (1967) and (Rice 1971). The emphasis here is on making the statistical mechanical connections to define some of the fundamental ingredients (internal energy, entropy) of any continuum thermodynamic framework. As mentioned earlier, resorting to a finite dimensional Hamiltonian microscopic model representing atomistic assemblies has a distinct advantage in making standard (nonequilibrium) thermodynamic formalism less abstract, especially ideas related to thermodynamic processes consisting of 'constrained equilibrium states.' Thus, a primary goal of this paper is to make clear how a real equilibrium state of an appropriate, constrained microscopic system can be made plausible, what this equilibrium exactly means and how such equilibria naturally form a process at macroscopic time scales, and why the resulting thermodynamics can actually be applied to continuum *dynamics* with inertia in many circumstances. Rice (1971) considers a thermodynamic model of plasticity arising from dislocations; the model here contains a more detailed consideration of dislocation kinematics (that accommodates the standard model of crystalline slip as one ingredient) leading to the representation of dislocation transport through wave-propagative effects and length-scale effects in mechanical response.

2. Specific internal energy of the continuum theory

Let $\boldsymbol{x}$ be a point in space occupied by a material point of a deforming body at time t. Consider a spatial volume $\Omega(\cdot, \boldsymbol{x})$ of fixed volume V around $\boldsymbol{x}$. Let the continuum mass density $\rho(\boldsymbol{x}, t)$ at the space-time location $(\boldsymbol{x}, t)$ be a piece of physical information available to us, for the moment from an unspecified source. Similarly, let us assume that the value of the continuum velocity $\boldsymbol{v}(\boldsymbol{x}, t)$ is also known. For simplicity we consider atoms of a single species with individual mass m.

The first objective is to state the physical assumptions behind defining a continuum specific internal energy (per unit mass) field. We now think of a collection of

$$N(\boldsymbol{x}, t) := \frac{\rho(\boldsymbol{x}, t)V}{m}$$

atoms indexed by I. Let $\tilde{V}_I$ be the velocity of the Ith atom. Let the mean velocity and fluctuations be defined as

$$\bar{V} = \frac{1}{N} \sum_{I=1}^{N} \tilde{V}_I \quad ; \quad V_I = \left(\tilde{V}_I - \bar{V} \right).$$

Then

$$\frac{1}{N} \sum_{I=1}^{N} \frac{m}{2} \tilde{V}_I \cdot \tilde{V}_I = \frac{1}{N} \sum_{I=1}^{N} \frac{m}{2} \left[\left\{ \left(\tilde{V}_I - \bar{V} \right) + \bar{V} \right\} \cdot \left\{ \left(\tilde{V}_I - \bar{V} \right) + \bar{V} \right\} \right] = \frac{m}{2} \bar{V} \cdot \bar{V} + \frac{1}{N} \sum_{I=1}^{N} \frac{m}{2} V_I \cdot V_I.$$

This implies that the total kinetic energy of the N atoms is given by

$$\frac{Nm}{2} \bar{V} \cdot \bar{V} + \sum_{I=1}^{N} \frac{m}{2} V_I \cdot V_I. \tag{1}$$

As for the 'potential' energy, let us assume that the entire body, viewed as a atomistic system, is endowed with a potential for generating interatomic forces which can be characterized as a function of number of atoms, say M (typically $M \gg N$), and the positions $r_j, j = 1$ to M, of the M atoms. Let this potential energy function be

$$U\left(M, \{ r_j, j = 1 \text{ to } M \} \right).$$

This prescription makes it clear that while the total potential energy of the body can be written down unambiguously, it is not so clear how one might define the potential energy of a certain subset of the atoms only in terms of the positions of that subset of atoms.

In the setting of continuum mechanics, we write the total energy of arbitrary subparts of the body, say Ω, as

$$\int_\Omega \rho \left(\frac{1}{2} v \cdot v + \varepsilon \right) dv,$$

where the first term in the parenthesis represents the kinetic energy per unit mass field and the second, the internal energy per unit mass field.

It seems natural then to associate

$$\int_\Omega \rho \left(\frac{1}{2} v \cdot v + \varepsilon \right) dv \quad \leftrightarrow \quad \frac{Nm}{2} \bar{V} \cdot \bar{V} + \sum_{I=1}^{N} \frac{m}{2} V_I \cdot V_I + U_c, \tag{2}$$

where U_c is an atomic interaction energy term that needs to be defined.

Motivated by the form of (2), we associate the continuum velocity field with the local mean atomic velocity, so that

$$v = \bar{V} \quad \Rightarrow \quad \frac{1}{2} v \cdot v = \frac{1}{2} \bar{V} \cdot \bar{V}. \tag{3}$$

Let the specific internal energy field (per unit mass) around (x, t), be denoted by $\varepsilon(x, t)$. We postulate that it corresponds to the total energy of a local, isolated, **constrained**, ergodic Hamiltonian system consisting of $N(x, t)$ atoms, with the potential of the original material. Thus for each $t \leq \tau \leq t + \Delta t$, given $\rho(x, t)$,

$$\rho(x, t) \varepsilon(x, t) V = E(x, t) := U\left(N(x, t), \{ r_j(\tau), j = 1 \text{ to } N(x, t) \} \right) + \sum_{I=1}^{N(x,t)} \frac{m}{2} V_I(\tau) \cdot V_I(\tau) \tag{4}$$

subject to appropriate constraints to be defined.

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The constraints are meant to represent the action of all the other atoms in the body on this set of $N(x,t)$ atoms beyond what can be represented through the specification of the value of the total energy, $E(x,t)$. These constraints have the following generic form: let a point of the $6N$ dimensional phase space of the Hamiltonian system be denoted by Y. The constraints are then written as

$$\Phi_i(Y) = z_i(x,t), i = 1 \text{ to } 2k, \ k \text{ a positive integer,} \qquad (5)$$

where Φ_i are real-valued functions of Y and z_i are values of macroscopic fields at the point (x,t). We discuss the specifics of these constraints in Section 6 in the context of a concrete example.

The manner in which (4) may be physically interpreted (and tested) as a definition of specific internal energy at (x,t) is as follows: given the mass density $\rho(x,t)$ consider the $N(x,t)$ nearest atoms to the point x at time t. Now assume that the positions and velocity *fluctuations* of these atoms satisfy (5) for the time interval $[t, t+\Delta t]$, given the values of $z_i(x,t)$; also, assume that the velocity *fluctuations* and the positions of these atoms are such that the extreme right-hand-side of (4) evaluated for these arguments attains a constant value, $E(x,t)$, over the time interval $[t, t+\Delta t]$. Then $\varepsilon(x,t)$ may be defined as $E(x,t)/(\rho(x,t)V)$.

Ergodicity is an abstract, but very useful, mathematical concept – for our purposes, we take it to be practically 'equivalent' to one of the most useful properties of an ergodic Hamiltonian system: consider a set A on the energy surface $\{Y : H(Y) = E\}$ of the system. Consider the time $\Delta\tau(\tau^*; A, Y)$ spent by a trajectory of the system in the set A starting from initial condition Y, over a total time of evolution τ^*. If the system has the property that

$$\lim_{\tau^* \to \infty} \frac{\Delta\tau(\tau^*; A, Y)}{\tau^*} = \mu(A)$$

independent of almost all trajectories with energy E used to generate it, where μ is a real-valued function on subsets A of the common energy surface, then we call the system ergodic.

3. Local equilibrium

A *primary assumption* we make here is that the local Hamiltonian system evolves on a time scale (~ femtoseconds) that is much smaller than the time scale of evolution (e.g. ~ microsecond) of the continuum theory; in particular, the separation is large enough such that for E held constant, the local atomistic system equilibrates on the macroscopic time-scale. By this, we mean the following: consider the $6N - 2k$ dimensional set of points forming the accessible states (or phase space) of the constrained Hamiltonian system. Consider further the $6n - 2k - 1$ dimensional subset of this constrained phase space, consistent with the prescribed value of the energy E, and consider an arbitrary subset A of it. Choose almost any trajectory of the constrained system with energy E and consider the ratio

$$\frac{\Delta\tau\left(\tau^*;A\right)}{\tau^*}$$

of the time $\Delta\tau$ spent by the trajectory in the set A, and the total time of evolution τ^* of the trajectory. Let Δt be a minimum interval of time on the t scale below which the continuum theory shows no appreciable evolution – this is an important conceptual ingredient, and we think of this as the time resolution of the continuum theory. Then, as a definition of microscopic equilibrium, we require that, given any A as defined above, there exists a constant $\mu(A)$ such that

$$\text{for any } \tau^* \geq \Delta t \qquad \left|\frac{\Delta\tau\left(\tau^*;A\right)}{\tau^*} - \mu(A)\right| < \varepsilon,$$

where $0 < \varepsilon \ll 1$ is a (user-specified) threshold. Of course, we keep in mind that the set A depends on E by definition, so the function μ really depends upon E for its definition.

4. Specific entropy field of the continuum theory

In defining a continuum entropy per unit mass field, we adapt the developments in Berdichevsky (1997) for our purposes. For each (x,t) in the body, define

$$H(Y) := U(X) + \sum_{I=1}^{N(x,t)} \frac{1}{2} m V_I \cdot V_I, \tag{6}$$

where Y is the list

$$Y = \left(X_1, X_2, \cdots, X_{N(x,t)}, V_1, V_2, \cdots, V_{N(x,t)}\right)$$

and we have used the shorthand

$$U(X) := U\left(N(x,t), \{r_j, j = 1 \text{ to } N(x,t)\}\right) \tag{7}$$

(cf. (4)).

Next a phase space region

$$\{Y : H(Y) \leq E(x,t), \Phi_i(Y) \leq z_i(x,t), i = 1 \text{ to } 2k\} \tag{8}$$

is defined.

Furthermore,

$$E(x,t) := \varepsilon(x,t)\rho(x,t)V,$$

where ε is the continuum internal energy per unit mass field. Let us assume that there is some invariant physical meaning that can be associated with volumes of regions in phase space. An important construct of the theory is the **volume** of the phase-space region defined by (8):

$$\Gamma\left(E(x,t), z(x,t); N(x,t)\right) := vol\{Y : H(Y) \leq E(x,t), \Phi_i(Y) \leq z_i(x,t), i = 1 \text{ to } 2k\} \tag{9}$$

In writing z, we mean the entire array $z_i, i = 1$ to $2k$.

Note that volumes in the $6N$ dimensional phase space of the above atomistic Hamiltonian system have physical units of $(momentum \times position)^{3N} = (Energy \times time)^{3N}$. We now assume that our microscopic measurements can only resolve an action scale, say $\bar{h}$, and above. Then,

following Berdichevsky (1997), *and all attendant assumptions therein* (nondegeneracy of constraints, incompressibility of phase flow of the constrained system and ergodicity of the constrained system being the main ones), given E, z, N it makes sense to define the entropy of the constrained Hamiltonian system as

$$S(E, z; N) := \ln\left(\frac{1}{\bar{h}^{3N(x,t)}} \frac{\partial^{2k}\Gamma}{\partial z_1 \cdots \partial z_{2k}}(E, z; N)\right).$$ (10)

$S(E, z, N)$ is simply a measure of the $6N - 2k$ dimensional volume of the constrained Hamiltonian system bounded by the energy surface E.

The objective of this paper until now has been to establish a procedure for defining point-wise values of the quantities E, z, N based on evaluations of the continuum fields ε, ρ, z. Thus, *we define the continuum entropy per unit mass field* from the entropy of the constrained Hamiltonian system defined above as

$$\eta(\rho(x,t), \varepsilon(x,t), z(x,t)) := \frac{C}{\rho(x,t)V} \ln\left(\frac{1}{\bar{h}^{3N(x,t)}} \frac{\partial^{2k}\Gamma}{\partial z_1 \cdots \partial z_{2k}}(E(x,t), z(x,t); N(x,t))\right),$$ (11)

where C is a constant with units of energy/absolute temperature. This expression for the specific entropy is simply a measure of the $6N - 2k$ dimensional volume of the constrained Hamiltonian system bounded by the energy surface E.

The motivation behind this definition is as follows; in the case of an unconstrained, ergodic, Hamiltonian system with Hamiltonian quadratic in the momenta, it is a principal result that the long-time average of the kinetic energy of any given particle along almost any trajectory with fixed energy is a constant (equipartition) and, by definition, this common value is called the absolute temperature, say T. This further definition is motivated from macroscopic thermodynamics where the result

$$\frac{1}{\theta} = \frac{\partial S}{\partial E}$$ (12)

where θ is the macroscopic temperature (i.e. the perceived level of hotness), S is the entropy of the system, and E is the energy. For the unconstrained Hamiltonian system, defining the phase space volume bounded by the E-energy surface as

$$\bar{\Gamma}(E) = vol\{Y : H(Y) \leq E\}$$ (13)

it can be shown (e.g. Berdichevsky, 1997) that

$$T(E) = \frac{\bar{\Gamma}(E)}{\frac{\partial\bar{\Gamma}}{\partial E}(E)}.$$ (14)

Therefore, defining entropy in microscopic terms (utilizing ideas going back to Boltzmann, Gibbs and Hertz, according to Berdichevsky, 1997) as

$$S(E) = \ln\left(\frac{\bar{\Gamma}(E)}{\Gamma_0}\right)$$

where Γ_0 is a constant required on dimensional grounds, implies $\theta = T(E)$.

In our case of the constrained Hamiltonian system, equipartition is not a derived result. However, macroscopic thermodynamics yields a result similar to (12), as we subsequently show.

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Moreover, in the (unconstrained) case where there is a formal proof, a natural geometric/physical interpretation of entropy arises as the $6N$ dimensional phase space volume of the system bounded by the energy surface E. These three facts motivate the definition (11).

We agree to pose the constraints in non-dimensional form by definition, so the logarithm makes sense. In general, a physically dimensional constraint, say $\tilde{\Phi} = \tilde{z}$, may be normalized arbitrarily so as to be stated in dimensionless form $\Phi = z$. Finally, it should be carefully noted that the dependence of the specific entropy field on the continuum mass density field goes far beyond what is apparent through its explicit appearance in the formula (11).

Turning to prospects for making the theory practical, it is clear that if the function S can be determined then the response function for the specific entropy of the material, $\eta(\rho, \varepsilon, z)$, is completely defined. There exists a great deal of expertise in the physics literature for calculating various energies and entropies of molecular systems, e.g. Frenkel and Smit (2002), mostly in the context of calculations with the canonical ensemble. It is conceivable that these strategies can be gainfully adapted to the specific problems mentioned herein. Practical approximation of the entropy function S, while an important subject in its own right, is beyond the scope of this paper. In the following section we mention a probabilistic interpretation of the entropy S that suggest some naïve methods for approaching the calculation of $S(z, E)$ that involve data collection from the unconstrained Hamiltonian system to yield information on the entropy of the constrained system.

5. Probabilistic interpretation of Entropy

We review some basic assumptions of equilibrium statistical mechanics in the microcanonical ensemble, following Berdichevsky (1997). Consider the unconstrained Hamiltonian system (6)-(7), assumed to be ergodic. Given phase functions $\Phi_i(Y), i = 1$ to P and a trajectory $Y(\cdot)$ with energy E we first define the amount of time $\Delta\tau(\tau^*)$, out of a total time of evolution τ^*, during which all the following relations

$$z_i \leq \Phi_i(Y(\tau)) \leq z_i + \Delta z_i, \quad i = 1 \text{ to } P$$

are satisfied. Let $\Delta = \Delta z_1 \times \Delta z_2 \cdots \times \Delta z_P$. We now assume that the limit

$$\lim_{\Delta \to 0} \frac{1}{\Delta} \lim_{\tau^* \to \infty} \frac{\Delta\tau(\tau^*)}{\tau^*} =: f(z_1, \cdots, z_P, E)$$

exists and, as shown in the notation, depends only on the $z_i, i = 1$ to P, and E, *and is independent of the trajectory used to define it.*

The function f is called the probability density of the characteristics Φ_i, $i = 1$ to P.
We recall the definition (13) and define

$$\Gamma(z_i, \cdots, z_P, E) := vol\{Y : H(Y) \leq E(x, t), \Phi_i(Y) \leq z_i(x, t), i = 1 \text{ to } P\}.$$

Then a fundamental result (under several strong assumptions) (Berdichevsky, 1997) is that

$$f(z_1, \cdots, z_P, E)\frac{\partial\bar{\Gamma}}{\partial E}(E) = \frac{\partial^{P+1}\Gamma}{\partial E \partial z_1 \cdots \partial z_P}(z_1, \cdots, z_P, E). \tag{15}$$

Now, (15) and (10) imply

$$f(z,E)\frac{\partial \bar{\Gamma}}{\partial E}(E) = \bar{h}^{3N}\frac{\partial}{\partial E}\exp\left(S(E,z;N)\right) \; ; \; z := (z_i, i = 1 \text{ to } 2k), \qquad (16)$$

where it is understood that the left hand side now refers to the unconstrained Hamiltonian system defined by (6)-(7); in particular, that the system contains N atoms.

Thus, if the probability density function of the $2k$ characteristics can be evaluated/approximated by some means (e.g. experimentally), then (16) provides a method of determining the entropy S of the local discrete system.

We note here that given the number of strong assumptions that have to hold to define the constrained Hamiltonian system and its entropy (11), it could just as well be as effective to simply define the entropy of a certain set of characteristics of an isolated system by the formula (16), thus bringing it closer in line with some other approaches to defining the entropy based on purely probabilistic grounds (Swendsen 2006). This would also then get rid of what appears to be a somewhat artificial constraint of having to deal with only an even number of characteristics (arising from the fact that the constrained system has to be Hamiltonian).

Molecular Dynamics (MD) based evaluation of $f(z,E;N)$

By definition, $f(z,E;N)$ can, *in principle*, be computed by integrating along representative MD trajectories for different values of E. However, as this may require long-time MD evolution, it is not clear how promising such an approach might be for practical evaluation of the probability density function for further utilization in (16) to determine $S(E,z;N)$.

Evaluation of $f(z;E)$ based on experimental observations in the large-N limit

Presumably, bodies with arbitrarily fixed values of energy E and a large number of atoms $(N \to \infty)$ admit the possibility of being obtained. Note that even with a large number of atoms, such bodies can serve as the isolated Hamiltonian systems discussed earlier. Consider one such value of E and let there be A bodies forming a sample space. We now make the following strong assumption: observing each body in the sample over a macroscopic time interval, say Δt, is equivalent to making A observations on a single trajectory with energy E, each observation consisting of a Δt time interval.

Let us index the specimens by $I = 1$ to A. Each has a set of values $z_i, i = 1$ to k associated with it, say $z_{iI}, i = 1$ to $2k, I = 1$ to A. Suppose B specimens were found to correspond to values of z_i^*, $i = 1$ to $2k$, for the constraints; i.e. $z_{iI_j} = z_i^*, i = 1$ to $2k, j = 1$ to B, with each $I_j \in \{1, 2, \ldots, A\}$. Under the stated assumptions, an approximation of the value of the probability density function f at the argument $(z^*;E)$ may be written as

$$f^h(z^*;E) = \frac{B\Delta t}{A\Delta t} = \frac{B}{A}.$$

The same procedure can then be repeated for all values of $(z; E)$ of interest.

Maximum Entropy states and most probable states

In closing, we note the following associations of the probabilistic interpretation of entropy with Gibbs's thermodynamic postulate about macroscopic equilibrium. Let us rewrite (16) in the form

$$f = \exp\left(S\left[1 + \frac{\ln\left\{\left(\partial \bar{\Gamma}/\partial E\right)^{-1} \bar{h}^{3N}\left(\partial S/\partial E\right)\right\}}{S}\right]\right). \tag{17}$$

When the fraction in the above expression is much smaller in magnitude w.r.t. unity, we obtain Boltzmann's expression for the entropy

$$\ln f(z, E) = S(z, E) \tag{18}$$

which expresses the relationship of the probability of observing the macroscopic state z with system energy E to the entropy of the system. In particular, Gibbs's postulate that for fixed energy, the macroscopic state (here z) that is observed (equilibrium) corresponds to the state that maximizes the entropy would suggest, according to (18) that Gibbs's *maximum entropy* equilibrium also corresponds to the most probable state(s), under the assumption leading to (18) from (17) (e.g. for large N, as shown by heuristic arguments in Berdichevsky (1997).

6. Example: Mesoscale Dislocation Mechanics

Up to the specification of constitutive equations, we assume that the following field equations are valid for describing the mechanics of a body containing dislocations, including resolving the mechanics of single dislocations (i.e. 'microscopic theory'):

$$\dot{\rho} + \rho\,div\,\boldsymbol{v} = 0 \Leftrightarrow \rho_{,t} = -div(\rho\boldsymbol{v}) \qquad \text{(Balance of Mass)} \tag{19}$$

$$\rho\dot{\boldsymbol{v}} = div\boldsymbol{T} \Leftrightarrow (\rho\boldsymbol{v})_{,t} = div[\boldsymbol{T} - \rho\boldsymbol{v}\otimes\boldsymbol{v}] \quad \text{(Balance of Linear Momentum)} \tag{20}$$

$$div\,\boldsymbol{\alpha} = \boldsymbol{0} \quad \text{(Dislocations cannot end in the material)} \tag{21}$$

$$curl\,\boldsymbol{W} = -\boldsymbol{\alpha} \quad \text{(Fundamental statement of elastic incompatibility and dislocations)} \tag{22}$$

$$\overset{\circ}{\boldsymbol{\alpha}} = -curl(\boldsymbol{\alpha}\times\boldsymbol{V}) \Leftrightarrow \boldsymbol{\alpha}_{,t} = -curl(\boldsymbol{\alpha}\times[\boldsymbol{v}+\boldsymbol{V}]) \quad \text{(Balance of Burgers vector content)} \tag{23}$$

$$div(\boldsymbol{v})\boldsymbol{\alpha} + \dot{\boldsymbol{\alpha}} - \boldsymbol{\alpha}\boldsymbol{L}^T =: \overset{\circ}{\boldsymbol{\alpha}}$$

$$\dot{\boldsymbol{W}} + \boldsymbol{W}\boldsymbol{L} = \boldsymbol{\alpha}\times\boldsymbol{V} . \tag{24}$$

Here, as in classical continuum mechanics, we assume that mass of arbitrarily small sets of particles in the body is conserved for all motions. In the above, ρ is the mass density, $\boldsymbol{v}$ is the material velocity, $\boldsymbol{T}$ is the Cauchy stress, $\boldsymbol{\alpha}$ is the dislocation density (Nye) tensor, $\boldsymbol{W}$ is the inverse elastic distortion tensor, $\boldsymbol{V}$ is the dislocation velocity field relative to the material, and $\boldsymbol{L}$ is the material velocity gradient. A superposed dot represents a material time derivative, whereas a subscript comma followed by a t represents differentiation with respect to time of the Eulerian representation of the field in question. All spatial derivative operators are defined on the

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current configuration. Equations (19)-(20) are familiar from standard continuum mechanics. For the derivation of (21)-(24), see Appendix B of this paper and Acharya (2007).

Our primary interest here is, of course, in mesoscale dislocation mechanics. We obtain the approximate governing partial differential equations for such a case, up to constitutive equations, by using the following simple technique.

For a microscopic field f given as a function on the current configuration and time, we define the mesoscopic space-time averaged field $\overline{f}$ as follows:

$$\overline{f}(\boldsymbol{x},t) := \frac{1}{\int_{I(t)}\int_{\Omega(x)} w(\boldsymbol{x}-\boldsymbol{x'},t-t')\,d\boldsymbol{x'}dt'} \int_{\Im}\int_{B} w(\boldsymbol{x}-\boldsymbol{x'},t-t') f(\boldsymbol{x'},t')\,d\boldsymbol{x'}dt', \qquad (25)$$

where B is the body and $\Im$ a sufficiently large interval of time. In the above, $\Omega(\boldsymbol{x})$ is a bounded region within the body around the point $\boldsymbol{x}$ with linear dimension of the order of the spatial resolution of the macroscopic model we seek, and $I(t)$ is a bounded interval in $\Im$ containing t. The averaged field $\overline{f}$ is simply a weighted, space-time, running average of the microscopic field f over regions whose scale is determined by the scale of spatial and temporal resolution of the averaged model one seeks. The weighting function w is non-dimensional, assumed to be smooth in the variables $\boldsymbol{x}, \boldsymbol{x'}, t, t'$ and, for fixed $\boldsymbol{x}$ and t, have support (i.e. to be non-zero) only in $\Omega(\boldsymbol{x}) \times I(t)$ when viewed as a function of $(\boldsymbol{x'}, t')$. We choose the volume of the region $\Omega(\boldsymbol{x})$

$$vol\{\boldsymbol{y} : \boldsymbol{y} \in \Omega(\boldsymbol{x})\} = V,$$

as used in defining the specific entropy and internal energy from atomistic considerations.

We assume that

$$\boldsymbol{v} = \overline{\boldsymbol{v}}$$

and that *averages of products are the product of averages* in all cases except

$$\overline{\boldsymbol{\alpha}\times\boldsymbol{V}} - \overline{\boldsymbol{\alpha}}\times\overline{\boldsymbol{V}} =: \tilde{\boldsymbol{L}}^{p}. \qquad (26)$$

In (26), the first term on the left-hand-side is the mesoscopic plastic distortion rate and the second term may be interpreted as the plastic distortion rate produced by the motion of the polar dislocation density (defined in the next section) moving with velocity $\overline{\boldsymbol{V}}$. Similarly, the term on the right-hand-side of (26) is the plastic distortion rate produced by the motion of the dislocation fluctuation density (also defined in the next section). $\tilde{\boldsymbol{L}}^{p}$ is a two point-tensor field from the current to the unstretched materially uniform elastic reference.

Applying the averaging operator (25) to the Eulerian form of the equations (19)-(24) under the above assumptions yield the following set of mesoscopic equations:

$$\dot{\overline{\rho}} \approx -\overline{\rho}\,div\,\overline{\boldsymbol{v}} \qquad (27)$$

$$\overline{\rho}\dot{\overline{\boldsymbol{v}}} \approx div\,\overline{\boldsymbol{T}} \qquad (28)$$

$$\dot{\overline{\boldsymbol{W}}} \approx \overline{\boldsymbol{\alpha}}\times\overline{\boldsymbol{V}} + \tilde{\boldsymbol{L}}^{p} - \overline{\boldsymbol{W}}\,\overline{\boldsymbol{L}} \qquad (29)$$

$$\dot{\overline{\boldsymbol{\alpha}}} \approx -curl\left(\overline{\boldsymbol{\alpha}}\times\overline{\boldsymbol{V}} + \tilde{\boldsymbol{L}}^{p}\right) - \overline{\boldsymbol{\alpha}}\otimes\boldsymbol{I} : \overline{\boldsymbol{L}} + \overline{\boldsymbol{\alpha}}\,\overline{\boldsymbol{L}}^{T}, \qquad (30)$$

where the $\approx$ signs reflect the fact that these averaged equations result from having made the assumptions on averaging products mentioned above.

6.1 Definition of local constraints for dislocation mechanics and thermodynamics

For the case of interest here, the $z_i(x,t), i = 1$ to 8 are defined as follows. Define
$$F^e := W^{-1}.$$
Let
$$C^e(x,t) := \overline{F^e}^T \overline{F^e}(x,t)$$
be the continuum elastic metric tensor at the point (x,t) corresponding to the space-time averaged continuum elastic distortion tensor $\overline{F^e}(x,t)$. This is a positive definite tensor resulting in six values of the array $z(x,t)$. We think of the $\Phi_i, i = 1$ to 6, as some correspondence rule that links the atomic positions of the $N(x,t)$ atoms to an average squared right stretch tensor. For example, at any given value of $E(x,t)$, let us consider an unstressed block of the N atoms in a perfect infinite lattice. Consider now an homogeneous deformation of this geometric shape with right Cauchy Green tensor given by $C^e(x,t)$. Now consider all possible placements of the $N(x,t)$ atoms within this deformed block (including defects in the lattice arrangement). We could consider all these arrangements as satisfying the constraints $\Phi_i(Y) = z_i(x,t), i = 1$ to 6. The same interpretation can be useful in determining the probability density function $f(z,E)$ from configurations along a trajectory of the unconstrained system with energy E.

For the next two values of the array z, we define
$$\overline{\alpha}$$
as the *polar dislocation density* at (x,t), also commonly referred to as the *geometrically necessary dislocation density (GND)* tensor. In terms of the polar dislocation density we also define the *dislocation fluctuation* tensor field, β, as the difference between the microscopic Nye tensor field and the polar dislocation density tensor field:
$$\beta(x,t) := \alpha(x,t) - \overline{\alpha}(x,t)$$
We now introduce a scalar field, $\kappa(x,t) = \overline{\alpha : \alpha}(x,t)$ which is the meso/macro space-time average of the square of the magnitude of the microscopic dislocation density tensor (Nye tensor) around (x,t). Notice that, by defining

$\kappa := \overline{\alpha : \alpha}$ (scalar total dislocation density),

$\kappa_g := \overline{\alpha} : \overline{\alpha}$ (scalar polar dislocation density), and   (31)

$\kappa_s := \overline{\beta : \beta}$ (scalar dislocation fluctuation density - commonly 'statistical density' SD)

we have the exact result
$$\overline{\alpha : \alpha} = \overline{\alpha} : \overline{\alpha} + \overline{\beta : \beta} \quad \Leftrightarrow \quad \kappa = \kappa_g + \kappa_s.$$
All of the scalar measures have physical dimensions of $[1/Length]^2$.

Under the product-averaging assumptions made, the evolution of the polar dislocation density tensor is given by

$$\dot{\bar{\alpha}} = \bar{\alpha}_{,t} + grad_x\bar{\alpha}\,\bar{v}$$

$$\Rightarrow \overline{\alpha_{ij\,,t'}} + \overline{\alpha_{ij\,,k'}v_{k'}} = \overline{\alpha_{ij\,,t'}} + \overline{\alpha_{ij\,,k'}\,v_{k'}} = \overline{\frac{d}{dt'}\alpha_{ij}}$$

$$\overline{\frac{d}{dt'}\alpha} = \overline{-curl_{x'}\left(\alpha \times V\right) - div_{x'}v\alpha + \alpha L^T}$$

$$\approx -curl_x\left(\bar{\alpha} \times \bar{V} + L^p\right) - \bar{\alpha} \otimes I : \bar{L} + \bar{\alpha}\bar{L}^T$$

$$\Rightarrow \dot{\bar{\alpha}} \approx -curl\left(\bar{\alpha} \times \bar{V} + L^p\right) - \bar{\alpha} \otimes I : \bar{L} + \bar{\alpha}\bar{L}^T , \tag{32}$$

where $(\cdot)_{,k'} = \partial(\cdot)/\partial x'_k$. Consequently the evolution of the scalar polar dislocation density is

$$\dot{\kappa}_g = 2\bar{\alpha} : \left[-curl\left(\bar{\alpha} \times \bar{V} + \tilde{L}^p\right)\right] - 2\left\{(\bar{\alpha} : \bar{\alpha})I - \bar{\alpha}^T\bar{\alpha}\right\} : \bar{L}^T . \tag{33}$$

We now assume that the mesoscale specific entropy field depends on

$$\eta\left(C^e\left(\bar{W}\right), \kappa_g, \kappa_s, \rho, \varepsilon\right). \tag{34}$$

We also assume that *Balance of energy and the Second Law hold in the same form for average fields, regardless of the length scale of averaging; the only change with length scale of averaging occurs in the actual details of the specific entropy response function, as defined in (34).*

From here onwards, we work with average fields but *drop the overhead bars for convenience*. Balance of energy takes the form

$$\rho\dot{\varepsilon} = T : L + div\,q + r , \tag{35}$$

where q is the heat flux vector[2] and r is the volumetric heat supply, and the Second Law is written as

$$\frac{d}{dt}\int_{B(t)}\rho\eta\,dv - \int_{\partial B(t)}\frac{q\cdot n}{\theta}da + \int_{B(t)}\frac{r}{\theta}dv =: H \geq 0 . \tag{36}$$

Using (34), and defining the *back-stress tensor*

$$B := -2\rho\frac{\partial\hat{\eta}}{\partial\kappa_g}\left(\alpha^T\alpha - (\alpha:\alpha)I\right) + \rho^2\frac{\partial\hat{\eta}}{\partial\rho}I + 2W^T curl\left(\rho\frac{\partial\hat{\eta}}{\partial\kappa_g}\alpha\right) \tag{37}$$

which is in general non-symmetric due to the last term, we have

---

[2] Where $q\cdot n$, n a unit vector, gives the heat flow per unit time in the direction $-n$, through unit area perpendicular to n.

$$H = \int_B \left[\frac{T}{\theta} - \left\{ \rho W^T \frac{\partial \eta}{\partial W} + 2\rho \frac{\partial \eta}{\partial \kappa_g} \left[(\boldsymbol{\alpha} : \boldsymbol{\alpha}) I - \boldsymbol{\alpha}^T \boldsymbol{\alpha} \right] + \rho^2 \frac{\partial \eta}{\partial \rho} I \right\} \right] : L \, dv$$

$$+ \int_B \rho \left(\frac{\partial \eta}{\partial \varepsilon} - \frac{1}{\theta} \right) \dot{\varepsilon} \, dv + \int_{B(t)} \frac{q \cdot grad \, \theta}{\theta^2} \, dv$$

$$+ \int_B X \left\{ \left(F^{eT} \left(\theta^{-1} T - B \right) \right)^T \boldsymbol{\alpha} \right\} \cdot V \, dv \quad + \quad \int_B F^{eT} \left(\theta^{-1} T - B \right) : \tilde{L}^p \, dv \qquad (38)$$

$$+ \int_B \rho \frac{\partial \eta}{\partial \kappa_s} \dot{\kappa}_s \, dv + \int_{\partial B} 2\rho \frac{\partial \eta}{\partial \kappa_g} \boldsymbol{\alpha} : \left[\left(\boldsymbol{\alpha} \times V + \tilde{L}^p \right) \times n \right] da,$$

where $(XAB)_i := e_{ijk} A_{jr} B_{rk}$.

Therefore, a sufficient condition for the satisfaction of the second law (36) for all processes of this model of dislocation mechanics is to require constitutive equations for $q, V, \tilde{L}^p, \dot{\kappa}_s, T, \theta$ to satisfy

$$q \cdot grad \, \theta \geq 0 \qquad (39)$$

$$X \left\{ (T - B)^T \left(F^e \boldsymbol{\alpha} \right) \right\} \cdot V \geq 0 \qquad (40)$$

$$F^{eT} (T - B) \cdot \tilde{L}^p \geq 0 \qquad (41)$$

$$\text{sgn} (\dot{\kappa}_s) = \text{sgn} \left(\rho \frac{\partial \eta}{\partial \kappa_s} \right) \qquad (42)$$

$$T = \theta \left\{ \rho W^T \frac{\partial \eta}{\partial W} + 2\rho \frac{\partial \eta}{\partial \kappa_g} \left[(\boldsymbol{\alpha} : \boldsymbol{\alpha}) I - \boldsymbol{\alpha}^T \boldsymbol{\alpha} \right] + \rho^2 \frac{\partial \eta}{\partial \rho} I \right\} \qquad (43)$$

$$\frac{1}{\theta} = \frac{\partial \eta}{\partial \varepsilon}. \qquad (44)$$

Of course, an implicit assumption in the above is that the stress response function depends on the list $(W, \boldsymbol{\alpha}, \kappa_s, \rho, \varepsilon)$. Also, we assume $\left| \rho \frac{\partial \hat{\eta}}{\partial \kappa_g} \boldsymbol{\alpha} \right|$ to be small in comparison to other stresses in the dissipative driving forces (40) and (41) so that the boundary term can be neglected with respect to considerations of ensuring non-negative entropy production in the body.

It can be shown that since η depends on W through C^e

$$W^T \frac{\partial \eta}{\partial W} = -2 F^e \frac{\partial \eta}{\partial C^e} F^{eT},$$

so that the stress tensor (43) is *symmetric*. The driving force for $\tilde{L}^p$ however is nonsymmetric, indicating that the skew-symmetric part of $\tilde{L}^p$ (*plastic spin*) affects the dissipative cost in the model in contrast to the conventional theory of crystal plasticity as well as 'isotropic' finite deformation plasticity theory.

Related to the shortcomings of the theory with regard to making fundamental suggestions on kinetic laws, we mention here that phenomenological models for the accumulation of scalar fluctuation dislocation density κ_s, e.g. the Voce law, see Kocks et al. (2000) or Guruprasad and

Benzerga (2008), and the averaged dislocation fluctuation plastic flow, $\tilde{L}^p$, can be accommodated within the thermodynamic restrictions mentioned above with straightforward modifications. As for $\tilde{L}^p$, thermodynamic restrictions for both 'isotropic' and crystal plasticity forms result.

In Acharya (2004) and Acharya and Roy (2006), a natural decomposition of W into compatible and incompatible parts is introduced that has practical advantages in solving for the state of internal stress corresponding to a given polar dislocation density distribution and in dealing with situations when the polar dislocation density field vanishes on the body. In Appendix C, the connection between what is presented above and that work is made.

Acknowledgment

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Appendix A: Thermodynamics in terms of the Helmholtz free energy and absolute temperature

Assume that we have the specific entropy function, $\tilde{\eta}$, defined as a function of (ε, d), where d is the collection of objects (ρ, z) interpreted as an array of numbers. Under the assumption that

$$\frac{\partial^2 \tilde{\eta}}{\partial \varepsilon^2} > 0$$

for all (ε, d), the temperature relation

$$\frac{1}{\theta} = \frac{\partial \tilde{\eta}}{\partial \varepsilon}(\varepsilon, d) \tag{45}$$

implies that there exists a function $\tilde{\varepsilon}$ such that

$$\varepsilon = \tilde{\varepsilon}(\theta, d).$$

Then, one can define the *Helmholtz free energy density* as

$$\psi = \tilde{\psi}(\theta, d) := \tilde{\varepsilon}(\theta, d) - \tilde{\eta}(\tilde{\varepsilon}(\theta, d), d) \theta. \tag{46}$$

Without loss of essential generality and to underplay the relevance of the heat supply term, we assume $r \equiv 0$. However, we proceed in the restricted case of $^m V \equiv 0$ for the sake of simplicity.

First, note that (45) and (46) imply

$$\frac{\partial \tilde{\psi}}{\partial \theta}(\theta, d) = -\tilde{\eta}(\tilde{\varepsilon}(\theta, d), d).$$

Consequently, we have

$$\dot{\varepsilon} = \frac{\partial \tilde{\psi}}{\partial d} \cdot \dot{d} + \theta \dot{\eta},$$

where the notation $\partial(\cdot)/\partial d$ implies the array of partial derivatives of the function $(\cdot)$ with respect to each entry of the array d. Therefore, balance of energy

$$\rho \dot{\varepsilon} = T : L + \operatorname{div} q$$

may be written in the alternate forms

$$\rho \theta \dot{\eta} = T : L - \rho \frac{\partial \tilde{\psi}}{\partial d} \cdot \dot{d} + \operatorname{div} q \quad \Leftrightarrow \quad -\rho \theta \frac{\partial^2 \tilde{\psi}}{\partial \theta^2} \dot{\theta} = \operatorname{div} q + \rho \theta \frac{\partial \tilde{\psi}}{\partial \theta \partial d} \cdot \dot{d} + \left(T : L - \rho \frac{\partial \tilde{\psi}}{\partial d} \cdot \dot{d} \right). \tag{47}$$

We now consider the following simple calculation implied by (46) and (45):

$$\frac{\partial \tilde{\psi}}{\partial d} = \frac{\partial \tilde{\varepsilon}}{\partial d} - \left[\frac{\partial \tilde{\eta}}{\partial \varepsilon} \frac{\partial \tilde{\varepsilon}}{\partial d} + \frac{\partial \tilde{\eta}}{\partial d} \right] \theta \Rightarrow \rho \frac{\partial \tilde{\psi}}{\partial d}(\theta, d) = -\rho \theta \frac{\partial \tilde{\eta}}{\partial d}(\tilde{\varepsilon}(\theta, d), d), \tag{48}$$

where $\dfrac{\partial \tilde{\eta}}{\partial d}(\tilde{\varepsilon}(\theta, d), d)$ has the regular meaning of being a partial derivative of the function $\tilde{\eta}$ with respect to d keeping ε fixed, and then evaluating at the pair at $(\tilde{\varepsilon}(\theta, d), d)$. Motivated by the second law of thermodynamics (see ((36), (38), and (44)), we now define the *mechanical dissipation* as

$$D := \rho \frac{\partial \tilde{\eta}}{\partial d} \cdot \dot{d} + \frac{T : L}{\theta} \geq 0,$$

to find the *temperature evolution equation* (47)$_2$ equivalent with balance of energy to be

$$\boxed{\rho c\dot{\theta} = div\,\boldsymbol{q} + \rho\theta\frac{\partial\tilde{\psi}}{\partial\theta\partial d}\cdot\dot{d} + \theta D}, \quad c := -\theta\frac{\partial^2\tilde{\psi}}{\partial\theta^2}. \tag{49}$$

The temperature evolution equation may be physically interpreted as a redistribution of the mechanically dissipated power plus the power received from heat into a change of entropy content at a point. It should be noted that while the mechanically dissipated power (and its corresponding entropy change, D) is necessarily non-negative, the entropy at a point can increase or decrease at any given instant depending on the entropy flux due to heat transfer. It should be noted that the Helmholtz-free energy defined here refers to an isolated constrained, Hamiltonian system.

Appendix B: Kinematics of Burgers vector conservation

We follow Fox (1966) and Acharya (2004) in this development. The dislocation density tensor is defined as the departure of the inverse elastic distortion from being a gradient of a vector field on the current configuration. So,

$$curl\,\boldsymbol{W} = -\boldsymbol{\alpha}\,. \tag{50}$$

Both $\boldsymbol{W}$ and $\boldsymbol{\alpha}$ are two-point tensor fields linking the current configuration to the, possibly incompatible, unstressed elastic reference (often referred to as the intermediate configuration – since we have no need to introduce an artificial reference configuration or the tensor field $\boldsymbol{F}^p$, the adjective 'intermediate' is superfluous).

Consider the case of finite elasticity without dislocations when $\boldsymbol{W}$ is a gradient of a vector field, i.e. an object that can be integrated on curves to produce a vector. This motivates the definition of $\boldsymbol{W}$, even in the presence of defects, to be a geometric object of the same kind.
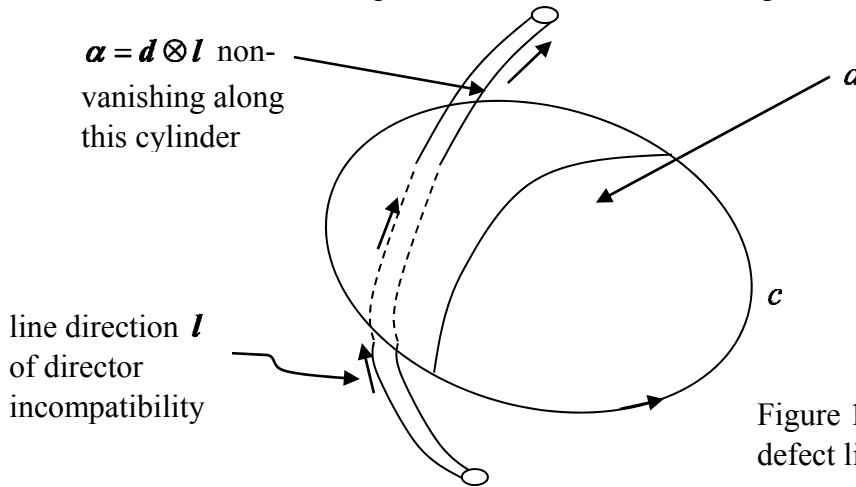

Figure 1. Dislocation density defect lines

Furthermore, by (50), then, $\boldsymbol{\alpha}$ is an areal density of defect lines, that represents elastic incompatibility. This is best appreciated at any spatial point where $\boldsymbol{\alpha}$ can be written as a tensor product of two vectors, so that the defect density may be visualized as a line carrying a vectorial attribute (Figure 1), the Burgers vector.

If a is *any* oriented area patch with unit normal field $\boldsymbol{v}$ and bounded by the closed curve c, and a has no defect lines intersecting it, then $\boldsymbol{W}$ can be written as a gradient on the patch. On the other hand, for an area patch intersected by the defect line, the integral

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$$\int_a \alpha \boldsymbol{v} \, da$$

quantifies the failure of W to define a single-valued (inverse) elastic deformation map when integrated along the closed curve c. *Thus*

$$\alpha \boldsymbol{v} \, da$$

characterizes the Burgers vector content in the oriented infinitesimal area element $\boldsymbol{v} da$. An immediate consequence of the definition (50) is that α is a solenoidal field and this implies that the dislocation density lines either end at boundaries or are closed loops.

It is natural to assume that these line-like dislocations move with a velocity and thus a velocity field, V *relative to the material*, can be attributed to the dislocation density field. The density field may also be integrated over an area and an accounting of the Burgers vector content of a particular area-patch of material particles over time can be carried out. This is the basis of the conservation law that provides the dynamics of the dislocation density field as

$$\overline{\int_{a(t)} \alpha \boldsymbol{v} \, da} = -\int_{c(t)} \alpha \times V \, d\boldsymbol{x}, \tag{51}$$

where $a(t)$ is the area patch occupied by an arbitrarily fixed set of material particles at time t and $c(t)$ is its closed bounding curve. The corresponding local form of (51) is given by

$$\overset{\circ}{\alpha} = -curl(\alpha \times V).$$

The right side of (51) represents the flux of Burgers vector carried by dislocations lines entering the material area patch a. This is best understood by decomposing α and V on a special orthonormal basis oriented with respect to an infinitesimal segment of the bounding curve c as shown in Figure 2.
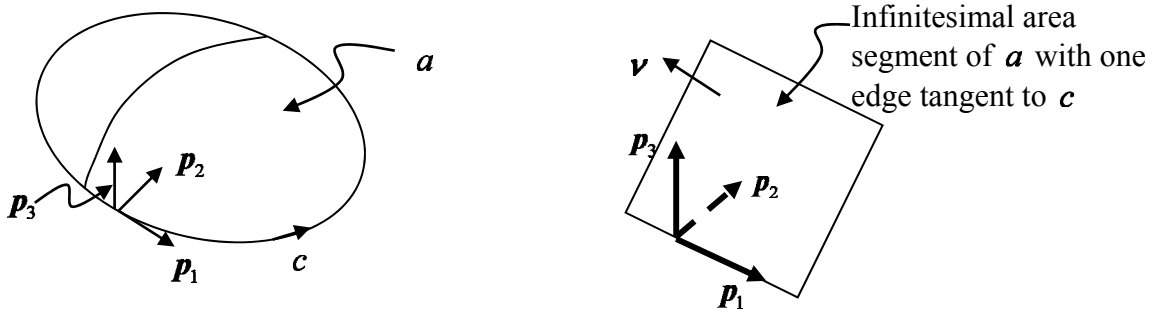

Figure 2. Orientation of local frame for understanding dislocation flow

$$(-\alpha \times V)d\boldsymbol{x} = -d\boldsymbol{x}\left[(\alpha \boldsymbol{p}_i) \otimes (\boldsymbol{p}_i \times V)\right]\boldsymbol{p}_1$$

$$= -(\alpha \boldsymbol{p}_1)d\boldsymbol{x}\left[\boldsymbol{p}_1 \times (V^1 \boldsymbol{p}_1 + V^2 \boldsymbol{p}_2 + V^3 \boldsymbol{p}_3)\right] \cdot \boldsymbol{p}_1$$

$$-(\alpha \boldsymbol{p}_2)d\boldsymbol{x}\left[\boldsymbol{p}_2 \times (V^1 \boldsymbol{p}_1 + V^2 \boldsymbol{p}_2 + V^3 \boldsymbol{p}_3)\right] \cdot \boldsymbol{p}_1$$

$$-(\alpha \boldsymbol{p}_3)d\boldsymbol{x}\left[\boldsymbol{p}_3 \times (V^1 \boldsymbol{p}_1 + V^2 \boldsymbol{p}_2 + V^3 \boldsymbol{p}_3)\right] \cdot \boldsymbol{p}_1$$

Without loss of generality, we also assume that the basis chosen is such that $\boldsymbol{\nu}$ of the infinitesimal area element at the boundary is not parallel to $\boldsymbol{p}_1 \times \boldsymbol{p}_2$ or $\boldsymbol{p}_1 \times \boldsymbol{p}_3$. Mathematically it is clear that there is no contribution to the flux from the first term on the right side above. Physically, this is understood as follows: the motion of any defect line along itself clearly produces no flux into the area element. Furthermore the motions, along directions $\boldsymbol{p}_2$ and $\boldsymbol{p}_3$, of the defect line component along $\boldsymbol{p}_1$ produce no intersection of this line component with the area element. Similar reasoning gives the physical meaning of

$$(-\boldsymbol{\alpha} \times V)\, d\boldsymbol{x} = -(\boldsymbol{\alpha} \boldsymbol{p}_2)\, d\boldsymbol{x}\, V^3 + (\boldsymbol{\alpha} \boldsymbol{p}_3)\, d\boldsymbol{x}\, V^2$$

(note that the signs are consistent with the chosen orientation of a and c).

The conservation law (51) implies a specific evolution for inverse elastic distortion as shown next. Arbitrarily fix an instant of time, say s, in the motion of a body and let $\boldsymbol{F}_s$ denote the time-dependent deformation gradient field corresponding to this motion with respect to the configuration at the time s. Denote positions on the configuration at time s as $\boldsymbol{x}_s$ and the image of the area patch $a(t)$ as $a(s)$. We similarly associate the closed curves $c(t)$ and $c(s)$. Then, using the definition (50) and Stokes's theorem, (51) can be written as

$$\overline{\int_{a(t)} \{-curl\, \boldsymbol{W}\}\boldsymbol{\nu}\, da}\;^{\boldsymbol{\cdot}} = -\int_{a(t)} curl\{\boldsymbol{\alpha} \times V\}\boldsymbol{\nu}\, da$$

$$\Rightarrow \overline{\int_{c(s)} \boldsymbol{W}\boldsymbol{F}\, d\boldsymbol{x}_s}\;^{\boldsymbol{\cdot}} = \int_{c(s)} [\boldsymbol{\alpha} \times V]\, \boldsymbol{F}_s\, d\boldsymbol{x}_s$$

$$\Rightarrow \int_{a(s)} curl\left(\overline{\boldsymbol{W}\boldsymbol{F}_s}\;^{\boldsymbol{\cdot}} - [\boldsymbol{\alpha} \times V]\boldsymbol{F}_s\right)\boldsymbol{\nu}\, da = \boldsymbol{0}$$

$$\Rightarrow \overline{\boldsymbol{W}\boldsymbol{F}_s}\;^{\boldsymbol{\cdot}} = [\boldsymbol{\alpha} \times {}^{\beta}V]\boldsymbol{F}_s$$

(52)

since the conservation law holds for all area patches. Without loss of generality we have made the assumption that a possibly additive gradient vanishes. Physically, this corresponds to the fact that at the 'microscopic' level no plastic deformation can occur at a point in the absence of dislocations at that location. Consequently, we have

$$\dot{\boldsymbol{W}}\boldsymbol{F}_s + \boldsymbol{W}\boldsymbol{L}\boldsymbol{F}_s = [\boldsymbol{\alpha} \times V]\boldsymbol{F}_s ,$$

and choosing $s = t$, we obtain

$$\dot{\boldsymbol{W}} + \boldsymbol{W}\boldsymbol{L} = \boldsymbol{\alpha} \times V .$$

(53)

Appendix C: An orthogonal decomposition for $\boldsymbol{W}$

Consider equations (22) and (24) or (29):

$$curl\, \boldsymbol{W} = -\boldsymbol{\alpha}$$

$$\dot{\boldsymbol{W}} + \boldsymbol{W}\boldsymbol{L} = \boldsymbol{\Pi} ,$$

where we have dropped overhead bars for convenience, and $\boldsymbol{\Pi}$ takes appropriate forms as described earlier.

Motivated by the question of determining the state of internal stress in a known body containing a given dislocation density distribution – which also translates to the question of setting up initial conditions on W consistent with that for $\boldsymbol{\alpha}$ in (19)-(24) or (27)-(30) – it is natural to introduce a decomposition of W into compatible and incompatible parts, most immediately on the current configuration. Thus we consider

$$\left.\begin{array}{c} W = \tilde{\chi} + grad\ f \\ div\ \tilde{\chi} = \boldsymbol{0} \end{array}\right\} \quad \text{on the current configuration}$$

$$\tilde{\chi}\boldsymbol{n} = \boldsymbol{0} \quad \text{on boundary of current configuration}$$

The goal now is to pose the theory in terms of $\tilde{\chi}$ and $grad\ f$ instead of W. The last two conditions above are designed to ensure that when $\boldsymbol{\alpha} \equiv \boldsymbol{0}$ on the body, the incompatible part of the inverse elastic distortion vanishes identically, since, with the decomposition in force, the incompatible part satisfies

$$curl\ \tilde{\chi} = -\boldsymbol{\alpha}\ .$$

Of course, for the current configuration known as well as the dislocation density field on it, the above specification also uniquely determines $\tilde{\chi}$ on it. It remains now to deduce the governing equation for $grad\ f$. For this, we consider

$$\dot{W} + WL = \dot{\tilde{\chi}} + grad\ \dot{f} - (grad\ f)L + (\tilde{\chi} + grad\ f)L = \Pi$$

$$\Rightarrow grad\ \dot{f} = \Pi - \dot{\tilde{\chi}} - \tilde{\chi}L$$

$$\Rightarrow \boxed{div\ grad\ \dot{f} = div\left(\Pi - \dot{\tilde{\chi}} - \tilde{\chi}L\right)}\ \text{on the current configuration.}$$

It is natural now to impose the boundary condition necessary for existence of solutions to the above component-wise Poisson equation for $\dot{f}$, i.e.

$$\left(grad\ \dot{f} - \left(\Pi - \dot{\tilde{\chi}} - \tilde{\chi}L\right)\right)\boldsymbol{n} = \boldsymbol{0} \quad \text{on the boundary of the current configuration.}$$

Thus, if instead of working with W one intends to work with the pair $\left(\tilde{\chi}, grad\ f\right)$, the governing equations for these fields would be

$$curl\ \tilde{\chi} = -\boldsymbol{\alpha}$$

$$div\ \tilde{\chi} = \boldsymbol{0} \qquad\qquad \text{on the current configuration}$$

$$div\ grad\ \dot{f} = div\left(\Pi - \dot{\tilde{\chi}} - \tilde{\chi}L\right)$$

and

$$\tilde{\chi}\boldsymbol{n} = \boldsymbol{0}$$

$$\left(grad\ \dot{f} - \left(\Pi - \dot{\tilde{\chi}} - \tilde{\chi}L\right)\right)\boldsymbol{n} = \boldsymbol{0} \qquad \text{on the boundary of the current configuration.}$$

These equations are the ones suggested in Acharya (2004) and Acharya and Roy (2006).