On thermodynamics of crystal plasticity

V.L. Berdichevsky

Mechanical Engineering, Wayne State University, 5050 Anthony Wayne, Detroit MI 48202, United States

Received 23 July 2005; received in revised form 7 October 2005; accepted 13 October 2005
Available online 10 November 2005

Abstract

It is argued in this paper that there are three distinctive physical situations in which the continuum descriptions of crystal plasticity are conceptually different. They are determined by the properties of the random field of dislocation density. One of the cases corresponds to conventional plasticity theory. In this case the system energy possesses the energy density, and a formula for energy density of the dislocation microstructure is derived. The phenomenology of the energy of microstructure is briefly discussed.

Keywords: Homogenization; Microstructure; Plasticity theory; Dislocation theory

1. Introduction

Thermodynamics is a theory of the slow variables of very complex systems. The goals of thermodynamics of crystal plasticity are to identify the slow characteristics of plastic flow and formulate the equations governing their evolution. The current understanding of the subject is still far from the level necessary to achieve these goals. In classical plasticity theory the basic slow variables are the fields of displacements, plastic strains, and entropy (or temperature). Classical plasticity ignores completely the microstructure and its evolution in the course of plastic flow, yet the evolution of microstructure is the reason for work hardening and many other plasticity phenomena. A physically adequate theory of plasticity should include the characteristics of microstructure and their interplay with macroscopic plastic flow. Some suggestions in this regard are made in this paper. We focus on the case when the only essential feature of the microstructure is the evolving dislocation network. The key question is: which characteristics of the dislocation network should enter into continuum plasticity theory? This question is inseparable from the question of how energy depends on the characteristics of the dislocation distribution. At first glance, the proper set of characteristics must determine the energy uniquely. For, in a conventional thermodynamics, energy is a deterministic functional of the basic kinematical fields. It turns out that the situation is, in fact, more complex: there are three essentially different physical situations specified by the relative order of the correlation radius of the dislocation network, \( a \), and the characteristic length of the problem, \( L \). If the correlation radius \( a \) is much smaller than the characteristic length \( L \), and there exists a characteristic length, \( l \), such that

\[
a \ll l \ll L
\]

(1)

then, as we will see, the system energy possesses an energy density which depends only on the local characteristics of the dislocation network.

Quite distinctive is the situation when

\[
a \ll L
\]

(2)

but the scale difference between \( a \) and \( L \) does not allow one to introduce \( l \) satisfying (1). A possibility for a continuum theory still exists but its meaning is essentially different from the conventional one.

In the third case,

\[
a \sim L
\]

(3)

the character of the theoretical description changes completely. A deterministic energy density as a function of...
local characteristics does not exist anymore. Total energy becomes an independent characteristic of the system which is additional to all other characteristics.

It was argued by Berdichevsky and Dimiduk [4] that in typical situations (turbulent plastic flow in Cottrell’s terminology [5]) the length \( a \) is on the order of tens of microns: the flow is highly intermittent with the characteristic size of inhomogeneity on the order of tens of microns. Some size-effect problems, like the dependence of hardness on the indenter size or yield stress on the specimen size, pertain, perhaps, to the third case. An approach to study the problems for the third case is outlined in [3], and we do not dwell on this case here. In laminar plastic flows the characteristic length \( a \) may be much less, and the cases 1 and 2 are possible even for microsamples.

In this paper, we briefly discuss the peculiarities of the first two cases and the corresponding formulas for the energy of the microstructure, and consider phenomenological models for the energy of microstructure. Most details of the derivations are omitted here due to the limited size of the paper; a complete treatment will be published elsewhere.

2. Energy of a crystal: The first case

We begin with the discussion of the first case. Consider a crystal occupying some region \( V \). In an initial stress-free state it does not contain defects. The energy of the initial state is the energy of thermal motion of the atoms, \( \mathcal{U}_{\text{th}} \). The displacements from the initial state to the actual state, \( u_i \), are assumed to be small (small Latin indices correspond to projections on a Cartesian observer’s frame and run through the values 1, 2, 3). Let one impose some prescribed displacements, \( u_{i|\partial V} \) at the boundary, \( \partial V \), of region \( V \),

\[
u_i = u_{i(\partial V)} \text{ at the boundary } \partial V \tag{4}\]

For simplicity, we neglect heat conductivity, so one can ignore the change of temperature. Then, in linear theory, the energy of the body, \( \mathcal{U} \), is determined by the variational problem

\[
\mathcal{U} = \min_{u \in \mathcal{W}} \int_V \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \, d^3x + \mathcal{U}_{\text{th}} \tag{5}
\]

where the minimum is taken with respect to all displacement fields \( u_i \) satisfying the constraint (4), \( C_{ijkl} \) are the components of the Young’s moduli tensor, and \( \varepsilon_{ij} \) are the strain tensor components,

\[
\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{6}
\]

We are going to show that, in the presence of dislocations, this formula is changed to

\[
\mathcal{U} = \min_{\varepsilon \in \mathcal{W}} \int_V \frac{1}{2} C_{ijkl} (\varepsilon_{ij} - \varepsilon_{ij}^{(p)}) (\varepsilon_{kl} - \varepsilon_{kl}^{(p)}) \, d^3x + \int_V U_m \, d^3x + \mathcal{U}_{\text{th}} \tag{7}
\]

where \( \varepsilon_{ij}^{(p)} \) are the averaged plastic strains associated with the dislocation distribution (bar denotes volume average), \( U_m \) the energy density of microstructure which is to be computed in the following way: to find \( U_m \), at point \( x \) one takes a box \( B \) of size \( l \) with the center at \( x \), remove all the dislocations outside of this box, assume in the box the dislocation density tensor equal to \( \varepsilon_{ij} - \bar{\varepsilon}_{ij} \), and find the energy of such a crystal, \( \mathcal{U}_{m} \), for zero displacements at the boundary; this energy, \( \mathcal{U}_{m} \), is a deterministic number in spite of the randomness of the field \( \varepsilon_{ij} \); finally, \( U_m = \mathcal{U}_{m}/|B|, |B| \) being the volume of the box \( B \). Energy density \( U_m \) may depend upon the position of the point \( x \) due to the interactions of the dislocations inside \( B \) with the boundary.

We begin with an easy justifiable relation for the energy of a crystal having dislocations

\[
\mathcal{U} = \mathcal{U}_0 - \int_V \sigma^{ij}_p \varepsilon_{ij}^{(p)} \, d^3x + \mathcal{U}_1 + \int_L \varepsilon_{ij} ds + \mathcal{U}_{\text{th}} \tag{8}
\]

Here \( \mathcal{U}_0 \) is the energy of the perfect crystal with the prescribed displacements at the boundary, \( \sigma^{ij}_p \) the corresponding stress field, \( \varepsilon_{ij}^{(p)} \) the field of plastic strains, \( \mathcal{U}_1 \) the energy of the crystal with the dislocation density tensor \( \varepsilon_{ij} \) and zero displacements at the boundary,

\[
\mathcal{U}_1 = \int_V \int_2 \frac{1}{2} R^{ijkl}(x,y)z_{ij}(x)z_{kl}(y) \, d^3x \, d^3y \tag{9}
\]

\( R^{ijkl}(x,y) \) a singular deterministic kernel depending on the geometry of region \( V \). The fourth term in (7) is the dislocation core energy, \( L \) being the set of all dislocation lines and \( e_0 \) the dislocation core energy per unit length. The dislocation density tensor is assumed to be desingularized by, for example, smearing out the delta functions over the tubes around the dislocation lines having a diameter on the order of the Burgers vector \( b \). Therefore, some dislocation core energy is contained in (8), and \( e_0 \) is to be understood as a necessary correction to obtain the proper value of the dislocation core energy.

Let us divide region \( V \) into a large number, \( N \), of small boxes \( B_x \), \( x = 1, 2, \ldots, N \). The volume of a box is \( |B| = |V|/N, |V| \) being the volume of region \( V \). Denote the space average over the box \( B_x \) by bar: for any function \( \varphi \)

\[
\bar{\varphi} = \frac{1}{|B_x|} \int_{B_x} \varphi \, d^3x
\]

The plastic strain field can be presented as a sum of the averaged plastic strains, \( \varepsilon_{ij}^{(p)} \), and fluctuations \( \varepsilon_{ij}^{(p)} = \varepsilon_{ij}^{(p)} + \xi_{ij}^{(p)} \). Similarly, \( \varepsilon_{ij} = \bar{\varepsilon}_{ij} + \bar{\xi}_{ij} \). The average value of fluctuating plastic strain and dislocation density is zero in each box. We assume that \( \varepsilon_{ij}^{(p)} \) and \( \bar{\varepsilon}_{ij} \) are slow variables, i.e. they change over distances which are much larger than the box size. The smooth functions which interpolate \( \varepsilon_{ij}^{(p)} \) and \( \bar{\varepsilon}_{ij} \) will also be denoted by \( \varepsilon_{ij}^{(p)} \) and \( \bar{\varepsilon}_{ij} \). Assume also that \( \varepsilon_{ij}^{(p)} \) and \( \bar{\varepsilon}_{ij} \) are random fields which possess the ergodic property: space average coincides with the mathematical expectation, in particular,

\[
\mathcal{M} \varepsilon_{ij}^{(p)} = \bar{\varepsilon}_{ij}^{(p)}, \quad \mathcal{M} \bar{\varepsilon}_{ij} = \bar{\varepsilon}_{ij} \text{ in each box } B_x
\]
Here $\mathcal{M}$ stands for the mathematical expectation. Consider the second term in (7)
\[
\int_V d^3x \frac{\delta e_{ij}(p)}{\delta x} = \int_V d^3x \frac{\delta e_{ij}(p)}{\delta x} + \sum_x \int_{B_x} d^3x \frac{\delta e_{ij}(p)}{\delta x}
\]

Let us choose the box size equal to the correlation radius of the dislocation network $a$ (thus, $N \sim (L/a)^3$). Then the values of the members of the sum are statistically independent and have zero mean value. Therefore, a typical value of the sum is of the order of $N^{-1/2}$; for small $a/L$ it is of the order of $(a/L)^{3/2}$. Thus, the sum can be neglected.

Consider now the third term in (7). It can be written as
\[
\mathcal{M}_1 = \int_V \int_V \frac{1}{2} R_{ijkl}(x, y) \bar{\omega}_{ij}(x) \bar{\omega}_{kl}(y) d^3x d^3y
+ \int_V \int_V \frac{1}{2} R_{ijkl}(x, y) \bar{\omega}_{ij}(y) \bar{\omega}_{kl}(y) d^3x d^3y
+ \sum_{x=1}^N \int_{B_x} \int_{B_x} \frac{1}{2} R_{ijkl}(x, y) \bar{\omega}_{ij}(x) \bar{\omega}_{kl}(y) d^3x d^3y
+ \sum_{x \neq y} \int_{B_x} \int_{B_y} \frac{1}{2} R_{ijkl}(x, y) \bar{\omega}_{ij}(y) \bar{\omega}_{kl}(y) d^3x d^3y
\]  

(9)

The second term is on the order of $N^{-1/2}$ as a sum of independent random variables with zero mean and can be neglected. The fourth term has a different structure of a double sum of the products of independent random variables. The sum contains about $N^2$ terms on the order of $|B|^2$. Therefore, the sum may be of the order of $N^2 \times |B|^2 \sim |V|^2$, i.e. finite. The probability of such an event is, however, very small because the average value of each member of the sum is zero, and the terms of the sum are statistically independent. Since the average value of the sum is zero, a typical value of the sum is on the order of the variance of the sum, which, as is easy to estimate, on the order of $N |B|^2 = |V|^2$. Therefore, the fourth term can be neglected as well. It should be emphasized that such simplifications can be made “in most cases”; however, for some rare realizations they yield a wrong answer. The similar issue is encountered in turbulence theory (see Berdichevsky [1]).

The third term in (9), after the addition of the dislocation core energy, is a sum of energies $\Delta \mathcal{M}_m$ for the boxes $B_x$; it converges to the second integral in (6). The proof of (6) is completed by referring to the relation
\[
\int_V \int_V \frac{1}{2} R_{ijkl}(x, y) \bar{\omega}_{ij}(x) \bar{\omega}_{kl}(y) d^3x d^3y
= \min_{a=0, \pi} \int_V \int_V \frac{1}{2} C_{ijkl}(\bar{\omega}_{ij} - \bar{\omega}_{ij}^{(a)})(\bar{\omega}_{kl} - \bar{\omega}_{kl}^{(a)}) d^3x
\]

and mentioning that adding to this energy the first two terms in (7) gives the first term in (6).

3. Energy of microstructure: Another derivation

Consider again energy $\mathcal{U}_1$ (8) with $x_{ij}$ being some random field. Let $z_{ij}$ mean the mathematical expectation of $z_{ij}$, and $x_{ij}'$ are, as before, fluctuations of the dislocation density. We have
\[
\mathcal{U}_1 = \int_V \int_V \frac{1}{2} R_{ijkl}(x, y) x_{ij}(x) x_{kl}(y) d^3x d^3y
= \int_V \int_V \frac{1}{2} R_{ijkl}(x, y) x_{ij}'(x) x_{kl}'(y) d^3x d^3y
+ \int_V \int_V R_{ijkl}(x, y) \bar{\omega}_{ij}(y) x_{kl}(y) d^3x d^3y
+ \int_V \int_V \frac{1}{2} R_{ijkl}(x, y) \bar{\omega}_{ij}(x) x_{kl}'(y) d^3x d^3y
\]

Suppose that, in spite of randomness of $x_{ij}$, $\mathcal{U}_1$ is practically deterministic, i.e. deviates only slightly from its average value $\mathcal{M}_1$. Then we may replace $\mathcal{U}_1$ with $\mathcal{M}_1$. Let $x_{ij}'$ be statistically independent in boxes $B_x$. Then, obviously,
\[
\mathcal{M}_1 = \int_V \int_V \frac{1}{2} R_{ijkl}(x, y) \bar{\omega}_{ij}(x) \bar{\omega}_{kl}(y) d^3x d^3y
+ \sum_{x=1}^N \int_{B_x} \int_{B_x} \frac{1}{2} R_{ijkl}(x, y) \bar{\omega}_{ij}(x) \bar{\omega}_{kl}(y) d^3x d^3y
\]

Each member of the sum is the mathematical expectation of energy $\Delta \mathcal{M}_m$ introduced in the previous section. The operation of the mathematical expectation may be dropped because $\Delta \mathcal{M}_m$ is practically deterministic: it is a sum of independent random variables, the energies of the boxes of the size $a$. Thus, we again arrive at (6). Another consequence of this reasoning is the relation
\[
\mathcal{M}_1 = \int_V \int_V \frac{1}{2} R_{ijkl}(x, y) \bar{\omega}_{ij}(x) \bar{\omega}_{kl}(y) d^3x d^3y
+ \int_V \int_V \frac{1}{2} R_{ijkl}(x, y) \bar{\omega}_{ij}(x) \bar{\omega}_{kl}(y) d^3x d^3y
\]

where $c_{ijkl}$ is the correlation tensor of dislocation density:
\[
c_{ijkl}(x, y) = \mathcal{M}_1 \bar{\omega}_{ij}'(x) \bar{\omega}_{kl}'(y)
\]

although its use is a complicated issue due to the singularities in both tensors $R_{ijkl}$ and $c_{ijkl}$.

4. Energy of a polycrystal

The derivation of a formula analogous to (6) for a polycrystal is a more difficult task. For polycrystals, the elastic moduli $C_{ijkl}$ are inhomogeneous random fields, and, what further complicates the problem is that the fields $C_{ijkl}$ and $x_{ij}$ might be correlated. In what follows, we assume that the formula for energy (6) holds true for polycrystals as well, if the average grain size $d$ is much smaller than $l$ and $C_{ijkl}$ in (6) are identified with the components of the effective elastic moduli. One cannot expect, however, such a simple recipe for computation of the energy of microstructure as the one given in Section 2 for crystals. A justification of Eq. (6) for polycrystals will be considered elsewhere.
5. Energy of microstructure: Phenomenology

In a phenomenological theory, energy density of microstructure, \( U_m \), is assumed to be a function of the local characteristics of the dislocation network, \( \rho_1, \rho_2, \ldots, \rho_n \). This function for a crystal can be computed in the following way: one takes the box \( B \) of the size \( a \), delete all dislocations outside \( B \), replace the dislocation density tensor by the difference \( \kappa_{ij} - \bar{\kappa}_{ij} \), and determine the average value of \( \Delta \mathcal{W}_m / |B| \) over all dislocation networks which are compatible with the given values of \( \rho_1, \rho_2, \ldots, \rho_n \). Such a problem seems solvable, at least in some cases, by means of the approach developed in [2]. A proper choice of \( \rho_1, \rho_2, \ldots, \rho_n \) for various plasticity phenomena is not known. It should be revealed by a detailed analysis of the dynamics of the dislocation networks. At the moment, we can only speculate on what such characteristics might be. Here we consider some simple phenomenological models which take into account only one or two parameters.

We begin with the simplest case of one-parameter modeling when the microstructure is characterized only by the total length of dislocation lines per unit volume, \( \rho \). The first contemporary models of this type were pioneered by Kocks [8] and Estrin and Mecking [6].

So, let the energy of microstructure per unit volume, \( U_m(\rho) \), be a function of only \( \rho \). The general features of the function \( U_m(\rho) \) are as follows.

First, \( U_m(\rho) \) must tend to zero as \( \rho \) tends to zero. If one takes into account only the core energy of the dislocation lines, then

\[
U_m(\rho) = \text{const} \mu b^2 \rho \quad (10)
\]

where a numerical constant is of the order of 0.1. An analysis of the dislocation interaction energy given for a random set of screw dislocations by Le and Berdichevsky [7] shows that the interaction energy is also linear in \( \rho \) for small \( \rho \). Thus, we adopt formula (10) for small \( \rho \).

If \( \rho \) increases, there must be some saturated value, \( \rho_s \), after which new dislocation structures develop, like subgrains and cell structures or new grain boundaries. Therefore, some additional parameters must come into play. If we prohibit such structures from developing, \( U_m(\rho) \) must tend to infinity as \( \rho \to \rho_s \). The transition near \( \rho = \rho_s \) must be quite sharp. A possible function \( U_m(\rho) \) is

\[
U_m(\rho) = k \mu \ln \left( \frac{1}{1 - \frac{\rho}{\rho_s}} \right) \quad (11)
\]

This model has two material constants, \( k \) and \( \rho_s \).

Let us show that to get the Voce law from the usual thermodynamic reasoning one has to change function (11) to

\[
U_m(\rho) = k \mu \left( \ln \left( \frac{1}{1 - \sqrt{\frac{\rho}{\rho_s}}} \right) - \sqrt{\frac{\rho}{\rho_s}} \right) \quad (12)
\]

which is linear with respect to \( \rho \) for small \( \rho \):

\[
U_m = k \mu \rho / 2 \rho_s \quad (13)
\]

Indeed, consider, for simplicity, a non-heat-conducting body, so that the energy supply to a material element (per unit volume per unit time) is just \( \sigma^i \kappa_{ij} \), \( \sigma^i \) being the stress tensor. The energy equation can be written as

\[
\frac{d}{dt} \left( U_0(\rho'_s, S_{th}) + U_m(\rho) \right) = \sigma^i \kappa_{ij}
\]

where \( \rho'_s = \rho_s - \rho'_{p} \) are elastic strains (we drop the average symbol, bar, since only the averaged parameters enter into a macroscopic theory), \( U_0 \) macroscopic energy density which is equal to \( \frac{1}{2} C_{ijkl}(\kappa_{ij} - \kappa_{ij}^p)(\kappa_{kl} - \kappa_{kl}^p) \) if one ignores thermal effects, \( S_{th} \) the entropy of thermal motion of atoms. Then,

\[
\frac{\partial U_0(\rho'_s, S_{th})}{\partial \rho'_s} \rho'_{s} + \frac{\partial U_0(\rho'_s, S_{th})}{\partial S_{th}} \frac{dS_{th}}{dt} + \int \frac{\partial U_m}{\partial \rho} \frac{d\rho}{dt} + \frac{d\rho}{dt} = \sigma^i \kappa_{ij}
\]

Since \( \partial U_0 / \partial S_{th} \) is equal to temperature, \( T \), and, by the standard reasoning, \( \sigma^i \) are equal to \( \partial U_0 / \partial \rho'_s \), we have

\[
T \frac{dS_{th}}{dt} + \frac{\partial U_m}{\partial \rho} \frac{d\rho}{dt} = \sigma^i \kappa_{ij} \quad (14)
\]

The work done by plastic deformation (the right hand side of (14)) heats the body (the first term in the left hand side) while some portion of the work transforms into the latent heat (the second term in the left hand side). It was experimentally established by Taylor and Quinney [10] that the latent heat is a certain portion of the work done:

\[
\frac{\partial U_m}{\partial \rho} \frac{d\rho}{dt} = \kappa \sigma^i \kappa_{ij} \quad (15)
\]

where \( \kappa \) is a constant of the order of 0.1–0.2. If the strain rates are linked to stresses, and \( U_m(\rho) \) is given, then Eq. (15) can be considered as a closing equation serving to find \( \rho \). For a simple shear with the only non-zero component of stresses, \( \gamma \), and (engineering) strains, \( \gamma \), we have

\[
\frac{\partial U_m}{\partial \rho} \frac{d\rho}{dt} = \kappa \gamma \quad (15)
\]

For the function (12) this transforms to the Voce law for the evolution of the yield strength, g, with strains \( (\gamma \geq 0) \):

\[
g = \frac{g_s - g}{g_s - g_0} \frac{d\gamma}{dt} = \frac{g_s - g_0}{g_s - g_0} \frac{d\gamma}{dt}
\]

using the following correspondences

\[
g = x \mu b \sqrt{\rho}, \quad k = x g_s (g_s - g_0) / \mu \theta_0, \quad \sqrt{\rho_s} = g_s / x \mu b
\]

where \( x \) is a constant, and \( \mu \) the shear modulus. In order to estimate the constants \( k \) and \( \rho_s \) for metals like Al or Ni we take the following values of the parameters: \( x = 1, b = 4 \times 10^{-10} \text{ m}, g_s = 160 \text{ MPa}, g_0 = 17 \text{ MPa}, \theta_0 = 392 \text{ MPa}, \mu = 23 \text{ GPa}, x = 0.15 \). Therefore, \( k = 0.00358, \rho_s = 3 \times 10^{14} \text{ m}^{-2} \). It is interesting to find the energy of microstructure using these data. According to (13) for small \( \rho \) it is equal to
$U_m = (k/2\rho b^2)\mu b^2 \rho = 3.96\mu b^2 \rho$; we see that the dislocation interaction energy is much bigger than the dislocation core energy ($\sim 0.1\mu b^2 \rho$) even for small $\rho$.

This model can be modified to provide a deeper meaning of the constraint $\rho \leq \rho_c$. For this we introduce an additional parameter, a characteristic length, $d$, which may be viewed, depending on a physical situation, as an average grain size or an average size of dislocation cells. We take, for definiteness, the former meaning. Then, the Hall–Petch effect suggests the following dependence of the saturated dislocation density on the grain size:

$$\rho_s(d) = \frac{k_1}{bd}$$

$k_1$ being a phenomenological constant. For the microstructure energy we have

$$U_m(\rho, d) = \dot{U}_m(\rho, \rho_s(d)) + \frac{\dot{\lambda}}{d}$$

(16)

where $\dot{U}_m(\rho, \rho_s)$ is a function (11) or (12), and $\dot{\lambda}$ is the average grain boundary energy per unit area. Instead of (14) one now obtains

$$\frac{dS_m}{dt} + \frac{\partial U_m}{\partial \rho} \dot{\rho} + \frac{\partial U_m}{\partial d} \dot{d} = \sigma_{ij}^\prime \epsilon_{ij}^\prime$$

(17)

A way of closure depends on the specifics of the material behavior to be described. For example, in equal channel angular extrusion that is used to obtain nano- and ultrafine grain materials [9] one observes the sharp decrease of the grain size which does not depend on the strain rate. It is believed that the sharp grain-size drop begins after the work-hardening process is practically completed. During work hardening the grain size does not change. After the completion of work hardening, a fast decay of the grain size sets on. If the completion of the work hardening is modeled by a criterion $\rho_s - \rho = k_2$, $k_2$ being a phenomenological constant, then a possible closure consistent with the thermodynamic Eq. (17) is

if $\rho_s - \rho < k_2$:

$$\frac{\partial U_m}{\partial \rho} \dot{\rho} = \kappa \sigma_{ij}^\prime \epsilon_{ij}^\prime, \quad \dot{d} = 0$$

(18)

if $\rho_s - \rho = k_2$:

$$\frac{\partial U_m}{\partial d} \dot{d} = \kappa \sigma_{ij}^\prime \epsilon_{ij}^\prime, \quad \dot{\rho} = 0$$

(19)

For an appropriate choice of parameters, $\partial U_m/\partial d$ is negative, therefore, after the completion of work hardening, all the work done will go to break up the grains ($\dot{d} < 0$). The closure (18), (19), however, might not be physically adequate: in rolling of metals the grains just elongate without breaking into the smaller ones. Perhaps, the difference between rolling and equal channel angular extrusion is in the character of the macroscopic plastic flow; an adequate thermodynamic theory of nanomaterial manufacturing, which does not exist at the moment, should include a thermodynamic parameter responsible for the grain elongation, i.e. the grain geometry is described, instead of by $d$, by a tensor characterizing the average orientations and dimensions of the grains.

This reasoning can be expanded into continuum theory of dislocations by the following remark: The total dislocation density, $\rho$, is a sum of the dislocation density of the stored dislocations, $\rho_s$, and the dislocation density of moving dislocations, denote it by $\dot{\rho}/b$. The parameter $\sigma$ can be modeled in the isotropic case as

$$\sigma = \sqrt{c_1 \sigma_{ij}^\prime \sigma_{ij}^\prime + c_2 \sigma_{ij}^\prime \sigma_{ij}^\prime}$$

(20)

c_1, c_2 being some phenomenological constants on the order of unity. Finally, one can put

$$\rho = \rho_s + \frac{\sigma}{b}$$

(21)

Eqs. (20) and (21) determine the dependence of energy on the dislocation density tensor.

6. The second case

The situation changes drastically in the case (2). One can repeat the reasoning of Section 2 choosing the box size equal to $a$ and arriving at the same recipe to determine the microstructure energy with the only one difference: $\Delta U_m$ is now the energy of the dislocation content of a box of the size $a$. Therefore, $U_m$ is, in general, random. The existence of the megaboxes of the size $l$ for the case (1) provided an additional averaging of $U_m$ over the megaboxes. This brings a deterministic value of the microstructure energy. In the case (2) megaboxes cannot be introduced, and we end up with the situation where $U_m$ is a random number. In fact, this situation is very close to the case (3). There is, however, an interesting class of problems where a deterministic continuum description may make sense. Let $U_m$ change slowly from box to box, i.e. it can be interpolated by a smooth function of space variables. Consider also an entropy of microstructure per unit volume, $S_m$, as the logarithm of the number of microstates which are compatible with the given values of $U_m, \rho_1, \rho_2, \ldots, \rho_n$. Then

$$S_m = S_m(U_m, \rho_1, \rho_2, \ldots, \rho_n)$$

(22)

Entropy of microstructure is also a slow variable. Instead of (22) one can write

$$U_m = U_m(S_m, \rho_1, \rho_2, \ldots, \rho_n)$$

Thus, we arrive at a class of continuum models which have an additional internal parameter, the entropy of microstructure. This entropy measures fluctuations which occur when one chooses various samples from the ensemble. For this case, the probability density function of the parameters $U_m, \rho_1, \rho_2, \ldots, \rho_n$ is given by the Einstein-type relation

$$f(U_m, \rho_1, \rho_2, \ldots, \rho_n) = \text{const} e^{S_m(U_m, \rho_1, \rho_2, \ldots, \rho_n)}$$

The possibilities and the scope of applications for this class of models have not been explored yet.
Acknowledgements

I thank D. Dimiduk, V.M. Segal and A. Acharia for useful discussions. Support from the Air Force Research Laboratory is gratefully acknowledged.

References