Homogenization in micro-plasticity

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Abstract

Homogenized descriptions of plasticity on micro- and macro-scale are essentially different. A key distinction is that the energy of micron-size specimens, in contrast to that of macro-specimens, is not a functional of integral characteristics of the dislocation networks. Thus, energy must be considered as an independent characteristic of the body which is additional to all other characteristics. In this paper, a homogenized description of dislocation motion on the micro-scale is proposed. The theory is considered for the case of anti-plane constrained shear which admits an analytical treatment.

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1. Introduction

Plasticity of crystalline bodies is caused by motion, multiplication and nucleation of defects of the crystal lattice. Macroscopic plasticity theory employs a homogenized description of the defect behavior. We focus here on dislocation plasticity neglecting the contributions from defects of other types. It was argued by Berdichevsky and Dimiduk (2005) that continuum theories cannot describe dislocation plasticity if the characteristic size of the problem becomes of the order

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of tens of microns: for such sizes “homogenized” characteristics of elastic and plastic fields fluctuate while a continuum theory being deterministic in its nature delivers some certain answers. Fluctuations of “homogenized” elastic and plastic fields make homogenization on the micro-scale fundamentally different from homogenization on the macro-scale. Here, an approach to a homogenized description of dislocation motion on the micro-scale is proposed. We discuss this approach for a simple situation of anti-plane constrained shear where each step can be evaluated analytically. In spite of its simplicity, the anti-plane problem seems to contain all the key ingredients of the general theory. The most essential one is the necessity to consider the energy of the body as an independent parameter which is additional to all other characteristics of the elastic and plastic fields. This is quite different from classical plasticity where energy is a functional of such characteristics.

2. Anti-plane constrained shear

The problem we are going to use as a trial example is as follows. Consider a crystal in the shape of a long circular cylinder. The ends of the cylinder are stress-free. At the lateral surface the displacements are prescribed. The displacement vector is directed along the cylinder axis, depends only on angle \( \theta \) (see Fig. 1), and, at some value of \( \theta \), has a jump \( N b, b \) being the interatomic distance. Then \( N \) screw dislocations enter the crystal to release the stress concentration at the jump. The dislocation positions can be described by points \( r_1, \ldots, r_N \) in the cross-sectional area \( \Omega \). Assume that the elastic properties of the bar are isotropic and characterized by the shear modulus \( G \). For a long bar, one may neglect the end effects and determine the stress state from the two-dimensional boundary-value problem for the stress.
function $\psi$:

$$\frac{1}{G}\triangle \psi = -\sum_{a=1}^{N} b \delta(x - r_a) \quad \text{in } \Omega, \quad \frac{1}{G} \frac{\partial \psi}{\partial n} = -\frac{du(s)}{ds} \quad \text{on } \partial \Omega. \quad (1)$$

Here $\triangle$ is the two-dimensional Laplace operator, $u(s)$ the boundary value of the axial displacement, $s$ the arc length along the boundary, $\partial / \partial n$ the normal derivative at the boundary, $\delta(x)$ the two-dimensional $\delta$-function smeared over a small circle of radius $\varepsilon$ with the center $x = 0$. The radius $\varepsilon$ plays the role of the dislocation core radius; it is in the order of $b$. The distances from the dislocations to the wall are assumed to be bigger than $\varepsilon$.

The function $u(s)$ must obey the condition

$$\int_{\partial \Omega} \frac{du}{ds} ds = Nb \quad (2)$$

which is the necessary condition for the boundary-value problem (1) to have a solution. Eq. (2) is satisfied because, as was assumed, the function $u(s)$ has a jump $Nb$.

The boundary shear strain $\gamma = du/\partial s$ may depend on $s$. Further analytical results pertain to the case of constant boundary shear strain $\gamma$.

The energy of the body per unit length, $H$, depends on the dislocation positions: $H = H(r_1, \ldots, r_N)$. We adopt the formula:

$$H(r_1, \ldots, r_N) = \frac{1}{2G} \int_{\Omega} (\nabla \psi)^2 \, d^2x. \quad (3)$$

In fact, there are additional contributions to the energy caused by the dislocation cores, but we ignore these contributions since they play a role of additive constants.

3. Homogenized description

It is seen from Eqs. (1) and (3) that any change of the dislocation positions affects the value of the energy. An immediate consequence of that feature of the system of dislocations is that energy cannot be considered as a function of any finite set of characteristics of the dislocation network. Suppose, say, we characterize the dislocation network by some set of integral characteristics like the total number of dislocations, the center of gravity of the dislocation cloud, the moments of inertia of the cloud, etc. Let the values of these characteristics be given. If the number of dislocations is bigger than the number of integral characteristics, there is freedom in changing the dislocation positions. This prevents energy from being a function of only the integral characteristics of the dislocation network.

The dependence of energy on the dislocation positions decays as the size of the body increases if the dislocation positions in various parts of the body are statistically independent: by the law of large numbers, the contributions to energy from the different parts of the body average out and bring a deterministic number which does not depend on the details of the dislocation distribution. For a body of
micron size the dislocation positions are not statistically independent, and the influence of the details of the dislocation network geometry on energy cannot be ignored. Since such details are never known, we come to a necessity to consider energy as an independent additional characteristic of the dislocation network.

Let the dislocation network be described by the value of its energy, $E$, and a number of characteristics $\rho_1, \ldots, \rho_m$ which can be measured experimentally and may include the number of dislocations of a certain sign, centers of gravity of dislocations of a certain sign, etc. We assume that the set of parameters $E, \rho_1, \ldots, \rho_m$ is complete, i.e. we know nothing more about the dislocation network besides this set. Thus, it is reasonable to consider an ensemble of all dislocation networks which have the same values of the parameters $E, \rho_1, \ldots, \rho_m$. All the members of the ensemble are assumed to be equally probable. For, an assignment of different probabilities to the members of the ensemble, i.e. saying that one member is more probable than another one, would mean that we know more about the ensemble than just the set of parameters $E, \rho_1, \ldots, \rho_m$, in contradiction with our starting point that this set is all that we know. In the example under consideration we take the simplest case when the only characteristics of the dislocation network are its energy, $E$, and the total number of dislocations, $N$.

4. Energy, entropy and probability

Let the value of energy, $E$, be known. Then not every dislocation network is admissible. Assuming that the number of dislocations is large one may ask, what is probability, $f(x)$, to find a dislocation at the point $x$? The answer to a similar question was obtained by Berdichevsky (1999) in a quite general setting. First, we formulate the results in that general case referring the reader to the original paper for further details.

Let energy be a negative minimum value in the variational problem:

$$-H = \min_{\psi} I(\psi),$$

$$I(\psi) = \frac{1}{2} (A\psi, \psi) - \frac{1}{N} \sum_{a=1}^{N} (l(r_a), \psi),$$

where $(A\psi, \psi)$ is a positive quadratic functional, $(l(r), \psi)$ a random linear functional depending on the “event” $r$. Random variables $r_1, \ldots, r_N$ are independent and identically distributed with probability density $f_0(r)$. The minimum value is a function of $r_1, \ldots, r_N$, and, thus, is random. For large $N$, the probability density function of energy, $f(E)$, has the form

$$f(E) = \text{const} \ e^{NS(E)}$$

Entropy per degree of freedom, $S(E)$, is the maximum stationary value of the functional

$$S(E, z, \psi) = Ez + \frac{z}{2} (A\psi, \psi) + \ln \int e^{-z(l(r), \psi)} f_0(r) dr.$$
Denote by $\beta$ and $\psi$ a stationary point of $S(E, z, \psi)$. If $\beta$ is positive, the corresponding stationary value of $S(E, z, \psi)$ is the maximum one. For positive $z$ the functional $S(E, z, \psi)$ is convex and, thus, has a unique minimizing element. We have

$$S(E) = \min_{\psi, z \geq 0} \left[ E z + \frac{z}{2} (A \psi, \psi) + \ln \int e^{-z(l(r), \psi)} f_0(r) \, dr \right].$$

(7)

The conditional probability density that, say, $r_1$ takes the value $r$ if energy has a prescribed value $E$, is

$$f(x) = \text{const} \, e^{-\beta(l(r), \psi)} f_0(r).$$

(8)

The energy of a body with dislocations can be written in form (4), (5); in particular, for anti-plane constrained shear, energy is the negative minimum value of the variational problem (4), (5) where the quadratic and the linear functionals are

$$(A \psi, \psi) = \frac{1}{G} \int_{\Omega} (\nabla \psi)^2 \, d^2x,$$

(9)

$$(l(r), \psi) = bN \langle \psi \rangle_r - \int_{\partial\Omega} \frac{du}{ds} \psi(s) \, ds.$$ (10)

Here we used the notation

$$\langle \psi \rangle_r = \int_{|x - r| \leq \varepsilon} \psi(x) \frac{d^2x}{\pi \varepsilon^2}.$$

Note that the product $bN$ is considered as finite for large $N$. The probability density $f_0(r)$ is constant.

The corresponding functional $S(E, z, \psi)$ depends smoothly on $\varepsilon$, and for $\varepsilon \to 0$ tends to the limit functional

$$E z + \frac{z}{2G} \int_{\Omega} (\nabla \psi)^2 \, d^2x + \ln \int_{\Omega} e^{-zhN\psi(x)} \frac{d^2x}{\pi R^2} + z \int_{\partial\Omega} \frac{du}{ds} \psi(s) \, ds.$$

$R$ being the radius of the cylinder. Therefore,

$$S(E) = \min_{\psi, z \geq 0} \left[ E z + \frac{z}{2G} \int_{\Omega} (\nabla \psi)^2 \, d^2x + \ln \int_{\Omega} e^{-zhN\psi(x)} \frac{d^2x}{\pi R^2} + z \int_{\partial\Omega} \frac{du}{ds} \psi(s) \, ds \right].$$

(11)

As follows from (8), (11) the probability density function of dislocation positions is

$$f(x) = \frac{e^{-\beta hN\psi(x)}}{\int_{\Omega} e^{-\beta hN\psi(\tilde{x})} \, d\tilde{x}}.$$ (12)
where $\psi(x)$ is the solution of the equation

$$\frac{1}{G} \Delta \psi = -Nb \frac{e^{-\beta b N \psi(x)}}{\int_{\Omega} e^{-\beta b N \psi(\tilde{x})} d\tilde{x}} \quad \text{in } \Omega,$$

(13)

with the boundary condition

$$\frac{1}{G} \frac{\partial \psi}{\partial n} = -\frac{du}{ds} \quad \text{on } \partial \Omega.$$

(14)

The solution to this boundary value problem, $\psi(x)$, has the meaning of the stress function averaged over all admissible dislocation networks.

The constant $\beta$ has the meaning of the inverse temperature of the dislocation ensemble: $\beta = 1/T$. The temperature of the dislocation ensemble, $T$, is defined as follows. Let $\Gamma$ be the number of all dislocation networks admissible for a given value of energy $E$:

$$\Gamma(E) = \int_{H(r_1, \ldots, r_N) < E} \frac{d^2r_1}{b^2} \cdots \frac{d^2r_N}{b^2}.$$

Then the entropy of this ensemble is, by definition,

$$NS(E) = \ln \Gamma(E).$$

Since

$$\frac{d\Gamma(E)}{dE} = \int \delta(E - H(r_1, \ldots, r_N)) \frac{d^2r_1}{b^2} \cdots \frac{d^2r_N}{b^2} = \left(\frac{\Omega}{b^2}\right)^N f(E),$$

we have from (6), up to small and/or constant terms,

$$\Gamma(E) = \text{const } e^{NS(E)}.$$

Therefore, for large $N$, entropy is given by Eq. (7).

The temperature of the ensemble is introduced by the formula

$$\beta = \frac{1}{T} = \frac{dS(E)}{dE}.$$

(15)

This parameter is presented in the boundary-value problem (13). The temperature $T$ is not equal to the thermodynamic temperature, $T_{th}$.

The additional equation allowing one to find the temperature of the dislocation ensemble follows from minimization with respect to $z$ in the variational problem (11):

$$\frac{1}{2G} \int_{\Omega} (\nabla \psi)^2 d^2x = E.$$

(16)

To obtain Eq. (16) directly without manipulating the Euler’s equations of the functional $S(E, z, \psi)$, one may vary $S(E, z, \psi)$ with respect to $z$ keeping the product $z\psi$ fixed.

The problem formulated is analogous to a problem encountered in statistical mechanics of point vortices (Montgomery and Joyce, 1974; Lundgren and Pointin,
There is a difference though in the boundary conditions.

The nonlinear Eq. (13) belongs to a class of equations studied by Liouville (see the review by Stuart, 1967). In the case of constant shear,

\[
\frac{du}{ds} = \text{const} = \gamma, \tag{17}
\]

the solution of the boundary value problem (13), (14) can be obtained analytically. First, note that from (17) and (2)

\[
\gamma \times 2\pi R = Nb. \tag{18}
\]

Note also that the solution of the boundary value problem (13) is determined up to an additive constant which obviously does not affect the stress state. We seek an axi-symmetric solution. If we find such a solution for a positive \( \beta \), it is the required one due to uniqueness. The axi-symmetric function \( \psi \) is constant on the boundary, and we can set \( \psi = 0 \) on \( \partial \Omega \). This allows us to use a known solution from the theory of point vortices:

\[
\psi(x) = \frac{2}{\beta bN} \ln \left[ 1 + \frac{1}{T^*} \left( 1 - \frac{r^2}{R^2} \right) \right], \tag{19}
\]

where \( r \) is the distance from the origin, and \( T^* \) is the dimensionless temperature

\[
T^* = \frac{T}{G \gamma^2 \pi R^2}. \tag{18}
\]

From (19) and (12) we find the probability distribution of dislocations:

\[
f(r) = \frac{1 + \frac{1}{T^*}}{\pi R^2 \left( 1 + \frac{1}{T^*} \left( 1 - \frac{r^2}{R^2} \right) \right)^2}. \tag{20}
\]

The probability density of dislocation positions is related to the dislocation density: \( Nf(x) \, d^2 x \) is equal to the number of dislocations in the vicinity of the point \( x \) which has the area \( d^2 x \).

The probability distribution of dislocations in terms of dimensionless temperature and dimensionless coordinates \( y = x/R \) is

\[
f(y) = \frac{1 + \frac{1}{T^*}}{\pi \left( 1 + \frac{1}{T^*} \left( 1 - |y|^2 \right) \right)^2}. \tag{21}
\]

It is convenient to introduce the dimensionless energy,

\[
E^* = \frac{E}{G \gamma^2 \pi R^2}. \tag{20}
\]
Then the inverse temperature is determined by the given value of energy from Eq. (16) which in the dimensionless variables takes the form

\[ T^* \left( 1 - T^* \ln \left( 1 + \frac{1}{T^*} \right) \right) = E^*. \]  

(22)

The dependence of energy on temperature is shown in Fig. 2. The dimensionless energy grows with temperature and tends to 1/2 when the temperature goes to infinity. Infinite temperature, according to (15), corresponds to the state with maximum entropy, i.e. to the state with maximum chaos. One may prefer to characterize it as the state with the zero value of \( \beta \). In this state, as follows from (12), all dislocations are homogeneously distributed over the crystal. Any finite temperature corresponds to a partially ordered dislocation network.

Fig. 3 shows how the system freezes when the dislocation ensemble temperature drops or, equivalently, energy decreases. It is seen that dislocations go to the boundary when energy (and temperature) decreases. At thermodynamic equilibrium all dislocations will be in a small vicinity of the boundary, i.e. repelling the dislocations from each other prevails over repelling of dislocations from the wall (recall that the wall is clamped; therefore, in contrast to a traction-free case, dislocations are repelled from the boundary).

5. Evolution to equilibrium

In the above consideration one parameter, energy, remained unspecified. If energy is known, one knows the dislocation density. To obtain a closed system of equations we need an equation to determine energy. This is, of course, the equation of the first law of thermodynamics. Since, according to (4), (5), (9), (10)

\[ \frac{\partial \tilde{H}}{\partial r_{(a)}^2} = b \frac{\partial \langle \psi \rangle_{r_a}}{\partial r_{(a)}^2} \]  

(23)

we have for the energy rate

\[ \frac{d\tilde{H}}{dt} = b \sum_{a=1}^{N} \frac{\partial \langle \psi \rangle_{r_a}}{\partial r_{(a)}^2} \frac{dr_{(a)}^2}{dt}. \]  

(24)

Greek indices run through the values 1,2. Let us use for the dislocation velocity the simplest law which warrants the decay of energy.

\[ \frac{dr_{(a)}^2}{dt} = -\frac{1}{B} \frac{\partial H}{\partial r_{(a)}^2} = -\frac{b}{B} \frac{\partial \langle \psi \rangle_{r_a}}{\partial r_{(a)}^2} \]  

(25)

where \( B \) is a positive constant. This law corresponds to the usual equation of dislocation dynamics while the constant \( B \) has the meaning of the dislocation mobility. Indeed, the stress function at the point \( r_a \) can be presented as a sum of the stress function, \( \tilde{\psi} \), of the dislocation located at \( r_a \) in an unbounded space, and a correction \( \psi' \). The correction describes the external field acting on the dislocation.
Obviously, \( \langle \psi' \rangle \), does not depend on \( r \), and its derivative with respect to \( r \) is zero. The correction \( \psi' \) is a smooth function which has a limit when \( \varepsilon \to 0 \). In this limit

\[
B \frac{d\psi'(a)}{dr} = -b \frac{\partial \psi'}{\partial r^2}.
\]  

(26)

The vector \( \frac{\partial \psi'}{\partial r^2} \) is directed along the line on which the resolved shear stress is maximum, and its magnitude is equal to the resolved shear stress. Thus Eq. (26) is the usual equation of dislocation dynamics (Nadgornyi, 1988).

From Eqs. (24) and (25) we find for the energy rate

\[
\frac{dH}{dt} = \frac{h^2}{B} \sum_{a=1}^{N} \frac{\partial \langle \psi \rangle_{r_a}}{\partial r^2_{a}} \frac{\partial \langle \psi \rangle_{r_a}}{\partial \psi}.
\]  

(27)

Since energy may be assumed a slow variable, averaging Eq. (27) we obtain

\[
\frac{dE}{dt} = -\frac{Nb^2}{B} \int_{\Omega} (\nabla \psi)^2 f(t, x) \, d^2 x.
\]  

(28)

So, the closed system of the equations for the evolution of the dislocation cloud consists of Eq. (28) and

\[
f(t, x) = \frac{e^{-\beta(t) b N \psi(t, x)}}{\int_{\Omega} e^{-\beta(t) b N \psi(t, x)}} \, d\tilde{x}.
\]  

(29)

\[
\frac{1}{G} \Delta \psi(t, x) = -Nb f(t, x) \quad \text{in} \quad \Omega, \quad \frac{1}{G} \frac{\partial \psi}{\partial n} = -\frac{d\mu}{ds} \quad \text{on} \quad \partial \Omega,
\]

\[
E(t) = \frac{1}{2G} \int_{\Omega} (\nabla \psi(t, x))^2 \, d^2 x.
\]

Eqs. (29) are, in fact, quasi-static, and for a circular cylinder we can use the solutions (19), (20) in which \( \beta \) must be considered as a function of time.

It is convenient to introduce the dimensionless time

\[
\tau = \frac{2Gb}{3RB} \gamma t.
\]

Then in dimensionless variables the energy Eq. (28) takes the form

\[
\frac{dE^*}{d\tau} = \frac{2 + 3T^*}{1 + T^*}.
\]  

(30)

This equation along with Eq. (22) determines the evolution of energy and temperature. The system of these two equations yields an ordinary differential equation for temperature:

\[
\frac{dT^*}{d\tau} = -\frac{2 + 3T^*}{2(1 + T^*)(1 - T^* \ln(1 + 1/T^*))} - 1.
\]  

(31)

Energy decays as the system goes to equilibrium. Fig. 2 shows that the temperature of the dislocation ensemble is also decaying. One may say that the system is freezing while going to equilibrium. A typical rate of freezing is shown in Fig. 4.
Eq. (31) predicts vanishing of temperature (and, hence, energy) at some instant \( \Theta \) and developing negative temperatures and energies for \( \tau > \Theta \). The reason for that is the failure of Eq. (28) near equilibrium when the dislocations are very close to the wall and/or each other. Nevertheless, one may try to estimate the time of approach to equilibrium as the time during which the solution of Eq. (31) changes from its initial value, \( a \), to zero. We have from Eq. (31)

\[
\Theta = \int_0^a \frac{2(1 + T^*)(1 - T^* \ln(1 + 1/T^*)) - 1}{2 + 3T^*} \, dT^*.
\]

The dependence of \( \Theta \) on the initial value of temperature can be presented also as the dependence on the initial value of energy since energy and temperature are linked by Eq. (22). This function is shown in Fig. 5.

All the curves in Figs. 2–5 are Master curves, i.e. they are universal due to the scaling chosen. If one uses the unscaled energy, temperature and time, then each Master curve splits into a bunch of curves and one would observe the dependence of the behavior of the system on the values of the parameters involved. Note that all the relations can be used formally for all values of the radius of the cylinder, \( R \), but the setting of the problem makes sense only for micro-samples: for macro-cylinders there are slow macroscopic deterministic parameters, like the field of plastic strain rate, which should be taken into account in addition to energy.

6. Some open issues

The problem considered may be generalized in several directions. One of the most interesting is a three-dimensional extension when the straight dislocation lines are changed to lines of arbitrary shape. A similar problem has been considered in

![Fig. 2. Dependence of dimensionless energy on dimensionless temperature.](image-url)
statistical mechanics of vortex lines in ideal fluid (Berdichevsky, 1998, 2002; Lions and Majda, 2000). The similarity between plasticity and turbulence is based on the fact that in both cases the “particles” of the system are lines; a vortex line in fluid mechanics is such a line that the velocity potential has a jump on any closed contour surrounding this line; for dislocations, the displacement vector has a jump. A dislocation is a slightly more complex object than a vortex line because it corresponds to a jump of a vector field, while for vortex lines the jump is

Fig. 3. Distribution of the dislocation density for different temperatures, $T = 0.1$ (the bottom curve for small $y$), $T = 0.5$ (middle curve) and $T = 1$ (upper curve).

Fig. 4. Dependence of dimensionless temperature of dislocation ensemble on dimensionless time in the course of evolution to equilibrium; the initial temperature value is 100.
experienced by a scalar, the velocity potential. Common features prevail, however, at least in the equilibrium case. As in fluid mechanics, one may expect that Schrödinger’s-type equation should appear as a part of the homogenized description. The reason for that is quite simple. As was discovered by R. Feynman, Schrödinger’s equation is intimately related to summation over all possible particle paths of some functional depending on the path. A very similar functional appears when one counts all dislocation lines compatible with the given value of energy. Summation over all admissible positions of dislocation lines is similar to summation over possible particle paths in quantum mechanics. Thus, an analogue of Schrödinger’s equation must emerge. These issues will be discussed elsewhere.

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References
