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Origin of gradient terms in plasticity at different length scales

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Abstract

The origins of gradient terms in plasticity are discussed for three different cases related to atomic distance, dislocations, and finite grain size.

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1. Introduction

In the recent years several attempts were made to introduce gradient terms into elasticity and plasticity (see e.g. [1,2]). Gradient terms are proved to be useful to account for experimental evidences, but their physical origins are often unclear. In most cases they are introduced heuristically. The purpose of the present paper is to demonstrate that for certain problems the precise form of gradient terms can be strictly derived.

In the following three strongly different problems (corresponding to different length scales), the consequences of finite lattice parameter, the influence of short range dislocation–dislocation correlation, and the influence of finite grain size on torsion deformation are analyzed. With these we intend to demonstrate that the introduction of gradient terms can be useful under much more general conditions than the ones which are related

to geometrically necessary dislocations. Since the different gradient terms are “derived” the corresponding coefficients can be directly related the appropriate intrinsic variable of the material considered.

2. Nonlocal effects due to finite lattice parameter

As it is well known, for a classical local continuum the speed of deformation waves does not depend on the frequency (there is no dispersion). However, for a crystalline material the dispersion relation $\omega(\vec{k})$ cannot be linear due to the finite lattice parameter (at the boundaries of the Brillouin-zone the $\omega(\vec{k})$ curve is always perpendicular to the surface of the Brillouin-zone). In order to take into account this in a continuum approach we need to assume that at a given point $\vec{r}$ the stress $t_{ij}(\vec{r})$ does not depend only on the local strain. The most general form of a nonlocal linear stress–strain relation is [3,4]

$$t_{ij}(\vec{r}) = \int C_{ijkl}(\vec{r} - \vec{r}') u_{k,l}(\vec{r}') d^3\vec{r}', \quad (1)$$

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where $u_k(\vec{r})$ is the displacement field, $C_{ijkl}(\vec{r})$ is the nonlocal elastic moduli tensor. (The indexes after comma always indicate derivatives with respect to the corresponding coordinates.) This leads to the equilibrium equation

$$t_{ij,i} + f_j = \int C_{ijkl,i}(\vec{r} - \vec{r}') u_{k,l}(\vec{r}') d^3\vec{r}' + f_j = 0 \quad (2)$$

in which J_j is the volume force density. If the system has infinite size and the displacement field $u_{k,l}(\vec{r})$ has unique value Eq. (2) can be rewritten as

$$\int C_{ijkl}(\vec{r} - \vec{r}') u_{k,l}(\vec{r}') d^3\vec{r}' + f_j = 0. \quad (3)$$

In the simplest isotropic case it can be assumed that

$$C_{ijkl}(\vec{r}) = C_{ijkl}^0 \alpha(\vec{r}), \quad (4)$$

where C_{ijkl}^0 is the elastic moduli tensor of an isotropic medium with Lamé constants λ^0 and μ^0 , and $\alpha(\vec{r})$ is a function accounting for the nonlocal interaction. (The classical local continuum description corresponds to $\alpha(\vec{r}) = \delta(\vec{r})$.) It is important to stress that the above form is a strong simplification restricting considerably the generality of the following analysis.

The concrete form of $\alpha(\vec{r})$ can be directly linked to the dispersion relation of the media considered. Namely, from Eq. (3) the Fourier transform of the Green-function of a nonlocal medium $G_{ij}^N(\vec{k})$ satisfies the condition

$$-k_m k_i C_{iklm}^0 G_{ij}^N(\vec{k}) \alpha(\vec{k}) + \delta_{jk} = 0. \quad (5)$$

It can be seen from Eq. (5) that the Green-function of a local medium $G_{ij}^L(\vec{k})$ (corresponding to $\alpha(\vec{k}) = 1$) is related to $G_{ij}^N(\vec{k})$ by the condition

$$G_{ij}^L(\vec{k}) = G_{ij}^N(\vec{k}) \alpha(\vec{k}). \quad (6)$$

According to Kunin [5] the Green-function of a nonlocal continuum can be given with the form

$$G_{ij}^N(\vec{k}) = \frac{k_i k_j}{\rho k^2} \frac{D^L(k^2)}{c^L k^2} + \frac{1}{\rho} \left\{ \delta_{ij} - \frac{k_i k_j}{k^2} \right\} \frac{D^T(k^2)}{c^T k^2} \quad (7)$$

with $|k| < k_B$,

where c_L and c_T are the two sound speeds, $D^L(k^2)$ and $D^T(k^2)$ are functions describing the dispersion of the longitudinal and transversal waves, ρ is the

density, and k_B is the radius of the Brillouin-zone. Assuming that $D^L(k^2) = D^T(k^2) = D(k^2)$ one can find that

$$G_{ij}^N(\vec{k}) = D(k^2) G_{ij}^L(\vec{k}). \quad (8)$$

By comparing Eqs. (6) and (8) we can conclude that

$$D(k^2) \alpha(\vec{k}) = 1. \quad (9)$$

From Eqs. (1), (4) and (9) the Fourier transform of the stress tensor is related to the strain as

$$t_{ik}(\vec{k}) = C_{iklm}^0 \frac{1}{D(k^2)} u_{l,m}(\vec{k}), \quad |k| < k_B, \quad (10)$$

According to this, the stress in the real space is written

$$t_{ik}(\vec{r}) = \int_{k_B} C_{iklm}^0 \frac{1}{D(k^2)} u_{l,m}(\vec{k}) \exp(i\vec{k}\vec{r}) d^3\vec{k}, \quad (11)$$

and the nonlocal interaction function reads

$$\alpha(\vec{r}) = \alpha(|\vec{r}|) = \int_{k_B} \frac{1}{D(k^2)} \exp(i\vec{k}\vec{r}) d^3\vec{k}. \quad (12)$$

(In the absence of dispersion $D(k^2) = 1$ and if $k_B \rightarrow \infty$ expression (11) gives back the stress in a local continuum.) With these we obtain

$$t_{ij}(\vec{r}) = C_{ijkl}^0 \int_{-\infty}^{\infty} \alpha(|\vec{s}|) u_{k,l}(\vec{r} - \vec{s}) d^3\vec{s}. \quad (13)$$

By the Taylor expansion or $u_{k,l}(r - s)$ around the points $s = 0$ we obtain

$$t_{ij}(\vec{r}) = C_{ijkl}^0 \left\{ u_{k,l}(\vec{r}) + \sum_{n=1}^{\infty} \beta_n \Delta^n u_{k,l}(\vec{r}) \right\} \quad (14)$$

with

$$\beta_n = \int_{-\infty}^{\infty} \alpha(|\vec{s}|) |\vec{s}|^{2n} d^3\vec{s}. \quad (15)$$

(Similar expression was proposed by Altan and Aifantis [6].) Since the only length scale introduced into the above consideration is $1/k_B$ which is proportional to the lattice parameter a , one can find from dimensionality that β_n is proportional to a^{2n} .

According to the results obtained above we can state that with a certain accuracy the consequences of the finite lattice parameter can be accounted by

the introduction of gradient terms in elasticity. Knowing the phonon dispersion relation, the coefficients of the gradient terms can be determined.

3. Diffusion term in dislocation dynamics

At scale of about 100 nm plasticity is controlled by the evolution of individual dislocations. In order to study much larger systems a continuum model needs to be developed. As it was shown by Groma et al. [7–9] for a system of straight parallel dislocations a continuum description can be directly derived from the equations of motion of individual dislocations. This builds up the link between micro- and meso-scales for only this extremely simplified situation, but gives the structure of evolution equations without ad hoc assumption.

Let us consider N parallel edge dislocations with Burgers vectors $\vec{b}_i = \pm \vec{b}$ positioned at the points $\{\vec{r}_i\}$, $i = 1, \dots, N$. With the commonly accepted assumption of over-damped dislocation motion the velocity of the i th dislocation is determined by the equation

$$\frac{d\vec{r}_i}{dt} = B \left(\sum_{j \neq i}^N \frac{\vec{b}_i \vec{b}_j}{|\vec{b}_j|} \tau_{\text{ind}}(\vec{r}_i - \vec{r}_j) + \vec{b}_i \tau_{\text{ext}} \right), \quad (16)$$

where B is the dislocation mobility, τ_{ext} is the external resolved shear stress, and

$$\tau_{\text{ind}}(\vec{r}) = \frac{\mu b}{2\pi(1-\nu)} \frac{x(x^2 - y^2)}{(x^2 + y^2)^2} \quad (17)$$

is the shear stress created by a dislocation at the point $\vec{r} = (x, y)$. As it is explained in details in [7], after multiplying Eq. (16) by the delta function $\delta(\vec{r} - \vec{r}_i)$ and performing a separate summation for the positive and negative sign dislocations we arrive at the evolution equations of the positive and negative sign dislocation densities $\rho_+(\vec{r})$, $\rho_-(\vec{r})$:

$$\begin{aligned} \frac{\partial \rho_+(\vec{r}_1, t)}{\partial t} + \int \frac{\partial}{\partial \vec{r}_1} \{ \rho_{++}(\vec{r}_1, \vec{r}_2, t) - \rho_{+-}(\vec{r}_1, \vec{r}_2, t) \} \\ \times \vec{b} \tau_{\text{ind}}(\vec{r}_1 - \vec{r}_2) d\vec{r}_2 = 0, \end{aligned} \quad (18)$$

$$\begin{aligned} \frac{\partial \rho_-(\vec{r}_1, t)}{\partial t} + \int \frac{\partial}{\partial \vec{r}_1} \{ \rho_{--}(\vec{r}_1, \vec{r}_2, t) - \rho_{-+}(\vec{r}_1, \vec{r}_2, t) \} \\ \times \vec{b} \tau_{\text{ind}}(\vec{r}_1 - \vec{r}_2) d\vec{r}_2 = 0, \end{aligned} \quad (19)$$

where $\rho_{++}, \rho_{+-}, \rho_{--}$ are the two-particle density functions with the corresponding signs. (Here the dislocation densities originally consisting of delta functions are replaced with their statistical average so, they are a smooth function of the space coordinates.)

For the further considerations it is useful to introduce the correlation functions d_{ij} defined by

$$\begin{aligned} \rho_{ij}(\vec{r}_1, \vec{r}_2, t) = \rho_i(\vec{r}_1) \rho_j(\vec{r}_2) (1 + d_{ij}(\vec{r}_1 - \vec{r}_2)) \\ i, j = +, -. \end{aligned} \quad (20)$$

By adding and subtracting Eqs. (18) and (19) the following evolution equations can be obtained for the total $\rho(\vec{r}, t) = \rho_+(\vec{r}, t) + \rho_-(\vec{r}, t)$ and the sign $\kappa(\vec{r}, t) = \rho_+(\vec{r}, t) - \rho_-(\vec{r}, t)$ dislocation densities (for details see [9]):

$$\frac{\partial \rho(\vec{r}, t)}{\partial t} + \frac{\partial}{\partial \vec{r}} \vec{b} [\kappa(\vec{r}, t) \{ \tau_{\text{int}}(\vec{r}, t) + \tau_{\text{ext}} + \tau_s(\vec{r}) \}] = 0 \quad (21)$$

$$\frac{\partial \kappa(\vec{r}, t)}{\partial t} + \frac{\partial}{\partial \vec{r}} \vec{b} [\rho(\vec{r}, t) \{ \tau_{\text{int}}(\vec{r}, t) + \tau_{\text{ext}} + \tau_s(\vec{r}) \}] = 0 \quad (22)$$

with

$$\tau_{\text{int}}(\vec{r}) = \int \kappa(\vec{r}_1) \tau_{\text{ind}}(\vec{r} - \vec{r}_1) d^p \vec{r}_1 \quad (23)$$

and

$$\tau_s(\vec{r}) = \int \kappa(\vec{r}_1) d^p(\vec{r} - \vec{r}_1) \tau_{\text{ind}}(\vec{r} - \vec{r}_1) d^p \vec{r}_1 \quad (24)$$

in which $d^p = 1/4(d_{++} + d_{--} + d_{+-} + d_{-+})$. The stress field $\tau_{\text{int}}(\vec{r})$ defined above can be considered as the self-consistent field created by the local excess of sign in the dislocation density. (In the framework outlined dislocation annihilation and multiplication can also be accounted by adding a source term to the right hand side of Eq. (21).)

The actual form of d^p is difficult to determine, but numerical studies show that it decays to zero within a few dislocation spacing. Because of this, in the integral in Eq. (24) the function $\kappa(\vec{r}_1)$ can be approximated by its Taylor expansion around the point $\vec{r}$. Keeping only the first nonvanishing term we arrive at

$$\tau_s(\vec{r}) = -\frac{\partial \kappa(\vec{r})}{\partial \vec{r}} \int (\vec{r} - \vec{r}_1) d^p(\vec{r} - \vec{r}_1) \tau_{\text{ind}}(\vec{r} - \vec{r}_1) d^2 \vec{r}_1. \quad (25)$$

Since $d^p(\vec{r})$ does not depend directly on $\vec{r}$ but on $\sqrt{\rho \vec{r}}$ by dimensionality reasons, and since the shear stress $\tau_{\text{ind}}(\vec{r})$ is proportional to $1/r$ Eq. (25) can be rewritten as

$$\tau_s(\vec{r}) = -\frac{\partial \kappa(\vec{r})}{\partial \vec{r}} \frac{1}{\rho(\vec{r})} \int \vec{x} d^p(\vec{x}) \tau_{\text{ind}}(\vec{x}) d^2 \vec{x}, \quad (26)$$

$$\vec{x} = \sqrt{\rho \vec{r}}.$$

From the symmetry properties of $d^p(\vec{r})$ (it is an even function) and from the actual form of $\tau_{\text{ind}}(\vec{r})$ one can conclude that

$$\tau_s(\vec{r}) = -\frac{\vec{b}\mu}{2\pi(1-\nu)\rho(\vec{r})} D \frac{\partial \kappa(\vec{r})}{\partial \vec{r}}, \quad (27)$$

where D is dimensionless constant. It is important to note that the self-consistent field $\tau_{\text{int}}(\vec{r})$ given by the expression (23) cannot be approximated by a gradient term since, as a consequence of $1/r$ decay of the kernel $\tau_{\text{ind}}(\vec{r})$, all of the expansion coefficients are infinite.

As it can be seen from the above given derivation of continuum description of dislocation evolution, in first approximation the short range dislocation–dislocation correlation effects can be accounted by introducing a gradient term. The length scale determining the strength of this diffusion like term is the dislocation spacing $1/\sqrt{\rho}$.

We would like to stress at this point that the quantity κ introduced above can be considered as geometrically necessary dislocation density. If it is nonzero at a certain point the dislocation ensemble has a “local” net Burgers vector (in the $\Delta \vec{A}$ infinitesimal surface element $\Delta \vec{b} = b\kappa \Delta \vec{A}$). According to Eq. (23), κ is the source of the long range internal stress. The term long range is used on the sense that the characteristic length scale of this stress component is longer than the dislocation spacing.

Concerning the problem whether at this length scale the gradient term is directly related to the existence of geometrically necessary dislocations we can say yes it is (see Eq. (27)). However, it is important to see clearly that the coefficient D is determined by the short range dislocation–dislo-

cation correlation properties (in the simplified case considered here it is described by the function d^p) and not by the geometrically necessary dislocations. So it can be stated that the gradient term in a continuum theory of dislocations describes a sort of coupling between the short range dislocation–dislocation correlation properties and the geometrically necessary dislocations.

4. Gradient effects due to finite grain size

Torsion deformation results in strongly inhomogeneous deformation inside the sample, so torsion test is ideal to study whether gradient terms need to be introduced in the stress–strain constitutive relation in a continuum plasticity model [2].

In order to investigate gradient effects which may appear on about 100 μm scale, cylindrical samples of electrolytic copper with diameter of 4 mm and a gauge length of 40 mm were deformed up to three different shear strain at the surface in a free-end torsion machine and with a constant shear rate of 0.014 s^{-1} . After these, microhardness measurements were carried out on the cross-section of the deformed samples with a Leitz hardness tester at 2 N load, resulting in indentation sizes of 50–100 μm and a Shimadzu DUH-202 dynamic hardness tester at 0.2 N load, producing indentation sizes of 10–20 μm .

The obtained microhardness versus distance from the torsional axis curves are plotted in Fig. 1. As it can be seen, the microhardness increases monotonously from the axis toward the surface. A very important feature of the observed results is that for the two samples deformed up to 3.2 and 6.33 surface strain the microhardnesses at the center differ from the microhardness of the undeformed sample. Since, due to simple symmetry reasons the strain has to vanish at the center, the results contradict with the assumption of traditional local plasticity, according to which the local flow stress depends only on the local strain. (As is discussed in details in [10], the above results cannot be due to the finite indentation size.)

In order to determine the physical origin of the nonlocal effect observed, microhardness measure-

Fig. 1. The microhardness versus distance from the origin for samples deformed in torsion up to the indicated surface shear strains. The microhardness measurements were performed with loads given between parentheses.

ments were performed on samples torsionally deformed up to the same surface strain but having different grain size (0.02–0.08 mm). It was found that the excess hardening at the torsional axis increases linearly with increasing grain size. So, the gradient effects observed in these measurements are clearly related to the finite grain size. On the basis of these results it can be stated that if we want to describe the properties of polycrystalline material within the framework of a constitutive stress–strain relation (i.e. the grains are not considered individually) under certain circumstances gradient effects need to be introduced with a characteristic length scale proportional to the grain size.

5. Summary and conclusions

It was demonstrated on three different cases that the collective nonlocal properties of systems

with high degrees of freedom can often be described by introducing gradient terms into the corresponding equations. However, the actual forms of the terms, and the values of the parameters depend on the problem investigated, so we believe there is no such a thing as a “general” gradient plasticity theory. The geometrically necessary dislocations represent only one possible sources of the gradient effects. Depending on the problem, among many other things the intrinsic length scale can be the lattice parameter, the dislocation spacing, or the grain size.

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