FROM DISCRETE DISLOCATION DYNAMICS TO A PHASE FIELD THEORY OF DISLOCATIONS

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ABSTRACT: A dislocation ensemble is a system of objects with long range interaction. So the traditional methods developed for atomic systems to derive a continuum theory from the equation of motion of the individual objects cannot be directly applied. We consider a set of parallel edge dislocations representing the simplest possible, but already rather complex system. It is shown, that based on discrete dislocation simulation results, a link between the microscopic and mesoscopic length-scale description of the collective behavior of dislocations can be established. It is found that the continuum theory of dislocations can be formulated as a phase field theory.

Keywords: dislocation dynamics, continuum theory, phase field theory

1 INTRODUCTION

In the past decade there has been a increasing activity to develop a continuum theory of dislocations. Theoretical investigations are largely motivated by the experimental finding that if the characteristic size of a specimen is less than about 10μm then the plastic response of the crystalline materials depends on the size (size effect). The simplest possible way to account for this effect is to add gradient terms to the "local" ones in the stress-strain relation. There are several different phenomenological propositions to incorporate gradient terms into continuum plasticity models. Although they are successfully applied to explain certain experimental results, the physical origin of the different gradient terms are not clear.

Since in crystalline materials the elementary carriers of plastic deformation are the dislocations, a continuum theory should be built up from the properties of individual dislocations. For a system of parallel edge dislocations with single slip Groma et al. [1] have established a systematic way to derive a continuum theory from the equation of motion of individual dislocations. The most important feature of this theory is that gradient terms appear naturally in the evolution equations of the different dislocation densities. At the moment, however, it is not clear how to extend the model for more complicated dislocation geometries and configurations. Recently, several new promising frameworks have been proposed for treating curved dislocation lines with statistical methods, but there are many open issues to be resolved before we can say we have a well established 3D continuum theory of dislocations. Constructing a continuum theory for even 2D multiple slip is far from straightforward.

In the paper we propose a phase field approach to derive continuum theory of straight edge dislocations

2 VARIATIONAL APPROACH

In order to derive a continuum theory, as a first step, we reformulate the Kröner-Kosevich [2] field theory of individual dislocations into a variational problem.

It is commonly assumed that the final state of a body, subject to shape change, is reached by two subsequent steps, a plastic and an elastic deformation. If we remain in small deformation the total deformation defined as

$$\epsilon^{\rm t}_{ij} = (\partial_i u_j + \partial_j u_i)/2, \tag{1}$$

is the sum of the elastic ϵ_{ij} and plastic $\epsilon^{\rm p}_{ij}$ deformations

$$\epsilon^{\rm t}_{i,j} = \epsilon_{ij} + \epsilon^{\rm p}_{ij} \tag{2}$$

where $u_i(\mathbf{r})$ is the displacement field.
According to the Kröner-Kosevich [2] the fundamental quantity determining the "plastic state" of a crystalline material is the incompatibility tensor η_{ij} defined as

$$\eta_{ij} = -\mathcal{I}_{ijmn}\epsilon^{\rm p}_{mn}, \tag{3}$$

where the $\mathcal{I}_{ijmn} = -e_{ikm}e_{jln}\partial_k\partial_l$ second order differential operator is the incompatibility operator with e_{ikm} denoting the antisymmetric tensor. (Double subscripts represent summation.) η_{ij} is related to the dislocation density tensor α_{ij} as [2]

$$\eta_{ij} = \frac{1}{2}\left(e_{jlm}\partial_l\alpha_{im} + e_{ilm}\partial_l\alpha_{jm}\right). \tag{4}$$

with

$$\alpha_{ij} = t_i b_j \delta^2(\xi) \tag{5}$$

where $\mathbf{t}$ is the line, $\mathbf{b}$ is the Burgers vector, and ξ is the distance from the dislocation line.
The elastic deformation ϵ_{ij} is generated by the stress field. For our further considerations the most convenient way is to give ϵ_{ij} as the functional derivative of the enthalpy functional $H[\sigma_{ij}]$ of the material, i.e.,

$$\epsilon_{ij} = -\frac{\delta H[\sigma_{ij}]}{\delta\sigma_{ij}}. \tag{6}$$

With the above relation Eq. (2) reads as

$$\epsilon^{\rm t}_{ij} = -\frac{\delta H}{\delta\sigma_{ij}} + \epsilon^{\rm p}_{ij}. \tag{7}$$

Since $\mathcal{I}_{ijmn}\epsilon^{\rm t}_{mn} = 0$, by taking the incompatibility of Eq. (7) we obtain that

$$\mathcal{I}_{ijmn}\frac{\delta H}{\delta\sigma_{mn}} = -\eta_{ij}. \tag{8}$$

Giving the stress tensor as the incompatibility of the stress potential χ_{ij},

$$\mathcal{I}_{ijmn}\chi_{mn} = \sigma_{ij}, \tag{9}$$

guarantees that the $\partial_i\sigma_{ij} = 0$ equilibrium condition is fulfilled, and Eq. (8) can be rewritten as

$$\frac{\delta H}{\delta\chi_{ij}} = -\eta_{ij}, \tag{10}$$

where H is a functional of $\mathcal{I}_{ijmn}\chi_{mn}$. By introducing the functional

$$E := H + \int \mathrm{d}V \eta_{ij}\chi_{ij}, \tag{11}$$

Eq. (10) can be reformulated as

$$\frac{\delta E}{\delta \chi_{ij}} = 0. \tag{12}$$

On the other hand, by substituting Eq. (8) into Eq. (11) and performing two partial integrations one can conclude that

$$E = H - \int \mathrm{d}V \frac{\delta H}{\delta \sigma_{ij}} \sigma_{ij}, \tag{13}$$

which is the elastic energy of the system. So, to calculate the stress field generated by a given incompatibility one has to determine the extremum of E given as a functional of the stress potential and the incompatibility tensor [3]. For our further considerations it is important to note, varying E with respect to the dislocation line position gives the Peach-Koehler force

$$F_i = e_{ikl} t_k \sigma_{lm} b_m \tag{14}$$

This means, the force acting on a dislocation segment is also ”coded” in the functional E.

In the considerations below we treat a set of parallel edge dislocations with line vectors $\mathbf{t} = (0, 0, -1)$. Denoting the position and Burgers vector of the jth dislocation by $\mathbf{r}^j$ and $\mathbf{b}^j$, respectively, for this plain problem [3]

$$E = \int \left[-\frac{D}{2} (\triangle\chi)^2 + \chi(\partial_i S_{ij} a_j) \right] \mathrm{d}^2 r \tag{15}$$

where $\chi = \chi_{33}$, $D = (1 - \nu)/2\mu$ with μ the shear modulus and ν Poisson's ratio, S_{ij} is the 90^0 rotation operator, and

$$a_i(\mathbf{r}) = \sum_j b_i^j \delta(\mathbf{r} - \mathbf{r}^j) \tag{16}$$

is the ” discrete” Burgers vector density.

One obtains from Eq. (12) that

$$\triangle^2 \chi = \frac{b}{D} \partial_i \left[\sum_j m_i^j \delta(\mathbf{r} - \mathbf{r}^j) \right] \tag{17}$$

where $\mathbf{m}^j$ is a unit vector perpendicular to $\mathbf{b}^j$ and from Eq. (9) the stress field generated by the dislocation system is

$$\sigma_{11} = -\partial_y \partial_y \chi, \quad \sigma_{22} = -\partial_x \partial_x \chi, \quad \sigma_{12} = \partial_x \partial_y \chi. \tag{18}$$

Furthermore, according to the above mentioned fact that the force acting on a dislocation can be obtained from E, the equation of motion of the jth dislocation reads as

$$\frac{dr_i^j}{dt} = \frac{b_i^j}{Bb^2} b_k^j \frac{dE}{dr_k^j} \tag{19}$$

where over-damped dislocation glide (climb is excluded) is assumed. B denotes the dislocation mobility.

3 COARSE GRAINED THEORY

The system of equation of motion given by Eq. (19) is a strongly coupled nonlinear system of ordinary differential equation which is difficult to solve. For many problems, however, we do not need that detailed description represented by Eq. (19). This means, like in many other problems, instead of dealing with the highly singular Burgers vector density function $\mathbf{a}(\mathbf{r})$ we can work with coarse grained (homogenized) density fields. They are obtained from the "discrete" densities by convolving them with an appropriate window function.

Let us consider a plain strain problem with M slip systems. Denote by $\rho^j_\pm(\mathbf{r})$ the coarse grained dislocation density with $+$ or $-$ sign in the jth slip plane. The simplest possible way to set up evolution equations for the densities introduced is to replace the discrete field in E by the coarse grained ones. With this

$$\bar{E} = \int \left\{ -\frac{D}{2}(\triangle\chi)^2 + b\chi \left[\sum_{j=1}^{M} \partial_i m_i^j \kappa^j \right] \right\} \mathrm{d}^2 r \tag{20}$$

where $\kappa^j = \rho^j_+ - \rho^j_-$. The "bar" sign in $\bar{E}$ indicates it depends on the coarse grained fields. (Certainly, in Eq. (20) χ corresponds also to the coarse grained field, but for simplicity this is not indicated explicitly.) Applying the standard formalism of phase field theories the evolution equations of the dislocation densities read as

$$\dot{\rho}^j_i - (\partial_k b_k) \left[\sum_{l=1,o=\pm}^{M} M^{j,l}_{i,o} (\partial_k b_k) \frac{\delta \bar{E}}{\delta \rho^l_o} \right] = 0 \tag{21}$$

in which we assumed that the number of dislocations is conserved. (The above equation simple means that the currents of the different dislocations are proportional to the gradient of the chemical potentials.) The mobilities $M^{j,l}_{i,o}$ introduced in the evolution equations cannot be determined from general principles. However, by comparing Eq. (21) with the dislocation evolution equations derived earlier from microscopic considerations for single slip [1] the unknown mobilities can be given. One can find that the only form physically reasonable is

$$\dot{\rho}^j_\pm \mp \frac{1}{Bb^2}(\partial_k b_k) \left[\rho^j_\pm (\partial_k b_k) \frac{\delta \bar{E}}{\delta \kappa_j} \right] = 0 \tag{22}$$

Substituting expression (20) into Eq. (22) we obtain

$$\dot{\rho}^j_\pm \mp \frac{1}{Bb}(\partial_k b_k) \left[\rho^j_\pm b^j_i \sigma_{ik} m^j_k \right] = 0. \tag{23}$$

in which σ_{ik} is given by the Eq. (18) with the stress function χ fulfilling the field equation

$$\frac{\delta \bar{E}}{\delta \chi} = 0 \implies \triangle^2 \chi = \frac{b}{D} \sum_{j=1}^{M} (\partial_i m_i^j) \kappa^j. \tag{24}$$

4 CORRELATION EFFECTS

Eq. (23) means that with the approximation applied above the evolution of the dislocation system is only determined by the stress generated by the coarse grained dislocation densities. As it was found earlier [1] the same evolution equations can be obtained

from microscopic considerations with neglecting the dislocation-dislocation correlations. With other words, simple replacing the "discrete" fields by coarse grained ones in the energy functional given by Eq. (15) results in dislocation evolution equations where the role of correlation effects are not taken into account. It is known, however, correlation effects play crucial role in the collective properties of dislocations. For example, the stored energy per unit volume corresponding to a completely random dislocation distribution would diverge logarithmically with the crystal size but there is no experimental evidence for this size dependence.
To take into dislocation correlation in the phase field theory proposed above one may try to add correction terms to the coarse grained energy functional $\bar{E}$. There is no general principle to determine the form of correction term but if the Burgers vector densities (GND density) in the different slip systems are much smaller than the stored densities it is reasonable to assume that the correction term is quadratic in κ^j. On the other hand we do not want to introduce other length scale but the dislocation spacing. It follows, that the correction term has to be inversely proportional to the total dislocation density [4]:

$$F_{\mathrm{corr}} = \int \frac{1}{\rho_{\mathrm{tot}}} \sum_{j,k}^{M} A^{jk} \kappa^j \kappa^k \mathrm{d}^2 r \tag{25}$$

where ρ_{tot} is the total dislocation density and A^{jk} is the coupling coefficient between the slip systems j and k. it may depend on the relative dislocation density populations (ρ^j/ρ^k) of the different slip systems. For the general case the actual form of dependence is not know but if the angle between the slip systems is $\Theta = 2\pi/M$ and the different slip systems are nearly equally populated from symmetry reason

$$F_{\mathrm{corr}} = T_{\mathrm{eff}} \int \frac{a_i(\mathbf{r}) a_i(\mathbf{r})}{b^2 \rho_{\mathrm{tot}}} \mathrm{d}^2 r \tag{26}$$

in which T_{eff} is the coupling coefficient between the correction and the "coarse grained" terms. It follows, the evolution equation of the 2D dislocation system is given by Eq. (22) but $\bar{E}$ has to be replaced by the functional

$$F = \int \left\{ -\frac{D}{2} (\triangle \chi)^2 + b\chi \left[\sum_{j=1}^{M} \partial_i m_i^j \kappa^j \right] + T_{\mathrm{eff}} \frac{a_i(\mathbf{r}) a_i(\mathbf{r})}{b^2 \rho_{\mathrm{tot}}} \right\} \mathrm{d}^2 r. \tag{27}$$

5 SCREENING & COMPARISON WITH DDD SIMULATIONS

To check if the continuum theory is able to account for the collective properties of dislocations its predictions were compared with discrete dislocation dynamics simulations for different static cases. The equilibrium in static are

$$\frac{\delta F}{\delta \chi} = 0, \quad \frac{\delta F}{\delta \kappa^j} = 0 \quad j = 1..M. \tag{28}$$

One can find from Eqs. (27,28) the stress function χ fulfills the equation

$$D \triangle^2 \chi - \frac{b^2 \rho_{\mathrm{tot}}}{T_{\mathrm{eff}}} \triangle \chi = 0. \tag{29}$$

It has to be noted that in the absence of dislocations Eq. (29) gives back the well known

$$\triangle^2 \chi = 0 \tag{30}$$

condition of plain strain problems. Dislocations result in a screening term proportional to $\triangle\chi$. It is the consequence of induced GNDs.
In the presence of an extra dislocation or a dislocation wall Eq. (29) has analytical solution which were compared with results of DDD simulations showing excellent agreement.

6 SUMMARY

It is shown that by applying the standard formalism of phase field theories the dynamics of a 2D dislocation ensemble can be derived from a scalar functional of the dislocation densities and the stress function. The theory presented serves as a "model" to develop a continuum theory of 3D dislocation ensembles in the future.

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