



# Dynamics of coarse grained dislocation densities from an effective free energy

Istvan Groma, Géza Györgyi, Benedek Kocsis

## ► To cite this version:

Istvan Groma, Géza Györgyi, Benedek Kocsis. Dynamics of coarse grained dislocation densities from an effective free energy. Philosophical Magazine, 2007, 87 (08-09), pp.1185-1199. 10.1080/14786430600835813 . hal-00513722

**HAL Id: hal-00513722**

**<https://hal.science/hal-00513722>**

Submitted on 1 Sep 2010

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



**Dynamics of coarse grained dislocation densities from an effective free energy**

Journal:	<i>Philosophical Magazine &amp; Philosophical Magazine Letters</i>
Manuscript ID:	TPHM-06-Mar-0051
Journal Selection:	Philosophical Magazine
Date Submitted by the Author:	07-Mar-2006
Complete List of Authors:	Groma, Istvan; Eötvös University, Budapest, Department of General Physics Györgyi, Géza; Eötvös University Budapest, Institute of Theoretical Physics, HAS Research Group Kocsis, Benedek; Eötvös University Budapest, Department of General Physics
Keywords:	dislocation dynamics, dislocation theory
Keywords (user supplied):	

# Dynamics of coarse grained dislocation densities from an effective free energy

I. Groma<sup>1</sup>, G. Györgyi<sup>2</sup>, and B. Kocsis<sup>1</sup>

<sup>1</sup>Department of General Physics, Eötvös University Budapest

P.O. Box 32, 1518 Budapest, Hungary

E-mail: groma@metal.elte.hu

<sup>2</sup>Institute of Theoretical Physics, HAS Research Group, Eötvös University Budapest

P.O. Box 32, 1518 Budapest, Hungary

E-mail: gyorgyi@glu.elte.hu

March 7, 2006

## Abstract

A continuum description of the time evolution of an ensemble of parallel straight dislocations has been recently derived from the equation of motions of individual dislocations. The predictions of the continuum model were compared to the results of discrete dislocation dynamics (DDD) simulations for several different boundary conditions. It was found that it is able to reproduce all the features of the dislocation ensembles obtained by DDD simulations. The continuum model, however, is systematically established only for single slip. Due to the complicated structure of the equations extending the derivation procedure for multiple slip is not straightforward.

In this paper an alternative approach based on a thermodynamics-like principle is proposed to derive continuum equations for single slip. An effective free energy is introduced even for zero physical temperature, which yields equilibrium conditions giving rise to Debye-like screening, furthermore, it generates

dynamical equations along the line of phase field theory. It is shown that this leads essentially to the same evolution equations as obtained earlier. In addition, it seems that this framework is extendable to multiple slip as well.

## 1 Introduction

In the past decade there has been a increasing activity to develop a continuum theory of dislocations. Theoretical investigations intensified due to an experimental finding, namely, if the characteristic size of a specimen is less than about  $10\mu\text{m}$  then the plastic response of the crystalline materials depends on the size [1, 2]. (The phenomenon is commonly called size effect). One can easily explain this size dependence by assuming that the crystalline materials have an internal degree of freedom which "feel" the sample surface. This immediately indicates that a theory able to account for the size effects has to be nonlocal, since the sample surface is "seen" from the bulk. 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 (Aifantis [3, 4, 5], Flack and Hutchinson [6], Gurtin [7], Svendsen [8]). 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. An appropriate continuum theory of dislocations should also be able to account for dislocation patterning which is a long standing challenge of dislocation theory.

Attempts to describing the time evolution of dislocation systems on a continuum level are not new (Kuhlmann-Wilsdorf et al. [9], Holt [10], Walgraef and Aifantis [11], Kratochvil et al. [12, 13]). However, these continuum theories either are based on questionable assumptions, or they depend on parameters which are difficult to determine.

For a system of parallel edge dislocations with single slip Groma et al. [14, 15, 16] have established a systematic way to build up a continuum theory from the equation

of motion of individual dislocation. 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, El-Azab [17], Kratochvil and Sedlacek [18], Koslowski et al. [19] and Zaiser and Hochrainer [20] have proposed promising frameworks 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.

A completely different approach based on thermodynamical considerations has been elaborated by Berdichevsky [21] for a system of uniform-sign screw dislocations in 2d. Although, 2d screw dislocations represent an extreme oversimplification, the variational method he applied seems to be promising to treat more realistic dislocation systems. Another important step forward was achieved by Sarafanov and Perevezentev [22]. Using a formal analogy with plasma systems, they determined the screening of a disclination by an ensemble of 2d edge dislocations. A general study of the Debye-like screening problem for 2d single slip geometry has been carried out by the present authors [23]. This involves an effective free energy whose variation leads to equilibrium equations, explicitly solvable under some physically important conditions. The results obtained were compared with DDD simulations and an experiment finding.

In this paper we construct evolution equations for dislocation densities resembling non-equilibrium thermodynamics. This is based on the effective free energy drawn from the aforementioned equilibrium theory [23]. Our main result is that the dynamical equations thus obtained reproduce the physically most important terms known from earlier studies [14, 15, 16].

First the method developed earlier to link the microscopic and mesoscopic description of the evolution of a 2d single slip dislocation system is summarized. The two subsequent sections present the new variational approach to the dynamical equations. Before the conclusion, the outlook of extending the model for double slip is

discussed.

## 2 Linking micro to mezoscale

In this section we recall the existing theory for the evolution of dislocation densities [14, 15, 16], which serves as the basis for comparison to our new approach as elucidated later. We start our analysis by considering the simplest possible dislocation ensemble, a system of  $N$  parallel edge dislocations with Burgers vectors  $\pm(b, 0, 0)$ . We assume that the temperature is low enough, so dislocation climb is negligible beside glide, i.e. dislocations can move only in their glide planes. As a first step, the equation of motion of individual dislocations has to be set up. Because of the dissipative nature of dislocation motion, beside the force acting on a dislocation due to the elastic field (Peach-Koehler force [24]), a friction force has to be taken into account. A frequently applied approximation is that the friction force is proportional to the velocity of a dislocation [25]. Since in the case of low deformation rate the inertia term can be neglected besides the friction force, the equation of motion of a dislocation is only a first order differential equation [14]:

$$\frac{d\vec{r}_i}{dt} = B^{-1}\vec{b}s_i \left[ \sum_{j \neq i}^N s_j \tau_{\text{ind}}(\vec{r}_i - \vec{r}_j) + \tau_{\text{ext}} \right], \quad (1)$$

where  $\vec{r}_i = \vec{r}_i(t)$  is the position of the  $i$ th dislocation in the plane perpendicular to the dislocation line direction,  $B$  is the dislocation mobility,  $s_i = \pm 1$  is the sign of the  $i$ th dislocation,  $\tau_{\text{ext}}$  is the external shear stress and

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

is the shear stress generated by an individual dislocation in an infinite medium. Here  $\mu$  is the shear modulus, and  $\nu$  is the Poisson's ratio.

In order to derive continuum equations let us multiply Eq. (1) with  $\delta(\vec{r} - \vec{r}_i)$ , and take its derivative with respect to  $\vec{r}$ :

$$\vec{\nabla} \left\{ \frac{d\vec{r}_i}{dt} \delta(\vec{r} - \vec{r}_i) \right\} = \vec{\nabla} \left\{ B^{-1}\vec{b}s_i \left[ \sum_{j \neq i}^N s_j \tau_{\text{ind}}(\vec{r}_i - \vec{r}_j) + \tau_{\text{ext}} \right] \delta(\vec{r} - \vec{r}_i) \right\}. \quad (3)$$

The left hand side of the above equation can be rewritten as

$$\vec{\nabla} \left\{ \frac{d\vec{r}_i}{dt} \delta(\vec{r} - \vec{r}_i) \right\} = -\frac{\vec{r}_i}{dt} \vec{\nabla}_i \delta(\vec{r} - \vec{r}_i) = -\frac{d}{dt} \delta(\vec{r} - \vec{r}_i). \quad (4)$$

For further considerations it is useful to introduce the discrete distribution functions corresponding to dislocations with positive and negative signs

$$\rho_{\pm}^d(\vec{r}) = \sum_{i=1}^N \Theta(\pm s_i) \delta(\vec{r} - \vec{r}_i), \quad (5)$$

where  $\Theta(x)$  is the Heaviside function. By multiplying Eq. (3) with  $\Theta(\pm s_i)$  and summing up with respect to  $i$  we get

$$\frac{d}{dt} \rho_{\pm}^d(\vec{r}) = \mp B^{-1}(\vec{b} \vec{\nabla}) \left\{ \left( \int \tau_{ind}(\vec{r} - \vec{r}') [\rho_{\pm}^d(\vec{r}') - \delta(\vec{r} - \vec{r}') - \rho_{\mp}^d(\vec{r}')] d^2 r' + \tau_{ext} \right) \rho_{\pm}^d(\vec{r}) \right\}, \quad (6)$$

(where  $\delta(\vec{r} - \vec{r}')$  beside  $\rho_{\pm}^d(\vec{r}')$  is needed to avoid dislocation self-interaction.) The above equation is a strongly nonlinear equation for the discrete dislocation densities  $\rho_{\pm}^d(\vec{r})$ , which is as difficult to solve as the original equation of motion (1). For many problems, however, we do not need such a detailed description of the dislocation system represented by the discrete density functions introduced above. We can get rid of the highly singular character of  $\rho_{\pm}^d(\vec{r}')$  convoluting Eq. (6) with a window function. In what follows, we shall denote the result of coarse graining on the quantity  $A$  by  $\langle A \rangle$ . One can immediately raise the question what is the appropriate function we should use for the shape of the windows function and what determines its 'half width'. There is no general recipe how to resolve this problem, but we can hope that within certain limits the results obtained by coarse graining are not sensitive to the actual shape and width of the window function.

After performing coarse graining on Eq. (6) we obtain that

$$\frac{\partial \rho_+(\vec{r}_1, t)}{\partial t} + B^{-1}(\vec{b} \vec{\nabla}_1) \left[ \rho_+(\vec{r}_1, t) \tau_{ext} + \int \{ \rho_{++}(\vec{r}_1, \vec{r}_2, t) - \rho_{+-}(\vec{r}_1, \vec{r}_2, t) \} \tau_{ind}(\vec{r}_1 - \vec{r}_2) d\vec{r}_2 \right] = 0 \quad (7)$$

$$\frac{\partial \rho_-(\vec{r}_1, t)}{\partial t} - B^{-1}(\vec{b} \vec{\nabla}_1) \left[ \rho_-(\vec{r}_1, t) \tau_{ext} - \int \{ \rho_{--}(\vec{r}_1, \vec{r}_2, t) - \rho_{-+}(\vec{r}_1, \vec{r}_2, t) \} \tau_{ind}(\vec{r}_1 - \vec{r}_2) d\vec{r}_2 \right] = 0 \quad (8)$$

where

$$\rho_{\pm}(\vec{r}) = \langle \rho_{\pm}^d(\vec{r}) \rangle \quad (9)$$

and

$$\rho_{\pm\pm}(\vec{r}_1, \vec{r}_2) = \langle \rho_{\pm}^d(\vec{r}_1) \rho_{\pm}^d(\vec{r}_2) - \rho_{\pm}^d(\vec{r}_1) \delta(\vec{r}_1 - \vec{r}_2) \rangle \quad (10)$$

are the coarse grained one and two-particle dislocation density functions corresponding to the signs indicated by the subscripts.

As it can be seen the equations derived above do not represent a closed set of equations because the time derivative of the one-particle density functions depend on the two-particles ones. In order to get closed evolution equations, the properties of the pair-correlation functions  $d_{ss'}$  defined as

$$\rho_{ss'}(\vec{r}_1, \vec{r}_2, t) = \rho_s(\vec{r}_1) \rho_{s'}(\vec{r}_2) (1 + d_{ss'}(\vec{r}_1, \vec{r}_2)) \quad s, s' \in \{+, -\} \quad (11)$$

have to be analyzed. According to discrete dislocation dynamics (DDD) simulations the pair-correlation functions defined above decay to zero within a few dislocation spacings [26]. As a result of this, if the total dislocation density  $\rho = \rho_+ + \rho_-$  varies slowly enough in space, we can assume that the correlation functions depend explicitly only on the relative coordinate  $\vec{r}_1 - \vec{r}_2$ . The direct  $\vec{r}_1$  (or  $\vec{r}_2$ ) dependence appears only through the local dislocation density i.e.

$$d_{ss'}(\vec{r}_1, \vec{r}_2) = d_{ss'}(\vec{r}_1 - \vec{r}_2, \rho(\vec{r}_1)) \quad s, s' \in \{+, -\}. \quad (12)$$

(Since  $d_{ss'}$  is short ranged in  $\vec{r}_1 - \vec{r}_2$ , it does not any make difference, if in the above expression  $\rho(\vec{r}_1)$  is replaced by  $\rho(\vec{r}_2)$ .) In the case  $\rho_+ - \rho_- \ll \rho$ , there is no other relevant length scale but the average dislocation spacing. So, for dimensionality reason the  $\rho$  dependence of  $d_{ss'}$  has to be the following:

$$d_{ss'}(\vec{r}_1, \vec{r}_2) = d_{ss'}((\vec{r}_1 - \vec{r}_2) \sqrt{\rho(\vec{r}_1)}) \quad s, s' \in \{+, -\}. \quad (13)$$

By substituting Eq. (13) into Eqs. (7,8) and (11) we conclude that the total and the  $\kappa = \rho_+ - \rho_-$  signed or geometrically necessary dislocation (GND) densities satisfy the evolution equations [16]

$$\frac{\partial \rho(\vec{r}, t)}{\partial t} + B^{-1}(\vec{b} \cdot \vec{\nabla})[\kappa(\vec{r}, t) \{\tau_{sc}(\vec{r}) + \tau_{ext} - \tau_f(\vec{r}) + \tau_b(\vec{r})\}] = 0, \quad (14)$$



$$\frac{\partial \kappa(\vec{r}, t)}{\partial t} + B^{-1}(\vec{b} \cdot \vec{\nabla})[\rho(\vec{r}, t) \{\tau_{sc}(\vec{r}) + \tau_{ext} - \tau_f(\vec{r}) + \tau_b(\vec{r})\}] = 0, \quad (15)$$

where

$$\tau_{sc}(\vec{r}) = \int \tau_{ind}(\vec{r} - \vec{r}_1) \kappa(\vec{r}_1) d^2 r_1, \quad (16)$$

$$\tau_f(\vec{r}) = \frac{1}{2} \int \rho(\vec{r} - \vec{r}_1) d^a(\vec{r}_1 \sqrt{\rho(\vec{r} - \vec{r}_1)}) \tau_{ind}(\vec{r}_1) d^2 r_1 \quad (17)$$

and

$$\tau_b(\vec{r}) = \int \kappa(\vec{r} - \vec{r}_1) d(\vec{r}_1 \sqrt{\rho(\vec{r} - \vec{r}_1)}) \tau_{ind}(\vec{r}_1) d^2 r_1, \quad (18)$$

in which the notations

$$d(\vec{r}) = 1/4[d_{++}(\vec{r}) + d_{--}(\vec{r}) + d_{+-}(\vec{r}) + d_{-+}(\vec{r})], \quad (19)$$

$$d^a(\vec{r}) = 1/2[d_{+-}(\vec{r}) - d_{-+}(\vec{r})] \quad (20)$$

are introduced. (For the sake of simplicity, the  $\rho$  dependence of the correlation functions are not indicated.) Due to the following obvious symmetry properties of the correlation functions

$$d_{+-}(\vec{r}) = d_{-+}(-\vec{r}), \quad d_{++}(\vec{r}) = d_{++}(-\vec{r}), \quad d_{--}(\vec{r}) = d_{--}(-\vec{r}) \quad (21)$$

$d(\vec{r})$  is an even, while  $d^a(\vec{r})$  is an odd function of  $\vec{r}$ .

Taking into account that the pair-correlation functions decay to zero within a few dislocation spacings the fields  $\kappa(\vec{r} - \vec{r}_1)$  and  $\rho(\vec{r} - \vec{r}_1)$  appearing in Eqs. (17,18) can be approximated by their Taylor expansion around the point  $\vec{r}$ . Keeping only the first nonvanishing terms and assuming that  $\frac{\partial \rho}{\partial r} \ll \rho^{3/2}$  we get

$$\tau_f(\vec{r}) = \frac{\rho(\vec{r})}{2} \int d^a(\vec{r}_1 \sqrt{\rho(\vec{r})}) \tau_{ind}(\vec{r}_1) d^2 r_1, \quad (22)$$

$$\tau_b(\vec{r}) = -\frac{\partial \kappa(\vec{r})}{\partial x} \int x_1 d(\vec{r}_1 \sqrt{\rho(\vec{r})}) \tau_{ind}(\vec{r}_1) d^2 r_1. \quad (23)$$

(To obtain expressions (22,23) one has to take into account the symmetry properties of  $d(\vec{r})$  and  $d^a(\vec{r})$  explained above, and that  $\tau_{ind}(\vec{r}) = -\tau_{ind}(-\vec{r})$ .) By the variable substitution  $\vec{\eta} = \sqrt{\rho} \vec{r}$   $\tau_f(\vec{r})$  and  $\tau_b(\vec{r})$  read as

$$\tau_f(\vec{r}) = \frac{\mu}{4\pi(1-\nu)} C_d b \sqrt{\rho(\vec{r})}, \quad (24)$$

and

$$\tau_b(\vec{r}) = -\frac{\mu}{2\pi(1-\nu)} D_d \frac{b}{\rho} \frac{\partial \kappa(\vec{r})}{\partial x}, \quad (25)$$

where

$$C_d = \int \frac{\eta_x(\eta_x^2 - \eta_y^2)}{(\eta_x^2 + \eta_y^2)^2} d^a(\eta_x, \eta_y) d\eta_x d\eta_y \quad (26)$$

and

$$D_d = \int \frac{\eta_x^2(\eta_x^2 - \eta_y^2)}{(\eta_x^2 + \eta_y^2)^2} d(\eta_x, \eta_y) d\eta_x d\eta_y \quad (27)$$

in which  $\vec{\eta}$  has to be measured in unit of dislocation spacing.

In order to understand the physical meaning of the different 'stress like' terms defined above we have to take into account that the correlation functions can depend on the external stress too. One can easily see, that  $d(x, y)$  (which is the sum of the four correlation functions) can have only a weak  $\tau_{\text{ext}}$  dependence. In the same time, however,  $d^a(x, y) = 1/2[d_{+-}(x, y) - d_{-+}(x, y)]$  varies strongly with  $\tau_{\text{ext}}$ . It follows, that  $D_d$  is a constant dimensionless material parameter, while  $C_d$  depends on the external stress. Beside this, according to Eq. (24),  $\tau_f$  scales with  $\sqrt{\rho(\vec{r})}$ . The actual stress dependence of  $C_d$  is difficult to determine, but from Eq. (24) we can speculate that  $\tau_f$  acts like the flow stress. This means, up to a certain stress level  $\tau_f^{\text{max}} \propto \sqrt{\rho}$ , it is as big as necessary to prevent dislocation motion. If, however, the local shear stress is larger than  $\tau_f^{\text{max}}$  it becomes a constant  $\tau_f = \tau_f^{\text{max}}$ . Certainly, we have to be careful with associating  $\tau_f$  with the flow stress. In real dislocation systems hardening is caused by forest dislocations not included into our model in any sense. Nevertheless, a stress like term showing similar properties as the flow stress appears naturally in the theory.

An important feature of the evolution equations obtained is that a term proportional to the gradient of the GND density appears naturally. There are several phenomenological attempts [3, 4, 6, 7, 8] to introduce similar gradient terms, but each of them suffers from the drawback that a length parameter  $l$  with unclear physical meaning has to be introduced. In contrast with this, in our theory there is a natural length parameter, namely, the dislocation spacing  $l = 1/\sqrt{\rho}$ . It has to be

emphasized that, unlike in phenomenological theories, our length parameter  $l$  is not a constant because  $\rho$  obeys the evolution equation Eq. (14).

For further considerations it is useful to note that for any 2d elastic problem the stress tensor can be obtained from a scalar function  $\chi$  (called stress potential or Airy's function) as [27]

$$\sigma_{11} = -\frac{\partial^2 \chi}{\partial y^2}, \quad \sigma_{22} = -\frac{\partial^2 \chi}{\partial x^2}, \quad \sigma_{12} = \frac{\partial^2 \chi}{\partial x \partial y}. \quad (28)$$

It follows from Eq. (28) that the

$$\frac{\partial}{\partial r_i} \sigma_{ij} = 0 \quad (29)$$

equilibrium condition is fulfilled. According to the field theory of dislocations by Kröner and Kosevich [27, 28], for the slip geometry considered in this paper,  $\chi$  is the solution of the biharmonic equation

$$\Delta^2 \chi(\vec{r}) = \frac{2\mu}{1-\nu} b \frac{\partial}{\partial y} \kappa(\vec{r}) \quad (30)$$

By solving the above equation one can find that for an infinite media  $\tau_{sc}$  given by Eq. (16) is equal to  $\sigma_{12}$ , i.e.  $\tau_{sc}$  appearing in the evolution equations derived is the coarse grained shear stress generated by the dislocation system. We mention that due to the long range nature of  $\tau_{ind}$ , in contrast with  $\tau_f$  and  $\tau_b$ ,  $\tau_{sc}$  cannot be approximated by a Taylor expansion

During the past couple of years the continuum theory explained above was solved for different nontrivial deformation geometries, like shear of a channel [16], bending [29] and shear of composite [30]. The results were compared with DDD simulations. It was found that the continuum model is able to reproduce not only the macroscopic (like stress strain curve) but the microscopic properties (dislocation density distributions, local shear rate, internal stress distribution) obtained by DDD simulations. At the moment, however, the continuum theory is well established only for single slip. Extending the theory just for 2d multiple slip (that is still a very strong simplification of the real dislocation geometry) is already far from trivial by a derivation procedure similar to the one outlined above. In order to establish a systematic way of setting up continuum equations for more complex situations, in the next part of the paper we propose a thermodynamics-like approach presented in a variational framework.

### 3 Variational approach

As the first step let us consider the following functional

$$E[\chi, \kappa] = \int \left[ -\frac{1-\nu}{4\mu} (\Delta\chi)^2 + b\chi' \frac{\partial\kappa}{\partial y} \right] d\vec{r}. \quad (31)$$

By varying  $E[\chi, \kappa]$  with respect to  $\chi$ , for an infinite medium (for which the surface terms vanish) we get, that at a given  $\kappa(\vec{r})$   $E[\chi, \kappa]$  has an extremum at a specific  $\chi$  satisfying the equilibrium Eq. (30). This means that the equilibrium condition (30) can be obtained from a variational principle. This simple finding will play a crucial role in the analysis below. It is easily seen from Eqs. (31) and (30) that the extremum of  $E[\chi, \kappa]$  is

$$E_{\min} = \int \left[ \frac{1-\nu}{4\mu} (\Delta\chi)^2 \right] d^2r. \quad (32)$$

Straightforward calculation shows that  $E_{\min}$  is the elastic energy of a deformed 2d system with Airy's function  $\chi(\vec{r})$ . This follows that if we consider a coarse grained GND density field  $\kappa(\vec{r})$  the energy functional given by Eq. (31) is minimized at the corresponding coarse grained Airy's function  $\chi(\vec{r})$ . We have to keep in mind, however, that since  $\kappa(\vec{r})$  and  $\chi(\vec{r})$  are coarse grained fields,  $E_{\min}$  is not the total elastic energy of a dislocation system.

The energy expression given by Eq. (31) has another important feature. The second term on the right hand side of (31)

$$E_{\text{int}} = \int \left[ b\chi \frac{\partial\kappa}{\partial y} \right] d^2r \quad (33)$$

is the interaction energy of dislocations with an external elastic field given by the Airy's function  $\chi(\vec{r})$ . In order to see that this is indeed the case, let us consider a single dislocation positioned at the point  $\vec{r}_0$ . Since for a single dislocation  $\kappa(\vec{r}) = \delta(\vec{r} - \vec{r}_0)$ , according to Eq. (33)

$$E_{\text{int}}(\vec{r}_0) = \int \left[ b\chi \frac{\partial}{\partial y} \delta(\vec{r} - \vec{r}_0) \right] d^2r. \quad (34)$$

Hence the force (per unit length) acting on the dislocation due to the elastic field is

$$\vec{F} = -\frac{d}{d^2r_0} E_{\text{int}}(\vec{r}_0) = b \left( \frac{\partial^2\chi}{\partial x_0 \partial y_0}, \frac{\partial^2\chi}{\partial y_0^2} \right) = b (\sigma_{12}(\vec{r}_0), -\sigma_{11}(\vec{r}_0)) \quad (35)$$

that is the Peach-Koehler force [24] for the dislocation geometry considered.

The next problem we are going to address is how to get evolution equations from the energy functional (31) introduced. For this we apply the standard method of phase field theories [31]. Assuming that the number of positive and negative dislocations are conserved, the evolution equations must have the form

$$\frac{\partial}{\partial t} \rho_{\pm} + \text{div} \vec{j}_{\pm} = 0, \quad (36)$$

where  $\vec{j}_{+}$  and  $\vec{j}_{-}$  are currents corresponding to positive and negative dislocations, respectively. Since in our present analysis dislocation climb is excluded, the currents have to be parallel to the Burgers vector so,  $\vec{j}_{\pm} = \vec{b}/|\vec{b}| j_{\pm}$  where  $j_{\pm}$  are scalar quantities.

Like in irreversible thermodynamics, we assume that the currents are linear functions of the gradient of the chemical potentials, i.e.

$$\begin{aligned} j_{+} &= M_{++} \frac{\partial}{\partial x} \frac{\delta E}{\delta \rho_{+}} + M_{+-} \frac{\partial}{\partial x} \frac{\delta E}{\delta \rho_{-}} \\ j_{-} &= M_{--} \frac{\partial}{\partial x} \frac{\delta E}{\delta \rho_{-}} + M_{-+} \frac{\partial}{\partial x} \frac{\delta E}{\delta \rho_{+}}, \end{aligned} \quad (37)$$

where  $M_{ij}$  ( $i, j = \pm$ ) are mobility parameters. The actual value of the mobilities cannot be determined from general considerations. They may depend on the dislocation densities, too. However, the evolution equations we obtain from Eqs. (36,37) should be the same as Eqs. (14,15) derived in the previous section from microscopic considerations. Taking the following forms for the currents

$$\begin{aligned} j_{+} &= \frac{B^{-1}}{2} \rho_{+} \frac{\partial}{\partial x} \left[ \frac{\delta E}{\delta \rho_{+}} - \frac{\delta E}{\delta \rho_{-}} \right] = B^{-1} \rho_{+} \frac{\partial}{\partial x} \frac{\delta E}{\delta \kappa} \\ j_{-} &= \frac{B^{-1}}{2} \rho_{-} \frac{\partial}{\partial x} \left[ \frac{\delta E}{\delta \rho_{-}} - \frac{\delta E}{\delta \rho_{+}} \right] = -B^{-1} \rho_{-} \frac{\partial}{\partial x} \frac{\delta E}{\delta \kappa} \end{aligned} \quad (38)$$

leads to the evolution equations for  $\rho = \rho_{+} - \rho_{-}$  and  $\kappa = \rho_{+} + \rho_{-}$  as

$$\frac{\partial \rho(\vec{r}, t)}{\partial t} + B^{-1} (\vec{b} \cdot \vec{\nabla}) [\kappa(\vec{r}, t) \tau_{sc}(\vec{r}, t)] = 0, \quad (39)$$

$$\frac{\partial \kappa(\vec{r}, t)}{\partial t} + B^{-1} (\vec{b} \cdot \vec{\nabla}) [\rho(\vec{r}, t) \tau_{sc}(\vec{r}, t)] = 0, \quad (40)$$

where  $\tau_{sc} = \partial^2 \chi / \partial x \partial y$  is the self-consistent shear stress introduced above. By comparing Eqs. (39,40) with Eqs. (14,15) we see that the  $\tau_f$  'flow' stress and the  $\tau_b$  gradient term related to the dislocation-dislocation correlation functions are not recovered by the considerations above. This means, that using the standard method of phase field theories, the dislocation dynamics we can obtain from the coarse grained energy functional  $E[\chi, \kappa]$  corresponds to the zeroth order approximation when the two-particle density functions are assumed to be the simple products of the one particle densities,  $\rho_{i,j}(\vec{r}_1, \vec{r}_2) = \rho_i(\vec{r}_1)\rho_j(\vec{r}_2)$ .

## 4 Effective free energy

As it is well known, if the dynamics of a system is influenced by thermal noise, the minimum of the free energy  $F = E - TS$  determines the equilibrium state, where  $T$  is the temperature characterizing the noise level, and  $S$  is the entropy. However, by estimating the order of magnitudes of the different terms in  $F$  one can find that for dislocation systems the  $TS$  term is negligible in most practical cases of plastic deformation. Nevertheless, as it is explained below in details, an effective temperature parameter  $T_{\text{eff}}$  can characterize the dislocation system, if dislocation glide dominates the dynamics. Remarkably, this effect holds even for zero physical temperature.

As the simplest possible assumption, the entropy of the dislocation system is approximated by

$$S[\rho_+, \rho_-] = - \int \left[ \rho_+ \ln \frac{\rho_+}{\rho_0} + \rho_- \ln \frac{\rho_-}{\rho_0} \right] d^2 r, \quad (41)$$

where  $\rho_0$  is a normalizing constant. If the GND density is small ( $|\kappa| \ll \rho$ ) up to quadratic term in  $\kappa$  the entropy is

$$S[\kappa, \rho] = \int \left[ \frac{\kappa^2}{2\rho} + \rho \ln \frac{\rho}{\rho_0} \right] d^2 r \quad (42)$$

With Eqs. (31,42) the effective free energy proposed reads as

$$F[\chi, \kappa, \rho] = \int \left[ -\frac{1-\nu}{4\mu} (\Delta \chi)^2 + b\chi \frac{\partial \kappa}{\partial y} + T_{\text{eff}} \frac{\kappa^2}{2\rho} \right] d^2 r + F'[\rho] \quad (43)$$

where  $F'[\rho]$  is a term depending only on  $\rho$ . Its actual form is not important for our further considerations.

Replacing  $E$  by  $F$  in expression (38) of the currents leads to the evolution equations

$$\frac{\partial \rho(\vec{r}, t)}{\partial t} + B^{-1}(\vec{b} \cdot \vec{\nabla}) \left[ \kappa(\vec{r}, t) \tau_{sc}(\vec{r}, t) + T_{eff} \frac{\partial}{\partial x} \left( \frac{\kappa}{\rho} \right) \right] = 0, \quad (44)$$

$$\frac{\partial \kappa(\vec{r}, t)}{\partial t} + B^{-1}(\vec{b} \cdot \vec{\nabla}) \left[ \rho(\vec{r}, t) \tau_{sc}(\vec{r}, t) + T_{eff} \frac{\partial}{\partial x} \left( \frac{\kappa}{\rho} \right) \right] = 0. \quad (45)$$

If we take

$$T_{eff} = \frac{\mu}{2\pi(1-\nu)} D_d, \quad (46)$$

and we assume that  $|\kappa| \ll \rho$  and  $\partial \rho / \partial x$  is in the same order as  $\partial \kappa / \partial x$ , the term beside  $\tau_{sc}$  in Eqs. (44,45) is equal to  $\tau_b$ , the gradient term obtained from microscopic considerations. This means, apart from the 'flow' stress  $\tau_f$ , the phase field theory based on the effective free energy functional given by Eq. (43) leads to the same evolution equations as the one derived by the coarse graining of the equations of motion of dislocations.

The result obtained can be summarized as follows: As it is expected, if in the energy expression of the dislocation system the fields  $\kappa$  and  $\chi$  corresponding to discrete dislocation distribution are replaced by coarse grained fields, effects related to dislocation-dislocation correlations are suppressed. Correlation effects manifested in the form of gradient of GND density, however, can be accounted for by an appropriate effective free energy. (We mention that the flow stress is not yet incorporated into the theory.)

A remarkable feature of the evolution equations derived here is that the dynamics is not influenced by the functional derivative of  $F$  with respect to the total dislocation density  $\rho$ . This follows that the conditions for equilibrium are

$$\frac{\delta F}{\delta \chi} = 0 \quad \frac{\delta F}{\delta \kappa} = 0, \quad (47)$$

i.e. the free energy is not minimized totally. Different initial configurations in  $\rho(\vec{r})$  may result in different equilibrium configurations.

We have to keep in mind that the theory is justified only by the fact that it gives the same evolution equations as the ones derived from discrete dislocation dynamics.

The main advantage of the formalism is in its potential to be extended to more complex dislocation configuration. Although the details are not developed at the moment, some of the aspects of the problem are discussed below.

## 5 Debye-like screening of dislocations

In order to demonstrate the capability of the variational approach proposed, we shortly discuss the problem of screening of the elastic field of a dislocation by a 'bath' of other dislocations. Here we only summarize the results compiled elsewhere [23].

Consider a 2d system of parallel edge dislocations distributed homogeneously with density  $\rho$ . Like before, we assume that the Burgers vector of the dislocations are  $\vec{b} = \pm(b, 0)$ . Then, let us add a single dislocation, fixed at the origin of the coordinate system. We ask for the induced GND density and internal stress. The effective free energy of the whole system is obviously

$$F'[\chi, \kappa] = F[\chi, \kappa] + \int b\chi \frac{\partial}{\partial y} \delta(\vec{r}) d^2r, \quad (48)$$

where the second term on the right hand side accounts for the interaction of the extra dislocation with the field created by the other dislocations. From the equilibrium conditions

$$\frac{\delta F'}{\delta \chi} = 0, \quad \frac{\delta F'}{\delta \kappa} = 0 \quad (49)$$

we get

$$\Delta^2 \chi = q \frac{\partial}{\partial y} [\kappa(\vec{r}) + \delta(\vec{r})] \quad (50)$$

and

$$b \frac{\partial \chi}{\partial y} = T_{\text{eff}} \frac{\kappa}{\rho}, \quad (51)$$

where  $q = 2b\mu/(1-\nu)$ . Differentiating with respect to  $y$  and assuming that  $\rho$  remains nearly constant, from (50) we conclude

$$\Delta^2 \chi = 4k_0^2 \frac{\partial^2 \chi}{\partial y^2} + q \frac{\partial}{\partial y} \delta(\vec{r}), \quad (52)$$



where

$$k_0 = \sqrt{\frac{b^2 \mu \rho}{2(1-\nu)T_{\text{eff}}}} \quad (53)$$

Its solution in an infinite medium is

$$\chi(\vec{r}) = -(4\pi k_0)^{-1} \sinh(k_0 y) K_0(k_0 r), \quad (54)$$

where  $K_0$  is the zeroth modified Bessel function of the second kind. Hence by Eq.

(51) the GND density induced is

$$\kappa(\vec{r}) = \frac{k_0^2}{\pi} \left[ \frac{y \sinh(k_0 y)}{r} K_1(k_0 r) - \cosh(k_0 y) K_0(k_0 r) \right]. \quad (55)$$

and by Eq. (28) the shear stress is

$$\sigma_{12} = \frac{q}{4\pi} \left[ \frac{K_1(k_0 r)}{r} \left( \cosh(k_0 y) k_0 x - \sinh(k_0 y) \frac{2xy}{r^2} \right) - \sinh(k_0 y) K_0(k_0 r) \frac{k_0 xy}{r^2} \right]. \quad (56)$$

It can be seen from the asymptotic forms of the Bessel functions, that near the origin the stress is equal to the unscreened stress, i.e., as it is expected, next to the dislocation the stress still decays with  $1/r$ . For large  $|x|$  values, however, both the induced GND and the stress decay like  $\exp(k_0 r)/\sqrt{r}$ . So within a couple of dislocation spacings ( $k_0 \propto \sqrt{\rho}$ ) they practically vanish. Remarkably, along the  $y$  axis  $\kappa$  has a power law asymptote

$$\kappa \approx \sqrt{\frac{k_0}{32\pi}} \frac{1}{|y|^{3/2}}. \quad (57)$$

In order to test the results obtained we performed DDD simulations (for details see [23]). The relaxed positions of 128 dislocations with 1000 different random initial configurations were computed. Then, the induced GND density  $\kappa(\vec{r}) \propto d_{++}(\vec{r}) - d_{+-}(\vec{r})$  was determined by counting the number of pairs of dislocations in a given vicinity of relative position  $\vec{r}$ . The comparison of the DDD and analytical results along the  $y$  axis can be seen in Fig. 1. It can be stated that the GND density values calculated by DDD follow the theoretical curve remarkably well. The only fitting parameter  $k_0$  was found to be  $k_0 = 4.2\sqrt{\rho}$ . We mention, that earlier investigations [23] also indicate that the continuum equations (14,15) are able to reproduce the properties observed by DDD under different conditions.

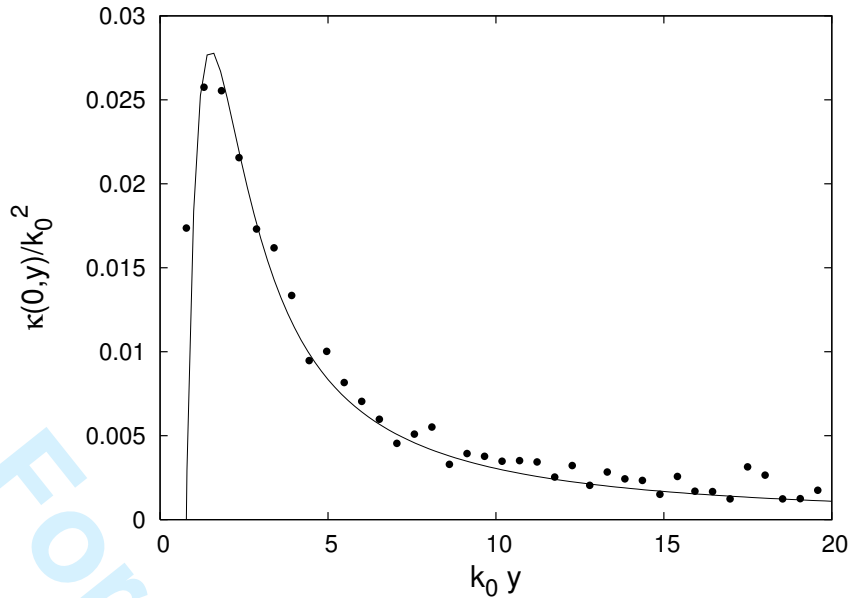


Figure 1: Induced GND along the  $y$  axis obtained by DDD simulation (circles) and the theoretical prediction (full line).

## 6 Double slip geometry

Several open issues have to be addressed before we can say we have an established continuum theory for double or multiple slip. The simplest possible way to extend the single slip equations to double slip is to assume that the GND-dependent part of the total effective free energy is the sum of the two respective terms corresponding to single slip

$$F_{d0}[\chi, \kappa_1, \kappa_2] = \int \left\{ -\frac{1-\nu}{4\mu}(\Delta\chi)^2 + \sum_{i=1}^2 \left[ b\chi(\vec{n}_i \vec{\nabla})\kappa_i + T_{\text{eff}} \frac{\kappa_i^2}{2\rho_i} \right] \right\} d^2r \quad (58)$$

and the currents of the four different type of dislocations are

$$\vec{j}_i^{\pm} = B^{-1} \rho_i^{\pm} (\vec{b}_i \vec{\nabla}) \frac{\delta F_{d0}}{\delta \kappa_i}, \quad i = 1, 2, \quad (59)$$

where quantities with subscript  $i = 1, 2$  correspond to the two-slip systems, and  $\vec{n}_i$  is a unit vector perpendicular to and  $\vec{b}_i$ .

In this case the dislocation evolutions in the two slip systems are coupled only through the Airy's function  $\chi$  (or the self-consistent stress field). According to earlier investigations [32] this does not give a satisfactory agreement with DDD simulations.

We speculate that a better agreement can be achieved by adding a 'cross' term  $F_{\text{cross}}$  to  $F_{d0}$ . If, like before, we assume that the GND densities are small compared to the total dislocation density, i.e., the equations are linear in  $\kappa_i$ , the 'cross' free energy has the form

$$F_{\text{cross}} = A(\rho_1, \rho_2, \varphi) \kappa_1 \kappa_2, \quad (60)$$

where  $A$  is symmetric in the two densities, its dimension is  $1/\rho$ , and  $\varphi$  is the angle between the Burgers vectors. The general form of the function  $A$  is not known, but in special cases simple arguments can help to determine it, and also numerical investigations are presently under way for that purpose.

## 7 Conclusions

A new variational approach, resembling non-equilibrium thermodynamics, is proposed to obtain evolution equations for the GND and the total dislocation densities for single slip. The key features can be summarized as follows.

Similarly to the equilibrium case studied earlier, also the dynamical equations can be derived from an effective free energy. The evolution equations are essentially the same as the ones obtained from microscopic considerations.

It is found, that the gradient term, which arose earlier due to the correlation of dislocations in the evolution equation, can also be accounted for by complementing the naive coarse grained energy by an appropriate term. Because of the formal analogy of the resulting quantity to the usual free energy, we called our formalism effective thermodynamics. It should be stressed, however, that the physical temperature of the system is zero, so in fact the effective free energy is a coarse grained energy computed more precisely than before. We surmise that the arising of a positive effective temperature is intimately related to the fact that dislocations are constrained to their glide planes. A notable outcome of the effective thermodynamics is the Debye-like screening of elastic stress fields by dislocations.

We suggest that the framework presented here opens a way to extend the theory of the single slip system to more general slip plane geometries.

## Acknowledgment

Financial supports of the European Community's Human Potential Programme under Contract No. HPRN-CT-2002-00198 [DEFINO] and MRTN-CT-2003-504634 [SizeDepEn] and the Hungarian Scientific Research Fund (OTKA) under Contract No. T 043519 and TS 044839 are gratefully acknowledged.

## References

- [1] N. Fleck and G. Müller, *Acta Mater.* **42** 475 (1994).
- [2] K. McElhaney, J. Vlassah and W. Nix, *J. Math. Res.* **13** 1300 (1998).
- [3] E. Aifantis, *Eng. Mater. Technol.* **106** 326 (1984).
- [4] E. Aifantis, *Int. J. Plast.* **2** 211 (1987).
- [5] E. Aifantis, *J. Mech. Behav. Mater.* **5** 335 (1994).
- [6] N. Fleck and J. Hutchinson, *J. Mech. Phys. Solids* **49** 2245 (2001).
- [7] M. Gurtin, *J. Mech. Phys. Solids* **50** 5 (2002).
- [8] B. Svendsen, *J. Mech. Phys. Solids* **50** 1297 (2002).
- [9] D. Kuhlmann-Wilsdorf, *Mat. Sci. Eng. A* **113** 1 (1989).
- [10] D. Holt, *Journal Appl. Phys.* **41** 3179 (1970).
- [11] D. Walgraef and E. Aifantis, *J. Appl. Phys.* **15** 688 (1985).
- [12] A. Franek, R. Kalus and J. Kratochvil, *Phil. Mag. A* **64** 497 (1991).
- [13] J. Kratochvil and M. Saxlova, *Scripta Met. Mater.* **26** 113 (1993).
- [14] I. Groma, *Phys. Rev. B* **56** 5807 (1997).
- [15] I. Groma and P. Balogh, *Acta Mater.* **47** 3647 (1999).
- [16] I. Groma, F. Csikor and M. Zaiser, *Acta. Mat.* **51** 1271 (2003).

[17] A. El-Azab, Phys. Rev. B **61** 11956 (2000).

[18] J. Kratochvil and R. Sedlacek, Phys.Rev.B **67** 094105 (2003).

[19] M. Koslowski, R. LeSar and R. Thomson, Phys. Rev. Letters **93** 265503 (2004).

[20] M. Zaiser and T. Hochrainer, Scripta Mater **5** 717 (2006).

[21] V. Berdichevsky, J. Mech. Phys. Solids **53** 2457 (2005).

[22] G. F. Sarafanov and V. Perevezentev, Tech. Phys. Letters **31** 936 (2005).

[23] I. Groma, G. Györgyi and B. Kocsis, submitted to Phys. Rev. Letters (2006).

[24] M. Peach and J. S. Koehler, Phys. Rev. **80** 486 (1950).

[25] W. Cai and V. Bulatov, Mat. Sci. Eng. A **387** 277 (2004).

[26] M. Zaiser, M. Miguel and I. Groma, Phys. Rev. B **64** 224102 (2001).

[27] E. Kröner, *Continuum Theory of Defects* in R. Balian et al., eds., *Physics of Defects* (Elsevier, 1981).

[28] L. D. Landau and E. M. Lifshitz, *Theory of elasticity* vol. 7 of *Course in theoretical physics* 3 ed. (Pergamon, Oxford, 1986).

[29] S. Y. S, E. V. der Giessen and I. Groma, Mod. Simul. Mat. Sci. Eng. **12** 1069 (2004).

[30] S. Y. S, I. Groma and E. V. der Giessen, J. Mech. Phys. Solids **52** 279 (2004).

[31] A. Finel, D. Maziere and M. Veron, eds. *Thermodynamics, Microstructures and Plasticity* NATO Science Series (Kluwer Academic Publisher, London, 2003).

[32] S. Yefimov and E. V. der Giessen, Int. J. Solids Struct. **42** 3375 (2005).