Statistical theory of dislocation

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Abstract The plastic deformation of materials are traditionally modeled by phenomenological crystal plasticity continuum theories. There are, however, several phenomena, like deformation size effect, hardening due to grain boundary, dislocation patter formation that cannot be described within this framework. One has to take into account that the stress-strain response of crystalline materials is determined by the collective motion of dislocations. The aim of the present chapter is to introduce a continuum theory of dislocation obtained by a systematic coarse-graining of the evolution equation of individual dislocations.

1 Introduction

The plastic deformation of crystalline materials is controlled by the collective motion of dislocations. So, to develop a comprehensive model for the stress-strain response of materials we have to understand the statistical properties of dislocations. Since dislocations form a complex network of line type objects, modeling the collective evolution of the dislocation network is a rather challenging problem. What make the issue even more difficult is that the dislocation motion is dissipative and the interaction between dislocations is long ranged. The statistical physics of line type dissipative systems with long range interaction is not developed.

One possibility is to study the evolution of the dislocation system with molecular dynamic (MD) simulation (Zepeda-Ruiz et al. (2016)). For details see Chapter V. With massive parallel computers it is feasible to perform MD simulation with 1000x1000x1000 atoms corresponding to a cube with about 200nm. By such a simulation one can study complex but still "elementary" dislocation phenomena like dislocation multiplication, junction formation, cross slip, *etc.*, but macroscopic properties of the system practically cannot be obtained.

With discrete dislocation dynamics (DDD) simulations (for details see Chapter II.) one can reach the order of $1\mu m$ sample size (Ghoniem and

Sun (1999); Kubin and Canova (1992); Rhee et al. (1998); Gomez-Garcia et al. (2006); Devincre et al. (2001); Bulatov et al. (2006), but for several important problems like dislocation patter formation or size effect we would need a system size minimum of $10\mu m$ because the characteristic size of dislocation patterns are about $1\mu m$.

In this chapter we discuss the statistical properties of a rather simplified dislocation system consisting of parallel edge dislocations. As it is explained below for this dislocation setup a continuum theory of the evolution of the different dislocation densities can be derived on a mathematically rigorous manner by a systematic coarse-graining of the equation of motion of dislocations. In order to get closed set of equations, however, requires some assumptions about the properties of dislocation-dislocation correlation functions. A key feature of the analysis is that these assumptions can be directly verified by DDD simulations. Moreover, the predictions of the continuum theory can be directly compared to DDD simulation results. So, the statistical continuum theory of dislocations presented is validated by DDD.

Although there are rather promising attempts to generalized the theory for more complex dislocation configurations, the 3D continuum theory of dislocations is much less developed. The 2D theory, established on a solid grounds, can help a lot in setting up the structure of the 3D continuum theory.

In the first part of the chapter the field theory of dislocations, developed by Nye, Kröner, and Kosevich, is summarized. It is explained how the stress or strain field generated by a dislocation system can be determined within the framework of a field theory. In the next part the link between the microscopic and mesoscopic descriptions of the evolution of a 2D dislocation system is established by a systematic coarse-graining. It is shown that the theory is able to predict dislocation patterning. In the last part current approaches for the 3D generalization of the theory are discussed.

2 Nye, Kröner, and Kosevich field theory of dislocations

2.1 Dislocation density tensor

Shortly after the concept of dislocation was introduced by Polanyi, Orovan and Taylor in 1934, it was recognized by the Burgers brothers that the elastic field generated by a straight dislocation was already determined by Vito Volterra in 1907 when he considered an elastic problem with a discontinuity on a half plane. (see for example Kovács and Zsoldos (1973)). In the 1950s Nye, Kröner and Kosevich reconsidered the problem and developed an extremely elegant formalism to determine the elastic properties of dislocated crystals (Kröner (1981); Landau and Lifshitz (1986)). In contrast to the **statistical theory of dislocations** (explained in details in this chapter) this theory does not consider the collective evolution of the dislocation network. It gives the different fields (stress, strain, etc.) generated by the dislocation system. So, it should be referred to as **field theory of dislocations**. Since, however, it is essential for the statistical theory, first it is shortly summarized. For more details the reader is referred to Kröner (1981); Landau and Lifshitz (1986); Kosevich (1979).

The deformation of a body can be given by the transformation $\vec{R}(\vec{r})$ where $\vec{R}$ is the deformed position of the point originally located at $\vec{r}$ in the reference (undeformed) system. Assuming that the transformation is differentiable, the transformation matrix defined as

$$dR_i = F_{ij} dx_j \tag{1}$$

is

$$F_{ij} = \partial_j R_i(\vec{r}). \tag{2}$$

(Throughout this chapter a double index implies summation according to Einstein summation convention.)

By introducing the displacement field $\vec{u}(\vec{r}) = \vec{R}(\vec{r}) - \vec{r}$ the matrix F_{ij} can be given as

$$F_{ij} = \delta_{ij} + \beta_{ji} \quad \text{with} \quad \beta_{ij} = \partial_i u_j(\vec{r}), \tag{3}$$

where β_{ij} is called the distortion tensor, and δ_{ij} is the unit tensor.

For an elastic body the internal stress σ_{ij} is completely determined by the deformation tensor $\epsilon_{ij} = (F_{ik}F_{jk} - \delta_{ij})/2$. If, however, plastic deformation is involved only a certain part of the deformation defined above generates stress. To account for this, it is assumed that the total deformation of the body is reached by two subsequent steps, a plastic and an elastic deformations. The first one given by the transformation matrix F^p_{ij} does not generate stress while the second one denoted by F^e_{ij} is related to the stress according to the constitutive equation of the material considered. So, the "starting" point of any plasticity theory of crystalline materials is that

$$F_{ij} = F^e_{ik} F^p_{kj}, \tag{4}$$

where neither F^e_{ij} nor F^p_{ij} is a derivative of a vector field (for details see Chapter VI.) It has to be mentioned that the definitions given above do not uniquely determine F^e_{ij} and F^p_{ij}. The issue is discussed below.

After introducing the plastic $\beta^p_{ij} = F^p_{ji} - \delta_{ij}$ and elastic $\beta^e_{ij} = F^e_{ji} - \delta_{ij}$ distortions Eq. (4) reads as

$$\partial_i u_j = \beta^e_{ij} + \beta^p_{ij} + \beta^e_{ik}\beta^p_{kj}. \tag{5}$$

In the rest of this chapter it is assumed that the distortions are small. So, the last term in the right hand side of the above equation is neglected (small deformation limit), i.e.

$$\partial_i u_j = \beta^e_{ij} + \beta^p_{ij}. \tag{6}$$

For a detailed introduction to the large deformation case see Chapter VI. It is important to stress, that so far, splitting $\partial_i u_j$ is just formal, we have to precisely defined β^e_{ij} and β^p_{ij}.

Since the total distortion $\beta_{ij} = \partial_i u_j$ is a gradient of a vector field its *curl* vanishes, $e_{ikl}\partial_k \beta_{lj} = 0$ where e_{ikl} is the permutation tensor. If, however, dislocations present in the crystal the plastic distortion is not *curl* free, its *curl*

$$\alpha_{ij} = -e_{ikl}\partial_k \beta^p_{lj} \tag{7}$$

is called Nye's dislocation density tensor. From Eq. (6) one can find that $\alpha_{ij} = e_{ikl}\partial_k \beta^e_{lj}$.

Taking the integral of α_{ij} for a surface

$$b_j = \int_A \alpha_{ij} dA_i = -\int_A e_{ikl}\partial_k \beta^p_{lj} dA_i = -\oint \beta^p_{ij} ds_i = -\oint du^p_j \tag{8}$$

gives the net Burgers vector of the dislocations crossing the surface. From this one can find that for a single dislocation

$$\alpha_{ij} = t_i b_j, \delta(\zeta) \tag{9}$$

where l_i is an unit vector in the direction of the dislocation line, and ζ is the distance from the dislocation line.

In the rest of this section we assume that the dislocation density tensor is given, its evolution will be discussed in the next section. In the following we concentrate on calculating the internal stress generated by the dislocation network. Before proceeding further, there are two important issues that have to be discussed:

- Since α_{ij} is the *curl* of the plastic distortion, β^p_{ij} is not uniquely defined by α_{ij}. For giving β^p_{ij} completely we have to put further physical input. The issue is discussed at the end of this section.

- In order to avoid that rigid body rotation generates internal stress, the stress cannot depend on the total elastic distortion β^e_{ij}, only its symmetric part, the elastic deformation $\epsilon^e_{ij} = (\beta^e_{ij} + \beta^e_{ji})/2$. It follows that the stress state does not uniquely determine β^e_{ij} only its symmetric part. Because of this, in the following the symmetric parts of the total, elastic, and plastic distortions are considered. From Eq. (6) they are related as

$$(\partial_j u_i + \partial_i u_j)/2 = \epsilon^e_{ij} + \epsilon^p_{ij}. \tag{10}$$

Assuming local linear elasticity the stress-strain relation (Hooke's law) is

$$\sigma_{ij} = L_{ijkl}\epsilon^e_{kl}, \tag{11}$$

where L_{ijkl} is the elastic modulus tensor. With Eq. (11) Eq. (10) reads as

$$(\partial_j u_i + \partial_i u_j)/2 = L^{-1}_{ijkl}\sigma_{kl} + \epsilon^p_{ij}. \tag{12}$$

In order to proceed further we introduce the incompatibility operator. It acts on a tensor field $\hat{A}$ as

$$(\mathrm{Inc}\hat{A})_{ij} = -e_{ikm}e_{jln}\partial_k\partial_l A_{mn}. \tag{13}$$

Two important properties of the *Inc* operator are:

- For any vector field $\vec{u}(\vec{r})$ the Inc of the symmetric part of its derivative vanishes:

$$\mathrm{Inc}\left(Sim\left[\frac{d\vec{u}}{d\vec{r}}\right]\right)_{ij} = 0, \tag{14}$$

  where

$$\left(Sim\left[\frac{d\vec{u}}{d\vec{r}}\right]\right)_{ij} = (\partial_i u_j + \partial_j u_i)/2. \tag{15}$$

- For any tensor field $\hat{A}(\vec{r})$

$$\partial_i(\mathrm{Inc}\hat{A})_{ij} = 0. \tag{16}$$

By taking the incompatibility of Eq. (12) one arrives at

$$-e_{ikm}e_{jln}\partial_k\partial_l L^{-1}_{mnop}\sigma_{op} = \eta_{ij}, \tag{17}$$

where the incompatibility field η_{ij} defined as

$$\eta_{ij} = -(\text{Inc}\hat{\epsilon}^p)_{ij} = e_{ikm}e_{jln}\partial_k\partial_l\epsilon^p_{mn} \tag{18}$$

is introduced. From Eq. (10) one gets that

$$\eta_{ij} = (\text{Inc}\hat{\epsilon}^e)_{ij}. \tag{19}$$

One can find that the incompatibility field is related to the dislocation density tensor as

$$\eta_{ij} = -\frac{1}{2}\left(e_{iln}\partial_n\alpha_{jl} + e_{jln}\partial_n\alpha_{il}\right), \tag{20}$$

but the source of incompatibility is not necessary related to dislocations. Any other defect such as grain boundary, disclination, stacking fault, inclusion, etc. also can be the source of incompatibility. According to the above equation the primary source of internal stress is the incompatibility field. Since, however, as it was mentioned above, the Inc of a symmetric part of a derivative of a vector filed vanishes, Eq. (17) is not sufficient to determine the stress field generated by η_{ij}. It has to be supplemented with the equilibrium equation

$$\partial_i\sigma_{ij} = 0, \tag{21}$$

the symmetry condition $\sigma_{ij} = \sigma_{ji}$, and the surface traction on the boundary (for other boundary conditions see below).

2.2 Second order stress function tensor

Like in electrodynamics it is useful to reformulate Eqs. (17, 21) into a potential theory. Let us introduce a second order stress function tensor χ_{ij} defined with the relation

$$\sigma_{ij} = (\text{Inc}\hat{\chi})_{ij} = -e_{ikm}e_{jln}\partial_k\partial_l\chi_{mn}. \tag{22}$$

Due to the identity (16) the (22) form of σ_{ij} guarantees that the equilibrium condition (21) is fulfilled. With the stress function tensor introduced above Eq. (17) reads as

$$\eta_{ij} \quad = \quad e_{ikm}e_{jln}e_{oqv}e_{puw}L^{-1}_{mnop}\partial_k\partial_l\partial_q\partial_u\chi_{vw}. \tag{23}$$

For an anisotropic medium the above equation is rather difficult to solve, but for isotropic materials, with shear modulus μ and Poisson's ratio ν, a general solution can be obtained. It is expedient to introduce another tensor potential χ'_{ij} defined as

$$\chi'_{ij} = \frac{1}{2\mu}\left(\chi_{ij} - \frac{\nu}{1+2\nu}\chi_{kk}\delta_{ij}\right) \tag{24}$$

$$\chi_{ij} = 2\mu\left(\chi'_{ij} + \frac{\nu}{1-\nu}\chi'_{kk}\delta_{ij}\right). \tag{25}$$

By inserting Eq. (25) into Eq. (23) one can find, if χ'_{ij} fulfills the gauge condition

$$\partial_i\chi'_{ij} = 0, \tag{26}$$

Eq. (22) simplifies to the biharmonic equation

$$\nabla^4\chi'_{ij} = \eta_{ij}. \tag{27}$$

A remarkable feature of this equation is that the different components of χ'_{ij} obey separate equations making the problem much easier to solve. For an infinite medium the general solution of Eq. (27) is

$$\chi'_{ij}(\vec{r}) = -\frac{1}{8\pi}\int\int\int|\vec{r}-\vec{r}'|\eta_{ij}(\vec{r}')dV' \tag{28}$$

2.3 2D problems

In the next section the statistical properties of an ensemble of parallel edge dislocations are discussed. In this case the stress and the strain do not vary along the dislocation line direction $\vec{l}$. Taking $\vec{l}$ parallel to the z axis (with $\vec{l} = (0, 0, -1)$) in the above expressions the derivatives with respect to z vanish ($\partial_z \equiv 0$). One can find that Eq. (22) simplifies to (Kröner (1981)):

$$\sigma_{11} = -\partial_y\partial_y\chi, \quad \sigma_{22} = -\partial_x\partial_x\chi, \quad \sigma_{12} = \partial_x\partial_y\chi, \quad \chi \equiv \chi_{33} \tag{29}$$

$$\sigma_{23} = -\partial_x\phi, \quad \sigma_{13} = \partial_y\phi, \quad \phi = -\partial_x\chi_{23} + \partial_y\chi_{31}. \tag{30}$$

Furthermore, from Eqs. (20, 23) one obtains that the two scalar fields χ and ϕ introduced above obey the equations

$$\nabla^4\chi = \frac{2\mu}{1-\nu}(b_1\partial_y - b_2\partial_x)(\rho_{d+} - \rho_{d-}) \tag{31}$$

$$\nabla^2\phi = \mu b_3(\rho_{d+} - \rho_{d-}), \tag{32}$$

where b_1, b_2, and b_3 are the x, y, and z directional components of the Burgers vector, respectively. The notations ρ_{d+} and ρ_{d-} stand for the dislocation densities with positive and negative signs, respectively. They are the sum of $\delta(\vec{r}-\vec{r}_i)$ Dirac delta functions, where $\vec{r}_i$ denotes the position of a dislocation. Here, for the sake of simplicity we assumed that all dislocations belong to the same slip system (single slip), but the expressions can be easily generalized for multiple slip.

For an infinite medium the solutions of Eqs. (31, 32) read as

$$\chi(\vec{r}) = \frac{\mu}{2\pi(1-\nu)} \int (b_1\partial_{y'} - b_2\partial_{x'}) \left[\rho_{d+}(\vec{r}') - \rho_{d-}(\vec{r}')\right] R^2 \ln R \; d^2\vec{r}' \tag{33}$$

and

$$\phi(\vec{r}) = -\frac{\mu b_3}{2\pi} \int \left[\rho_{d+}(\vec{r}') - \rho_{d-}(\vec{r}')\right] \ln(R) \; d^2\vec{r}', \tag{34}$$

where $R = |\vec{r} - \vec{r}'|$.

2.4 Variational approach I.

For developing the statistical theory of dislocations it is useful to formulate the results explained above to a variational formalism. We are going to explain two possible approaches. In the first one the elastic deformation ϵ^e_{ij} is considered as the variational field, while in the second one the stress plays the role of independent variable.

Let us first consider the defect free situation. According to thermodynamics principles if the Helmholtz free energy as a functional of the deformation tensor ϵ_{ij} is given the elastic response of the material considered is determined. It should be stressed that we do not have to restrict our considerations to linear elasticity, nonlinearity and nonlocality (the free energy may depend on the derivatives of the deformation tensor) can be allowed. For simplicity here, however, we exclude further possible fields, like curvature, dependence of the free energy. For a general description see Chapter VI..

The stress is the functional derivative of the free energy:

$$\sigma_{ij} = \frac{\delta A}{\delta \epsilon_{ij}}. \tag{35}$$

Since $\epsilon_{ij} = (\partial_i u_j + \partial_j u_i)/2$, the minimum condition

$$-\frac{\delta A}{\delta u_i} = 0 \tag{36}$$

leads to the common equilibrium equation

$$-\frac{\delta A}{\delta u_i} = \partial_j \frac{\delta A}{\delta \epsilon_{ij}} = \partial_j \sigma_{ij} = 0, \tag{37}$$

where for simplicity body force is neglected and surface terms are not discussed.

One arrives at an equivalent result minimizing the free energy with respect to the elastic deformation with the additional condition that Inc of ϵ_{ij} vanishes, ensuring that ϵ_{ij} is the symmetric part of the derivative of the vector field u_i. The additional condition can be taken into account by minimizing the functional

$$Q[\epsilon_{ij}, \chi_{ij}] = A(\epsilon_{ij}) - \int \chi_{ij} (\mathrm{Inc}\hat{\epsilon})_{ij} dV \tag{38}$$

with respect to ϵ_{ij} and the Lagrangian multiplier χ_{ij} (Gröger et al. (2010)), leading to

$$\frac{\delta Q}{\delta \epsilon_{ij}} = \frac{\delta A}{\delta \epsilon_{ij}} - (\mathrm{Inc}\chi)_{ij} = \sigma_{ij} - (\mathrm{Inc}\hat{\chi})_{ij} = 0, \tag{39}$$

and

$$\frac{\delta Q}{\delta \chi_{ij}} = (\mathrm{Inc}\hat{\epsilon})_{ij} = 0. \tag{40}$$

It can bee seen from Eq. (39) that the Lagrangian multiplier introduced is the second order stress function and the equilibrium condition $\partial_j \sigma_{ij} = 0$ is automatically fulfilled.

Generalizing the method for defected media is straightforward. If one simply considers the functional

$$Q[\epsilon^e_{ij}, \chi_{ij}] = A(\epsilon^e_{ij}) - \int \chi_{ij} \left[(\mathrm{Inc}\hat{\epsilon}^e)_{ij} - \eta_{ij} \right] dV \tag{41}$$

the variations with respect to ϵ^e_{ij} and χ_{ij} lead to the bulk equations obtained above for dislocated media.

It should be mentioned, however, that in the above derivation surface terms appearing during the variations were not considered. So, the results obtained are valid only for infinite body with fields go to zero at infinity or for periodic boundary conditions. With other words, the variational method explained gives only the bulk equations, boundary conditions have to be handled separately.

2.5 Variational approach II.

In order to derive the other variational method (Groma et al. (2006, 2010)) let us consider the Gibbs free energy G that is a functional of the stress. Its functional derivative with respect to the stress is the negative elastic strain:

$$-\frac{\delta G}{\delta \sigma_{ij}} = \epsilon^e_{ij}.$$

To ensure the equilibrium condition let us use the second order stress function ($\sigma_{ij} = (\mathrm{Inc}\hat{\chi})_{ij}$) and introduce the functional

$$P[\chi_{ij}] = G((\mathrm{Inc}\hat{\chi})_{ij}) + \int \chi_{ij}\eta_{ij} dV \tag{42}$$

called as "plastic potential" hereafter.

The minimum condition

$$\frac{\delta P}{\delta \chi_{ij}} = 0 \tag{43}$$

leads to

$$\frac{\delta P}{\delta \chi_{ij}} = \left(\mathrm{Inc}\frac{\delta G}{\delta \hat{\sigma}}\right)_{ij} + \eta_{ij} = -(\mathrm{Inc}\hat{\epsilon}^e)_{ij} + \eta_{ij} = 0. \tag{44}$$

This means, in accordance with the definition of the incompatibility field η_{ij}, the plastic potential is minimized with respect to χ_{ij} so that the incompatibility is the Inc of the elastic deformation. Like for the other variational method explained above, surface terms are not taken into account. So, it is assumed that the different fields go to zero at infinity.

For the further considerations it is important to realize that the value of the plastic potential $P[\chi_{ij}]$ at its minimum χ^{eq}_{ij} is the Helmholtz free energy of the system. In order to see this, let us substitute the relation (19) into Eq. (42):

$$P[\chi^{eq}_{ij}] = G(\sigma^{eq}_{ij}) + \int \chi^{eq}_{ij}(\mathrm{Inc}\epsilon^e)_{ij} dV. \tag{45}$$

After a double partial integration in the second term of the right hand side we arrive at

$$P[\chi^{eq}_{ij}] = G(\sigma^{eq}_{ij}) + \int \sigma^{eq}_{ij}\epsilon^e_{ij} dV. \tag{46}$$

From Eq. (42) one concludes

$$P[\chi_{ij}^{eq}] = G(\sigma_{ij}^{eq}) - \int \sigma_{ij}^{eq} \frac{\delta G}{\delta \sigma_{ij}^{eq}} dV, \tag{47}$$

i.e. $P[\chi_{ij}^{eq}]$ is the Legendre transform of the Gibbs free energy that is the Helmholtz free energy. So, the plastic potential at its minimum is the free energy of the system at the given incompatibility η_{ij}. It follows that the negative gradient of $P[\chi_{ij}^{eq}]$ with respect to the dislocation segment position $\vec{r}^{seg}$ is the Peach Koehler force acting on the dislocation segment

$$F_i = -\frac{dP}{dr_i^{seg}} = e_{ikl} t_k \sigma_{lm} b_m. \tag{48}$$

2.6 Local linear medium

We first demonstrate the variational principle on the elementary example of a local, linear material obeying Hooke's law (Groma et al. (2010)). In this case the Gibbs free energy is a quadratic functional of the stress as

$$G_0[\sigma] := -\int \frac{1}{2} \sigma_{ij} L_{ijkl}^{-1} \sigma_{kl} \mathrm{d}V, \tag{49}$$

where L_{ijkl}^{-1} is the elastic compliance tensor. Hence, the plastic potential given by equation (42) reads as

$$P[\chi, \eta] = \int \left[-\frac{1}{2} e_{iop} e_{jqr} (\partial_o \partial_q \chi_{pr}) L_{ijkl}^{-1} e_{kst} e_{luz} \partial_s \partial_u \chi_{tz} + \chi_{ij} \eta_{ji} \right] \mathrm{d}V. \tag{50}$$

One can find that the plastic potential given above gets its minimum if χ_{ij} fulfills Eq. (23).

2.7 Variation for plane problems

In the statistical theory of dislocations, plane (2D) problems play an important role. In this section we discuss the variational method outline above for a systems of straight dislocations extending parallel to the z direction (Groma et al. (2010)).

After a long but straightforward calculation one can find that for edge dislocations the plastic potential functional reads as

$$P[\chi, \alpha] = \int \left[-\frac{1-\nu}{4\mu} (\triangle \chi)^2 + \chi (\partial_2 \alpha_{31} - \partial_1 \alpha_{32}) \right] \mathrm{d}^2 r, \tag{51}$$

where $\chi := \chi_{33}$ is now a single component stress function (the other components of χ_{ij} vanish). The components of the stress tensor are given by

Eq. (29). In $P[\chi, \alpha]$ the incompatibility tensor η_{ij} has been expressed by the dislocation density tensor α_{ij}, which now has only two nonvanishing components. The minimum condition $\delta P/\delta\chi = 0$ leads to the fourth order partial differential equation:

$$\frac{1-\nu}{2\mu} \triangle^2 \chi = \partial_2 \alpha_{31} - \partial_1 \alpha_{32}. \tag{52}$$

Although later in this chapter we do not consider screw dislocations, we summarize their case as well (this variational problem was first discussed by Berdichevsky (2005)). The plastic potential now is

$$P[\phi, \alpha] = \int \left[-\frac{1}{2\mu} |\nabla \phi|^2 + \phi \alpha_{33} \right] \mathrm{d}^2 r \tag{53}$$

with

$$\phi := -\partial_1 \chi_{23} + \partial_2 \chi_{31}. \tag{54}$$

The relevant stress components are

$$\sigma_{23} = -\partial_1 \phi, \quad \sigma_{13} = \partial_2 \phi. \tag{55}$$

The corresponding minimum condition leads to the Poisson's equation

$$\frac{1}{\mu} \triangle \phi = -\alpha_{33}. \tag{56}$$

It has to be mentioned that Eqs. (52, 56) obtained by the variational approach are certainly equivalent with the ones derived earlier. In this section we just demonstrated how the variational method works for a classical local linear medium.

2.8 Dislocation core regularization

The significance of dislocation core regularization is widely known. It is not only necessary to account for core effects, but also to eliminate singularities in a physically well founded manner in numerical simulations. There are many different propositions for dislocation core regularization (Aifantis (1999); Gutkin and E.C. (1999); Lasar (2003)) but, as it is explained below, the variational approach offers a natural way to regularize the singular stress at the dislocation line.

It is common in phase field theories that surface or size effects are captured by introducing appropriate 'gradient terms' in the energy functional. The concept can be applied in dislocation theory too, but as we have recognized above, the physical properties of a material are determined by the functional form of the Gibbs free energy–stress relation. So, the gradient terms have to be introduced in the Gibbs free energy by adding terms that depend on the gradient of the stress. In first order linear approximation one can consider the 'nonlocal' Gibbs free energy

$$G_{nonlocal}[\sigma] = G_0 - b^2 \int N_{ijklmn}(\partial_i \sigma_{jk}) \partial_l \sigma_{mn} \mathrm{d}V, \tag{57}$$

where N_{ijklmn} is a constant tensor with inverse stress dimension and b is the Burgers vector. (b^2 is separated from N_{ijklmn} to indicate the relative order between G_0 and the gradient dependent term.) From $G_{nonlocal}[\sigma]$ the corresponding $P[\chi, \eta]$ has to be constructed as it is explained above.

It should be mentioned that nonlocality could be introduced on a much more general way by taking the Gibbs free energy in the form

$$G_{nonlocal}[\sigma] = -\int \frac{1}{2} \sigma_{ij}(\vec{r}) S_{ijkl}(\vec{r} - \vec{r}') \sigma_{kl}(\vec{r}') \mathrm{d}V \mathrm{d}V', \tag{58}$$

where $S_{ijkl}(\vec{r}')$ is a function which goes to zero fast enough if $|\vec{r}| \to \infty$, but in a first order approximation, if its range is of the order of the lattice constant, it obviously gives the same as Eq. (57).

To demonstrate how the nonlocal term introduced above results in dislocation core regularization let us consider a single straight dislocation. From Eqs. (51) and (57) for a single edge dislocation at the origin

$$P[\chi] = \int \left\{ -\frac{1-\nu}{4\mu} \left[|\triangle \chi|^2 + a^2 |\nabla \triangle \chi|^2 \right] + \chi \partial_2 \delta(\vec{r}) \right\} \mathrm{d}^2 r, \tag{59}$$

where a is a parameter with length dimension that is in the order of the lattice constant. Here, for the sake of simplicity, we considered only the simplest possible isotropic gradient term from Eq. (57) but the general case can be treated in a similar way. The corresponding equilibrium equation has the form

$$\triangle^2 \chi - a^2 \triangle^3 \chi = \frac{2b\mu}{1-\nu} \partial_2 \delta(\vec{r}). \tag{60}$$

The above equation has analytical solution. By taking its Fourier transform one can find that

$$\chi^F(q_1, q_2) = \frac{2b\mu}{1-\nu} \frac{i q_y}{(q_x^2 + q_y^2)^4 + a^2 (q_x^2 + q_y^2)^6} \tag{61}$$

from which, according to equation (29), the Fourier transform of the resolved shear stress reads as

$$\sigma_{12}^{\mathrm{r},F}(q_1, q_2) = -\frac{2b\mu}{1-\nu} \frac{i q_x q_y^2}{(q_x^2 + q_y^2)^4 + a^2 (q_x^2 + q_y^2)^6}. \tag{62}$$

By inverse Fourier transformation we obtain

$$\chi = \frac{b\mu}{2\pi(1-\nu)} \frac{ay}{r} \left[-2K_1\left(\frac{r}{a}\right) + 2\frac{a}{r} + \frac{r}{a} \ln\left(\frac{r}{a}\right) \right], \tag{63}$$

where $K_1(x)$ is the modified Bessel function of the second kind. To demonstrate the difference between the regularized and the "classical" solutions more explicitly the shear stress along the x axis is plotted in Fig. 1. As it

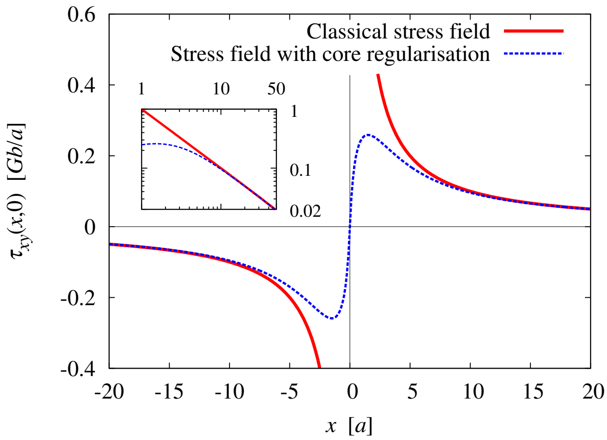


Figure 1. Shear stress along the x axis obtained with and without core regularization. ($G := \mu/[2\pi(1-\nu)]$.)

can be seen, for x larger than about $10\,a$, σ^{r}_{12} is close to the classical stress field $\sigma_{12} \propto 1/r$. So as it is expected, the 'gradient term' introduced above influences only the central core region.

In a similar way, for screw dislocations from Eqs. (53) and (57)

$$P = \int \left\{ -\frac{1}{2\mu} \left[|\nabla\phi|^2 + c^2(\triangle\phi)^2 \right] + b\phi\delta(\vec{r}) \right\} \mathrm{d}^2 r, \tag{64}$$

where c is a constant (see Berdichevsky (2005)). One can obtain that the minimum condition $\delta P/\delta\phi = 0$ is fulfilled if ϕ satisfies the equation

$$\triangle\phi - c^2\triangle^2\phi = -b\mu\delta(\vec{r}). \tag{65}$$

Like for edge dislocations, numerical solution of the above equation shows that the second term of the left hand side of the equation results in stress regularization in the vicinity of the dislocation line.

Comparing the present approach with other methods suggested by Aifantis (1999); Gutkin and E.C. (1999); Lasar (2003), although one can find some similarities, but the major difference is that in these works the core region is regularized by spreading out the dislocation density tensor α_{ij}, while in our analysis the dislocation density tensor remains proportional to a Dirac delta, like in the classical non-regularized case. The core is regularized by the nonlocallity in the Gibbs free energy.

2.9 Dislocation-solute atom interaction

Solute atoms can strongly modify the collective properties of dislocations. Among other things they can lead to plastic instabilities (for a recent review see Ananthakrishna (2007)). In this section we show that the effect of solute atoms can be easily incorporated into the variational framework (Groma et al. (2007)). We restrict our consideration for straight edge dislocations with Burgers vectors parallel to the x axis, but it is straightforward to generalize the method for 3D.

The Gibbs free energy of a coupled system can be always given as the sum of the Gibbs free energy of the two uncoupled systems and a coupling term. Therefore, if we add to the plastic potential the Gibbs free energy contribution of the solute atoms we arrive at the 'plastic potential' of the dislocation-solute system. According to Eq. (51) the plastic potential of the parallel edge dislocation system considered is

$$P_{\mathrm{d}}[\chi, \kappa] = \int \left[-\frac{1-\nu}{4\mu} (\triangle \chi)^2 + b\chi(\partial_2 \kappa) \right] \mathrm{d}^2 r, \tag{66}$$

where κ is the signed dislocation density (geometrically necessary density, GND) defined as $\alpha_{31} = b\kappa$ that is the only nonvanishing component of the dislocation density tensor for the dislocation geometry considered.

For the solute atoms we assume that their concentration c is close to the equilibrium concentration c_∞. In this case the Gibbs free energy of the solute atoms can be given with the quadratic form

$$G_{\mathrm{c}}[c] = \int \alpha (c - c_\infty)^2 \mathrm{d}^2 r, \tag{67}$$

where α is a constant (which may depend on c_∞).

To determine the form of the coupling term we use the well-known fact that beside concentration gradient, the pressure gradient also causes solute atom diffusion. According to the principles of irreversible thermodynamics the solute atom current is proportional to the gradient of the chemical potential $\mu_c = \frac{\delta G}{\delta c}$. So, taking the coupling term in the form

$$G_{cp}[\chi, c] = \int \beta c p \, \mathrm{d}^2 r, \tag{68}$$

where β is constant, the total plastic potential reads as

$$P[\chi, \kappa, c] = P_{\mathrm{d}}[\chi, \kappa] + G_{\mathrm{c}}[c] + G_{cp}[\chi, c] \tag{69}$$

$$= \int \left[-\frac{1-\nu}{4\mu} (\triangle \chi)^2 + b\chi(\partial_2 \kappa) + \alpha(c - c_\infty)^2 - \beta c \triangle \chi \right] \mathrm{d}^2 r, \tag{70}$$

and

$$\frac{\delta P}{\delta c} = \frac{\delta G_c + G_{cp}}{\delta c} = \mu_c. \tag{71}$$

It should be mentioned that Eq. (70) results in linear equations for the stress and the solute atom concentration. Nonlinearity can also be treated within the framework proposed, but it is out of the scope of the paper.

Since the purpose of the subsection is to demonstrate the way the variational approach works, we now restrict our analysis only to static problems. One can find from the equilibrium conditions $\frac{\delta P}{\delta \chi} = 0$ and $\frac{\delta P}{\delta c} = \mu_0$ that

$$\frac{1-\nu}{2\mu} \triangle^2 \chi + \beta \triangle c = b \, \partial_2 \kappa \tag{72}$$

and

$$\alpha(c - c_\infty) = \beta \triangle \chi + \mu_0, \tag{73}$$

where μ_0 is the constant equlibrion chemical potential. By combining the two equations we get that

$$\left[\frac{1-\nu}{2\mu} + \frac{\beta^2}{\alpha} \right] \triangle^2 \chi = b \partial_2 \kappa. \tag{74}$$

A remarkable feature of the above equation is that, apart from a constant multiplier, the functional form of the stress function χ is not affected by the solute atoms. Moreover, the solute atom concentration is proportional to the pressure caused by the dislocations. Certainly the result obtained is not new, it is the well know Cottrell atmosphere of solute atoms around dislocation lines (Cottrell and Bilby (1949)), but it illustrates very well the fact that the coupled system of dislocations and solute atoms can be treated with the variational framework suggested.

2.10 Time evolution of the dislocation density tensor

As it is explained above, if we know the dislocation density tensor (i.e. we know the dislocation line geometry) the internal stress field can be determined from Eq. (23). This is however, only a "static" description. In order to be able to describe the response of the dislocation system to external signals, the governing equations of the time evolution of the dislocation density tensor should be determined. Moreover, as it was mentioned earlier the dislocation density tensor α_{ij} does not determine completely the plastic distortion β^p_{ij}, however, the stress state is uniquely given by α_{ij} or more precisely by the incompatibility tensor η_{ij}. So, one have to put some additional physical input that determine the plastic distortion completely.

For this goal let us take the time derivative (denoted by " $\cdot$ ") of Eq. (7):

$$\dot{\alpha}_{ij} + e_{ikl}\partial_k j_{lj} = 0, \tag{75}$$

where

$$j_{ij} = -\dot{\beta}^p_{ij} \tag{76}$$

is called dislocation current density (Landau and Lifshitz (1986)). The above equation is the "conservation law of the Burgers vector" in differential form. Indeed, if we integrate both sides of Eq. (75) for an arbitrary area contoured by the closed curve L, according to Eq. (8), we obtain that

$$\frac{db_j}{dt} = -\oint_L j_{ij} ds_i \tag{77}$$

It is obvious from this relation that $\hat{j}$ is the Burgers vector carried by the dislocations crossing a unit length part of the contour line L per unit time.

For an individual dislocation one can find that

$$j_{ik} = e_{ilm} l_t v_m b_k \delta^{(2)}(\xi), \tag{78}$$

where $\vec{v}$ is the velocity of the dislocation line at a given point. It is important to note that if we added the gradient of an arbitrary vector field to j_{ij} given above, this would also satisfy the conservation law (75). The problem is obviously related to the non-uniqueness of the plastic distortion discussed earlier. However, expression (78) is the only one which is physically meaningful. One expects that there is no plastic current anywhere else but at the dislocation line. Nevertheless, strictly speaking we have to postulate this.

With this postulation the plastic distortion is given by the time integration of j_{ij} if β^p_{ij} is known at a given moment. (One can often assume that the plastic distortion vanishes initially.)

For the better understanding of the problem related to the nonuniqueness of β^p_{ij} let us consider a dislocation loop. One has to take into account that a defect in the materials is determined completely only if the cut of surface (where we have the jump in the displacement) is given. Taking another cut of surface ended on the same line corresponds to another defect. As it was explained above, however, the stress generated by the two defects is the same, it is determined only by the dislocation line loop. Nevertheless, there is a “natural” cut of surface that is generated during the expansion of the loop, i.e. the surface the dislocation line passed while the loop is formed.

The above results clearly show that j_{ij} has to be considered as an independent quantity. In order to be able to describe the time evolution of the dislocation system we have to set up a constitutive relation giving how j_{ij} depends on the dislocation density tensor and the external stress. Due to the long range nature of the dislocation-dislocation interaction, the constitutive relation is obviously non-local in α_{ij} and should also depend on the total amount of dislocation line per unit volume commonly called the statistically stored dislocation density. Beside this, the constitutive relation has to be able to account for several different "local" phenomena (self loop interaction, junction formation, annihilation etc.) making even more difficult to determine its form.

One possible approach to handle this problem is to set up the constitutive relation from phenomenological considerations. During the past years several phenomenological expressions were proposed and successfully applied for modeling certain phenomena (Aifantis (1984, 1987, 1994); Fleck and Hutchinson (2001); Gurtin (2002); Svendsen (2002)) but the problem is far not completely solved.

Another widely used approach to study the time evolution of dislocation systems is discrete dislocation dynamics (DDD) simulation in which the dislocation loops are considered individually. After setting up velocity laws for the dislocation segments the dislocation loop geometry is updated numerically. Describing the actual numerical techniques used in DDD simulations is out of the scope of this chapter. The details can be found in Chapter II.

2.11 Time evolution of the displacement field

In the previous part we have discussed how the stress field generated by the dislocations can be determined and what can be said in general about the time evolution of the dislocation density tensor. However, in many applications it is important to determine the displacement field $\vec{u}(\vec{r})$, too.

Let us go back to our starting equation (6), multiply it with the elastic modulus tensor L_{ijkl}, and take the div of the equation. With Eqs. (11, 21) one obtains

$$\partial_i L_{ijkl} \partial_l u_k = \partial_i L_{ijkl} \beta^p_{kl}. \tag{79}$$

This is formally equivalent with the common equilibrium equation of elasticity with body force density

$$f_j = -\partial_i L_{ijkl} \beta^p_{kl}. \tag{80}$$

Since, as it is explained earlier, the dislocation density tensor does not determine the plastic distortion uniquely, the above equation is not enough to determine the displacement field. Taking, however, the time derivative of Eq. (79), with the (76) definition of j_{ij}, one arrives at

$$\partial_i L_{ijkl} \partial_l \dot{u}_k = \partial_i L_{ijkl} j_{kl}. \tag{81}$$

As it is discussed above, based on physical arguments, j_{ij} can be uniquely defined, so the deformation velocity field $\dot{u}_i$ can already be determined if j_{ij} is known. Integrating it with respect to time gives the change of the displacement field that is the quantity one can really measure.

3 Statistical continuum theory of dislocations

3.1 General issues

In this section we analyze in details the statistical properties of a system of straight parallel edge dislocations in single slip, that is the simplest possible dislocation configuration one can envisage, but as it is demonstrated by DDD simulations (Kubin and Canova (1992); Rhee et al. (1998); Ghoniem and Sun (1999); Groma and Bakó (2000); Devincre et al. (2001); Gomez-Garcia et al. (2006); Ispánovity et al. (2010); Ispanovity et al. (2014)) this system can reproduce several key properties of the dislocation system. Moreover, the structure of the continuum evolution equations derived on a systematic manner can guide us to develop a more general statistical continuum theory of dislocations. Possible directions of the generalization are discussed in the last section.

Before we start to derive the statistical continuum theory we shortly summarize those key issues one faces developing a theory for the collective behavior of dislocations:

- The dislocation-dislocation interaction is long range. The force acting between two straight parallel dislocations is inversely proportional to their distance $F \propto 1/r$.

- The dislocation motion is strongly dissipative. It is commonly assumed that the dislocation motion is over-damped meaning that the inertial term (ma) is negligible beside the friction force. For small dislocation velocity one can assume that the friction force is proportional to the dislocation velocity. So, in our considerations the velocity is taken to be proportional to the Peach Koehler force, $v \propto F$ resulting that the equation of motion of a dislocation is a first order ordinary differential equation. Generalization is discussed in Chapter II.

- At low enough temperature dislocation climb is negligible beside glide. In our considerations climb will be neglected. As a consequence dislocations cannot leave their slip plane. From statistical physics point of view this means that there is a quenched disorder in the system defined at the generation of the initial dislocation configuration. Since there is no any physical reason introducing a characteristic length scale but the average dislocation spacing the slip planes are assumed to be placed randomly.

- The last issue we have to investigate in more details is the role of thermal noise on the motion of dislocations.

Let us consider N parallel edge dislocations with dislocation line direction parallel to the z and Burger vector parallel to the x axes, respectively (see Fig. 2).

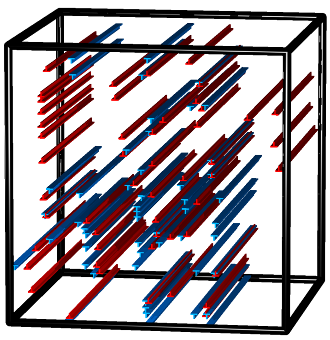


Figure 2. 2D dislocation configuration

With the over-damped dynamics the equations of motion of the dislocation system is

$$\frac{dx_i}{dt} = M_0 b s_i \left(\sum_{j=1}^{N} s_j \tau_{ind}(\vec{r}_i - \vec{r}_j) + \tau_{ext} \right), \tag{82}$$

where $\vec{r}_i$ is the position, $s_i = \pm 1$ is the sign of the ith dislocation, M_0 is the dislocation mobility, b is the Burgers vector, τ_{ext} is the external shear stress, and $\tau_{ind}(\vec{r})$ is the shear stress generated by a dislocation at point $\vec{r}$ (Groma et al. (2003)). The above equation is the one solved numerically in 2D discrete dislocation dynamics (DDD) simulations.

According to Eq. (29) $\tau_{ind}(\vec{r} - \vec{r}_j)$ is related to the second order stress function χ_{ind} as

$$\tau_{ind}(\vec{r}) = \partial_x \partial_y \chi_{ind}(\vec{r}) \tag{83}$$

with χ_{ind} fulfilling the biharmonic equation

$$\bigtriangledown^4 \chi_{ind} = \frac{2\mu}{1-\nu} b \partial_y \delta(\vec{r}) \tag{84}$$

obtained from Eq. (31). Denoting

$$U_{ind}(\vec{r}) = -\partial_y \chi_{ind}(\vec{r}) \tag{85}$$

one gets

$$\tau_{ind}(\vec{r}) = -\partial_x U_{ind}(\vec{r}). \tag{86}$$

By introducing the dislocation-dislocation interaction energy

$$V(\vec{r}_1, \vec{r}_2, ...\vec{r}_N) = \frac{b}{2\sqrt{\rho}} \sum_{i \neq j} s_i s_j U_{ind}(\vec{r}_i - \vec{r}_j) \tag{87}$$

Eq. (82) can be given as

$$\frac{dx_i}{dt} = -M_\rho b \frac{\partial V}{\partial x_i}. \tag{88}$$

with $M_\rho = M_0 \sqrt{\rho}$. It should be noted that since bU_{ind} is energy per unit length, for the further analysis it is useful to multiply it with a characteristic length scale of the problem leading to a quantity with energy dimension. A natural characteristic length scale for the problem is the dislocation spacing $1/\sqrt{\rho}$. This is why $1/\sqrt{\rho}$ is introduced in V.

Thermal noise can be incorporated into the equation of motion of dislocation by adding a random force term to Eq. (88):

$$\frac{dx_i}{dt} = -M_\rho b \partial_{x_i} V + \sqrt{2 M_\rho k_b T} \zeta_i(t), \tag{89}$$

where $\zeta_i(t)$ is a random noise with time correlation $< \zeta_i(t)\zeta_j(0) >= \delta_{ij}\delta(t)$, T is the temperature, and k_b is the Boltzmann constant.

For the probability density $p_N(t, \vec{r}_1, \vec{r}_2, ...\vec{r}_N)$ the Fokker-Planck equation corresponding to the stochastic differential equation (89) reads as

$$\frac{\partial p_N}{\partial t} = M_\rho \sum_{i=1}^{N} \partial_{x_i} \left((\partial_{x_i} V) p_N + k_b T \partial_{x_i} p_N \right). \tag{90}$$

One can easily see that the steady state solution of the above equation is

$$p_N^\infty(\vec{r}_1, \vec{r}_2, ...\vec{r}_N) = \frac{1}{Z} e^{-\frac{V}{k_b T}}, \tag{91}$$

where Z is a normalizing factor. This means, although a dislocation ensemble is not a Hamiltonian system, so the common methods of statistical physics cannot be applied, the probability of a given dislocation configuration is proportional to a Boltzmann factor. In many theories developed for describing the collective properties of dislocations Eq. (91) is used as starting point.

There is, however, an issue related to time scales one has to take into account. The right hand side of Eq. (90) contains two terms. Taking into account that energy of the dislocation system introduced above $V \propto \mu b^2/\sqrt{\rho}$ and the characteristic length scale of the problem $l \propto 1/\sqrt{\rho}$ one can introduce two characteristic time scales

$$t_V = \frac{1}{M_\rho \mu b^2 \sqrt{\rho}} \quad \text{and} \quad t_T = \frac{1}{M_\rho k_b T \rho} \tag{92}$$

corresponding to the firs and second term of the right hand side of Eq. (90), respectively. With typical values the ration

$$\frac{t_V}{t_T} = \frac{k_b T}{\mu b^2} \sqrt{\rho} \tag{93}$$

is less than 10^{-4}, i.e. the characteristic time related to thermal noise is much longer than the one corresponding to elastic dislocation-dislocation interaction. This is why for most of the problems the thermal noise is negligible in the equation of motion of dislocations. So, by neglecting the noise term, from Eqs. (87, 90) the time evolution equation of the N particle probability density $p_N(t, \vec{r}_1, \vec{r}_2, ...\vec{r}_N)$ reads as

$$\begin{aligned} \frac{\partial p_N}{\partial t} &= M_0 b \sum_{i \neq j}^{N} \partial_{x_i} \left[s_i s_j \left(\partial_{x_i} U_{ind}(\vec{r}_i - \vec{r}_j) \right) p_N \right] \\ &= -M_0 b \sum_{i \neq j}^{N} \partial_{x_i} \left[s_i s_j \tau_{ind}(\vec{r}_i - \vec{r}_j) p_N \right]. \end{aligned} \tag{94}$$

It should be noted, that the above equation is mathematically equivalent with the equation of motion of dislocations given by the Eq. (82), its solution can be easily constructed from the solution of Eq. (82). Eq. (94) acts, however, as the "starting" equation of the statistical physics based continuum theory of dislocations.

The result obtained that the thermal noise is often negligible beside the elastic interaction force has an important consequence for the time dependence of the elastic energy $E(t) = V(\vec{r}_1(t), \vec{r}_2(t), ...\vec{r}_N(t))$ of the dislocation system. Let us calculate the rate of energy change:

$$\frac{dE}{dt} = \frac{d}{dt} V(\vec{r}_1(t), \vec{r}_2(t), ...\vec{r}_N(t)) = \sum_{i=1}^{N} \frac{dx_i}{dt} \frac{\partial}{\partial x_i} V(\vec{r}_1, \vec{r}_2, ...\vec{r}_N). \tag{95}$$

From Eq. (88) one obtains

$$\frac{dE}{dt} = -\frac{1}{M_\rho b} \sum_{i=1}^{N} \frac{dx_i}{dt} \frac{dx_i}{dt} \leqslant 0 \tag{96}$$

meaning that the elastic energy of the dislocation system cannot increase during the evolution of the system. So, the dislocation system stacks in the "closest" local energy minimum. Unlike a classical thermal system it cannot leave the local energy minimum by thermal fluctuation (or more precisely, the time needed to overcome an energy barrier is much longer than the elastic relaxation time).

3.2 Coarse-graining

The dislocation density tensor introduced above is a highly singular quantity. It is infinite along the dislocation lines and vanishes elsewhere. More precisely, it is proportional to a delta function along the dislocation lines. The same holds for the dislocation current density. The conservation law (94) guarantees that during the evolution of the dislocation system this delta function does not "spread out", only the shape of the loops can change. This is certainly what we expect physically. This means, if we want to follow the evolution of the system we have to follow the track of each dislocation loop as it is done in DDD simulations.

We may hope, like for many other physical systems, to predict the macroscopic response of the dislocation system, we do not need this detailed knowledge of the evolution of the dislocation configuration. One should try to operate with locally averaged quantities. Locally averaged fields for the dislocation density tensor, stress, dislocation, current density, etc., can be obtained from the “singular” ones by convolving them with a window function. This is commonly called as ”coarse-graining” or “homogenization”.

One can immediately raise the question what is the appropriate function we should use for the shape of the window function, and what determines its half width. There is not a general recipe how to resolve these problems. Nevertheless, we can hope that within certain limits the result obtained by the coarse-graining is not sensitive to the actual window function shape and its width. If this is not the case, this clearly indicates that all the microscopical details are important. So, the coarse-graining procedure always requires extra care. It is important to stress that, before the equations obtained by coarse-graining are applied for a given problem, one always has to study the relevance of the homogenization.

In order to indicate the difficulties, as a simple example (see Groma et al. (2007)), let us consider again a set of parallel edge dislocations with $\pm\vec{b}$ Burgers vectors parallel to the x axis. For this case Eq. (31) simplifies to

$$\nabla^4\chi = \frac{2\mu b}{1-\nu}\partial_y\kappa_d, \tag{97}$$

where $\kappa_d = \rho_{d+} - \rho_{d-}$ is the signed dislocation density that is a sum of delta functions. If we take the convolution of Eq. (97) with a window function $w(\vec{r})$ we obtain that

$$\int w(\vec{r}-\vec{r}')\nabla'^4\chi(\vec{r}')d^2r' = \frac{2\mu b}{1-\nu}\int w(\vec{r}-\vec{r}')\partial y'\kappa_d(\vec{r})d^2r'. \tag{98}$$

After partial integrations we get that

$$\nabla^4\int w(\vec{r}-\vec{r}')\chi(\vec{r}')d^2r' = \frac{2\mu b}{1-\nu}\partial y\int w(\vec{r}-\vec{r}')\kappa_d(\vec{r})d^2r'. \tag{99}$$

As it can be seen, the coarse-grained fields denoted by

$$<\chi>=\int w(\vec{r}-\vec{r}')\chi(\vec{r}')d^2r' \qquad <\kappa>=\int w(\vec{r}-\vec{r}')\kappa_d(\vec{r}')d^2r' \tag{100}$$

are related to each other as

$$\nabla^4<\chi>=\frac{\mu b}{1-\nu}\partial y<\kappa> \tag{101}$$

which is formally equivalent with Eq. (97). With a similar argument, from Eq. (29) one can find that

$$\begin{aligned} <\sigma>_{11} &= -\partial_y\partial_y<\chi>, \\ <\sigma>_{22} &= -\partial_x\partial_x<\chi>, \\ <\sigma>_{12} &= \partial_x\partial_y<\chi>. \end{aligned} \tag{102}$$

We can see, the coarse-grained fields are related to each other as the "discrete" ones.

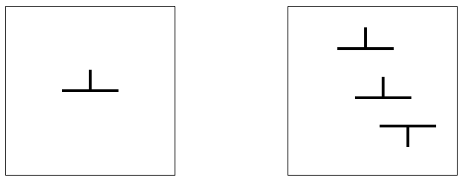


Figure 3. Two strongly different dislocation configurations giving the same κ if they are coarse-grained for the areas indicated by the boxes.

We can see, however, important information is lost during coarse-graining. If we consider two dislocation configurations indicated in Figure 3 and coarse-grain them for the square area indicated by the boxes, we get the same signed dislocation density value. On the other hand, it is obvious that the response of the two configurations are strongly different, if one applies an external shear. So, in a continuum theory of dislocations, in which we operate with smooth fields, the coarse-grained dislocation density tensor is not enough to characterize the state of the system. In the next subsection we discuss how a continuum theory can be derived from the equation of motion of straight parallel dislocations and what relevant quantities are needed to have an appropriate description of this simple dislocation system on the mesoscopic scale.

3.3 Coarse-graining of the equations of motion of dislocations

In order to derive the statistical physics based continuum theory of dislocation we have to link directly the microscale description of the evolution of the dislocation system to a mesoscopic scale where we operate with continuous dislocation density fields. This goal can be achieved by a systematic coarse-graining of the equations of motion of dislocation given by Eq. (82) (Groma (1997); Zaiser et al. (2001); Groma et al. (2003, 2006, 2007, 2010, 2015, 2016); Valdenaire et al. (2016)).

For simplicity let us first assume that each dislocation has the same sign ($s_i = 1$) and the external load is zero (see Groma et al. (2007)). In this case

Eq. (82) reads as

$$\frac{dx_i}{dt} = M_0 \left(\sum_{j=1}^{N} F(\vec{r}_i - \vec{r}_j) \right) \tag{103}$$

with $F = b\tau_{ind}$.

As a first step let us multiply Eq. (103) with $\delta(\vec{r} - \vec{r}_i)$ and take its derivative with respect to x:

$$\partial_x \left\{ \frac{dx_i}{dt} \delta(\vec{r} - \vec{r}_i) \right\} = M_0 \partial_x \left\{ \left(\sum_{j \neq i}^{N} F(\vec{r}_i - \vec{r}_j) \right) \delta(\vec{r} - \vec{r}_i) \right\}, \tag{104}$$

where $\vec{r} = (x, y)$ is an arbitrary point. It is useful to introduce the "discrete" dislocation density

$$\rho_d(\vec{r}) \quad = \quad \sum_{i=1}^{N} \delta(\vec{r} - \vec{r}_i) \tag{105}$$

that is the same as ρ_{d+} defined in subsection 2.3, but since in the present analysis only one type of dislocation is considered, the subscript $+$ is dropped. With this, the summation on the right hand side of Eq. (104) can be replaced by a weighted integral. Furthermore, taking into account that

$$\partial_x \left\{ \frac{dx_i}{dt} \delta(\vec{r} - \vec{r}_i) \right\} = -\frac{dx_i}{dt} \partial_{x_i} \delta(\vec{r} - \vec{r}_i) = -\frac{d}{dt} \delta(\vec{r} - \vec{r}_i), \tag{106}$$

from Eq. (104) we get that

$$\begin{aligned} & -\frac{d}{dt} \delta(\vec{r} - \vec{r}_i) \qquad\qquad (107) \\ &= \quad M_0 \partial_x \left\{ \left(\int F(\vec{r} - \vec{r}')[\rho_d(\vec{r}') - \delta(\vec{r} - \vec{r}')] d^2\vec{r}' \right) \delta(\vec{r} - \vec{r}_i) \right\}, \end{aligned}$$

where $\delta(\vec{r} - \vec{r}')$ beside $\rho_d(\vec{r}')$ is needed to avoid self dislocation interaction. By summing up with respect to i we conclude

$$-\frac{d}{dt} \rho_d(\vec{r}) = M_0 \partial_x \left\{ \left(\int F(\vec{r} - \vec{r}')[\rho_d(\vec{r}') - \delta(\vec{r} - \vec{r}')] d^2\vec{r}' \right) \rho_d(\vec{r}) \right\}, \tag{108}$$

which is a nonlinear strongly non-local equation for the "discrete" dislocation density $\rho_d(\vec{r})$. Like it was done with the field equation (97), to get rid of the singular character of $\rho_d(\vec{r})$ we can coarse-grain Eq. (108). By introducing the coarse-grained quantities

$$\rho_1(\vec{r}) = < \rho_{disc}(\vec{r}) > \tag{109}$$

$$\rho_2(\vec{r}_1, \vec{r}_2) =< \rho_{disc}(\vec{r}_1)\rho_{disc}(\vec{r}_2) - \rho_{disc}(\vec{r}_1)\delta(\vec{r}_1 - \vec{r}_2) >, \tag{110}$$

we get

$$\frac{\partial \rho_1(\vec{r}_1, t)}{\partial t} + \int \partial_{x_1} \left\{\rho_2(\vec{r}_1, \vec{r}_2, t) F(\vec{r}_1 - \vec{r}_2)\right\} d^2 r_2 = 0. \tag{111}$$

The procedure applied above clearly shows that the form of Eq. (111) does not depend on the actual form of the window function applied for the coarse-graining. The densities $\rho_1(\vec{r})$ and $\rho_2(\vec{r}_1, \vec{r}_2)$, however, can certainly depend on $w(\vec{r})$. This is not a problem until we do not assume some relation between $\rho_1(\vec{r})$ and $\rho_2(\vec{r}_1, \vec{r}_2)$. We can say that Eq. (111) is exact but it is not enough to describe the time evolution of the dislocation density because the time derivative of the one particle density $\rho_1(\vec{r})$ depend on the two particle density $\rho_2(\vec{r}_1, \vec{r}_2)$. One can derive equation for $\rho_2(\vec{r}_1, \vec{r}_2)$ but it depends on the 3 particle density function. In general one can obtain a hierarchy of equations where the time derivative of the k particle density depends on the $k + 1$ particle density (see below).

In order to get a closed theory we need a closure approximation. Before we discuss how this can be obtained, the above results have to be generalized for the case where Burgers vector of the dislocations are not the same. The simplest generalization is if we allow that the Burgers vectors of the dislocations can differ in sign (Groma et al. (2007)). This is still a strong simplification of a real dislocation ensemble but an important step forward. Without going into the details with a similar procedure explained above one can find that

$$\begin{aligned} \frac{\partial \rho_+(\vec{r}_1, t)}{\partial t} &= \\ &-M_0 \partial_{x_1} \left[\rho_+(\vec{r}_1) b \tau_{ext} + \int \left\{\rho_{++}(\vec{r}_1, \vec{r}_2) - \rho_{+-}(\vec{r}_1, \vec{r}_2)\right\} F(\vec{r}_1 - \vec{r}_2) d^2 r_2\right] \end{aligned} \tag{112}$$

$$\begin{aligned} \frac{\partial \rho_-(\vec{r}_1, t)}{\partial t} &= \\ &+M_0 \partial_{x_1} \left[\rho_-(\vec{r}_1) b \tau_{ext} - \int \left\{\rho_{--}(\vec{r}_1, \vec{r}_2) - \rho_{-+}(\vec{r}_1, \vec{r}_2)\right\} F(\vec{r}_1 - \vec{r}_2) d^2 r_2\right], \end{aligned} \tag{113}$$

where the subscripts "+" and "-" indicate the sign of the Burgers vector the different density functions are corresponding to. External load is also added. We mention here that the negative signs in front of ρ_{+-} and ρ_{-+} in Eqs. (112) and (113) come from the simple fact that the interaction force acting between dislocations with opposite signs is $-F$.

By adding and substituting the two equations one arrives at:

$$\frac{\partial\rho(\vec{r}_1,t)}{\partial t} \quad +M_0 b\partial_{x_1}[\kappa(\vec{r}_1,t)\tau_{ext} + \int\{\rho_{++}(\vec{r}_1,\vec{r}_2,t) + \rho_{--}(\vec{r}_1,\vec{r}_2,t) \\ -\rho_{+-}(\vec{r}_1,\vec{r}_2,t) - \rho_{-+}(\vec{r}_1,\vec{r}_2,t)\}\tau_{ind}\vec{r}_1 - \vec{r}_2)d^2r_2] = 0, \quad (114)$$

$$\frac{\partial\kappa(\vec{r}_1,t)}{\partial t} \quad +M_0 b\partial_{x_1}[\rho(\vec{r}_1,t)\tau_{ext} + \int\{\rho_{++}(\vec{r}_1,\vec{r}_2,t) - \rho_{--}(\vec{r}_1,\vec{r}_2,t) \\ -\rho_{+-}(\vec{r}_1,\vec{r}_2,t) + \rho_{-+}(\vec{r}_1,\vec{r}_2,t)\}\tau_{ind}(\vec{r}_1 - \vec{r}_2)d^2r_2] = 0, \quad (115)$$

where $\rho(\vec{r},t) = \rho_+(\vec{r},t)+\rho_-(\vec{r},t)$ is the total and $\kappa(\vec{r},t) = \rho_+(\vec{r},t)-\rho_-(\vec{r},t)$ is the signed dislocation density. (κ is the same as $<\kappa>$ introduced in Eq. (100) but to have shorter equations the brackets $< .. >$ were omitted)

3.4 Direct averaging of p_N

Equations (111) derived by the direct coarse-graining of the equations of motion of dislocations can be obtained from the evolution equation of the N particle probability density p_N given by Eq. (94) too (Groma (1997)). For one type of dislocations it reads as

$$\frac{\partial p_N}{\partial t} = -M_0 \sum_{i\neq j}^{N} \partial_{x_i}\left[F(\vec{r}_i - \vec{r}_j)p_N\right]. \quad (116)$$

As it was mentioned earlier for many applications we do not need that detailed description represented by the N particle probability density function. A less detailed description of the system is the k-th order probability density function defined as

$$p_k(\vec{r}_1,\vec{r}_2,..,\vec{r}_k) = \int\int ... \int p_N(t,\vec{r}_1,\vec{r}_2...\vec{r}_N)d^2\vec{r}_{k+1}d^2\vec{r}_{k+2}...d^2\vec{r}_N. \quad (117)$$

After integrating Eq. (116) with respect to the variables $\vec{r}_{k+1},\vec{r}_{k+2},...\vec{r}_N$, from the above definition of p_k (117) we obtain that

$$\frac{\partial p_k}{\partial t} = -M_0 \sum_{i=1}^{N}\sum_{j=1,j\neq i}^{N} \int \partial_{x_i}\left\{p_N F(\vec{r}_i - \vec{r}_j)\right\} d^2\vec{r}_{k+1}d^2\vec{r}_{k+2}...d^2r_N. \quad (118)$$

After a long but straightforward calculation (for details see Groma (1997)) we get that

$$\frac{\partial p_k}{\partial t} + M_0 \sum_{i=1}^{k}\sum_{j=1,j\neq i}^{k} \partial_{x_i}\left\{p_k F(\vec{r}_i - \vec{r}_j)\right\} \quad (119) \\ +(N-k)\int \partial_{x_i}\left\{p_{k+1}F(\vec{r}_i - \vec{r}_{k+1})\right\} d^2\vec{r}_{k+1} = 0.$$

As it can be seen, equation for the k-th order probability distribution function depends on the $k+1$-th order one. So, the reduction procedure applied results in a hierarchy of the equations. In fluid dynamics and plasma physics this is called as BBGKY hierarchy.

For our further consideration the equations for p_1 and p_2 play an important role, so we give their explicit forms (Groma (1997)):

$$\frac{\partial \rho_1(\vec{r}_1, t)}{\partial t} + M_0 \int \partial_{x_1} \{\rho_2(\vec{r}_1, \vec{r}_2, t) F(\vec{r}_1 - \vec{r}_2)\} \, d^2\vec{r}_2 \quad = \quad 0 \qquad (120)$$

and

$$\frac{\partial \rho_2(\vec{r}_1, \vec{r}_2, t)}{\partial t} + (\partial_{x_1} - \partial_{x_2}) \rho_2(\vec{r}_1, \vec{r}_2, t) F(\vec{r}_1 - \vec{r}_2) + \partial_{x_1} \int \rho_3(\vec{r}_1, \vec{r}_2, \vec{r}_3, t) F(\vec{r}_1 - \vec{r}_3) d^2\vec{r}_3 + 1 \leftrightarrow 2 = 0, \qquad (121)$$

where the notations $\rho_1 = Np_1, \rho_2 = N(N-1)p_2, \rho_3 = N(N-1)(N-2)p_3$ were introduced. As it can be seen for ρ_1 Eq. (111) is recovered indicating that the course graining procedure and the averaging method explained here are equivalent.

3.5 Evolution of the plastic shear

Before we discuss how a closed theory can be obtained for the evolution of ρ and κ it is useful to analyze the evolution of plastic shear. For the dislocation geometry considered the only non-vanishing component of the dislocation density tensor is

$$\alpha_{31} = b\kappa. \qquad (122)$$

For the plane problem considered the only component of the plastic distortion contributing to α_{31} is β_{21}^p and

$$b\kappa = -\partial_x \gamma, \qquad (123)$$

where the notation $\gamma = \beta_{21}^p$ commonly used is introduced. Eq. (123) means, to get spatially varying plastic shear one has to introduce dislocations. This is why κ is often called geometrically necessary dislocation (GND) density.

Taking the time derivative of Eq. (123) we get

$$\frac{\partial \kappa}{\partial t} = -\partial_x \dot{\gamma}. \qquad (124)$$

By comparing this with Eq. (115) we obtain an explicit expression for the plastic shear rate $\dot{\gamma}$:

$$\begin{aligned}&\dot{\gamma} = \rho(\vec{r_1})b^2\tau_{ext} \\ &+\int\{\rho_{++}(\vec{r}_1,\vec{r}_2) - \rho_{--}(\vec{r}_1,\vec{r}_2) - \rho_{+-}(\vec{r}_1,\vec{r}_2) \\ &+\rho_{-+}(\vec{r}_1,\vec{r}_2)\}b^2\tau_{ind}(\vec{r}_1 - \vec{r}_2)d\vec{r}_2.\end{aligned} \tag{125}$$

3.6 Self-consistent field approximation

In order to have a closed continuum theory describing the evolution of the dislocation system, the (119) hierarchy of equations has to be cut at some order k. For this, from some considerations independent from the Eq. (119), we have to give how the $k+1$ order density function can be built from the lower order ones. The simplest possible assumption is that the two particle density functions are the products of the one particle density functions (Groma (1997); Groma and Balogh (1999)), i.e.

$$\rho_{ss'}(\vec{r}_1,\vec{r}_2,t) = \rho_s(\vec{r}_1)\rho_{s'}(\vec{r}_2), \quad s,s' \ \in\{+,-\}. \tag{126}$$

This means, dislocation-dislocation correlations are neglected. As it is explained below this leads to a self-consistent field theory. Similar approximation is often used in other fields of physics.

By substituting Eq. (126) into Eqs. (114, 115) we arrive at

$$\frac{\partial\rho(\vec{r},t)}{\partial t} + M_0 b\partial_x[\kappa(\vec{r},t)\{\tau_{sc}(\vec{r},t)+\tau_{ext}\}] = 0, \tag{127}$$

$$\frac{\partial\kappa(\vec{r},t)}{\partial t} + M_0 b\partial_x[\rho(\vec{r},t)\{\tau_{sc}(\vec{r},t)+\tau_{ext}\}] = 0, \tag{128}$$

where

$$\tau_{sc}(\vec{r}) = \int\kappa(\vec{r}_1,t)\tau_{ind}(\vec{r}-\vec{r}_1)d^2r_1 \tag{129}$$

is the shear stress field generated by the coarse-grained signed dislocation density. This is why τ_{sc} is often called as self-consistent or mean stress field. The quantity τ_{sc}, however, is not a "new" quantity. From Eqs. (82-86) one can see that τ_{sc} fulfill the field equations

$$\Delta^2\chi \quad = \quad \frac{2b\mu}{(1-\nu)}\partial_y\kappa(\vec{r}), \qquad \tau_{sc} = \partial_x\partial_y\chi \tag{130}$$

By comparing Eq. (130) with Eqs. (101, 102) we can see that τ_{sc} is nothing but the coarse-grained shear stress $< \sigma >_{12}$.

It is important to note that dislocation multiplication and annihilation can also be taken into account by adding a source term $f(\rho, \tau_{ext} + \tau_{sc}, ...)$ to the right hand side of Eq. (127):

$$\frac{\partial \rho(\vec{r}, t)}{\partial t} + M_0 b \partial_x [\kappa(\vec{r}, t) \{\tau_{sc}(\vec{r}, t) + \tau_{ext}\}] = f(\rho, \tau_{ext} + \tau_{sc}, ...). \tag{131}$$

Determining the actual form of the source term is a difficult issue, that is out of the scope of this paper.

3.7 Dislocation-dislocation correlation

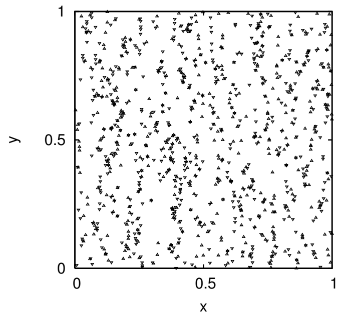
The self-consistent field theory explained above was obtained by assuming that the two particle density functions are the product of the corresponding one particle densities. This means that the probability finding two dislocations at points $\vec{r}_1$ and $\vec{r}_2$ is simple the product of finding one in point $\vec{r}_1$ and another one in point $\vec{r}_2$, i.e. we neglect any effects related to dislocation-dislocation correlation. This is obviously a strong simplification leading to effects not observed experimentally. Just to mention one, the elastic energy of dislocations placed into a box randomly diverges logarithmically with the system size (Zaiser (2013)) resulting that the energy of a dislocation system is not en extensive variable. There is not any experimental evidence indicating this. An appropriate form of dislocation-dislocation correlation, however, can resolve the problem.

Without restricting generality, the two particle density functions can be given in the form:

$$\rho_{ss'}(\vec{r}_1, \vec{r}_2, t) = \rho_s(\vec{r}_1)\rho_{s'}(\vec{r}_2)(1 + d_{ss'}(\vec{r}_1, \vec{r}_2)) \quad s, s' \in \{+, -\}, \tag{132}$$

where $d_{ss'}$ is called dislocation-dislocation correlation function. In order to be able to say something about the correlation function as a first step it is useful to analyze the properties of dislocation-dislocation correlations in an originally homogeneous relaxed dislocation system (Zaiser et al. (2001); Groma et al. (2003)). Although the BBGKY hierarchy (see Eq. (121)) explained earlier gives the possibility to investigate the properties of $d_{ss'}$ analytically (assuming something about the three particle density functions), but due to the complicated nonlinear character of the equations, apart from some simple general statements, it is rather difficult to say anything about $d_{ss'}$.

For initially homogeneous, relaxed dislocation systems $d_{ss'}$ can be determined by solving numerically Eq. (82). Details of the appropriate numerical methods can be found in (Ispánovity et al. (2008)). For determining the correlation functions we do not have to study extremely large systems (about 500 dislocations is already enough), but we need several (around 1000) relaxed configurations to have the necessary statistics. Knowing the relaxed positions of dislocations $d_{ss'}$ can be obtained by simply counting the number of dislocation pairs at different relative positions. In the simulations presented parallel straight edge dislocations were considered at single slip geometry ($\vec{b}$ is parallel to the x axis). The number of dislocations was kept constant. Initially the dislocations were randomly distributed. By the numerical integration of Eq. (82) the relaxed dislocation configuration was determined at zero external stress. Figure 4 shows the correlation function d_{+-} obtained numerically (Zaiser et al. (2001)).



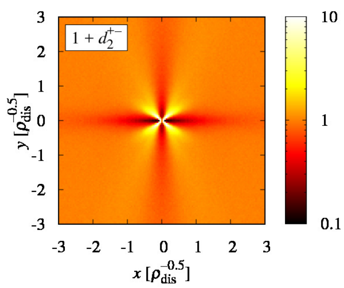


Figure 4. Typical relaxed 2D dislocation configuration (left box) and the d_{+-} dislocation-dislocation correlation function (right box) determined numerically at single slip geometry.

For our considerations the most important properties of the correlation function is that it decays to zero exponentially within a couple of average dislocation spacing. So, for originally random, relaxed dislocation configurations the dislocation-dislocation correlation is short-ranged. With other words, if the distance of two dislocations is larger than a couple of times the average dislocation spacing the correlation between them is negligible (Zaiser et al. (2001); Groma et al. (2003)). We have to keep in mind, however, that this is valid only if the relaxed configuration is obtained from an initially random dislocation distribution. One can obviously set up initial configuration that relaxes to a strongly correlated state like for example a Taylor lattice. The problem is related to the constrained motion of dislocations. Since in the simulations only dislocation glide is allowed and dislocation multiplication is excluded, the number of dislocations in any narrow strip parallel to the Burgers vector cannot change during the relaxation of the system. It is determined by the initial configuration. The system does not "forget" fully the initial configuration. In reality, of course, the number of dislocations in a strip is determined by the dislocation multiplication. Since, however in 2D there is no "natural" law for dislocation multiplication one should investigate the correlation properties in 3D, but there is not any comprehensive result reported so far.

3.8 Local density approximation

Based on the results of the 2D simulations we can state that the dislocation-dislocation correlation functions are short range. So, it is plausible to assume that the correlation functions $d_{ss'}(\vec{r}_1, \vec{r}_2)$ defined by the Eq. (132) can be approximated with the correlation function corresponding to a homogeneous system with dislocation density $\rho(\vec{r}_1)$. It follows that $d_{ss'}(\vec{r}_1, \vec{r}_2)$ practically depends only on $(\vec{r}_1 - \vec{r}_2)$, the direct $\vec{r}_1$ or $\vec{r}_2$ dependence is weak, it appears only through the spatial variation of the dislocation density, i.e.

$$\rho_{ss'}(\vec{r}_1, \vec{r}_2, t) = \rho_s(\vec{r}_1)\rho_{s'}(\vec{r}_2)(1 + d_{ss'}(\vec{r}_1 - \vec{r}_2, \rho(\vec{r}_1)) \quad s, s' \in \{+, -\}, \tag{133}$$

where we indicated that the correlation function certainly depends on the dislocation density. One can certainly raise the question if in $d_{ss'}(\vec{r}_1 - \vec{r}_2, \rho)$ one should take the dislocation density in point $\vec{r}_1$ or $\vec{r}_2$. Assuming, however, that the dislocation density varies slowly in the length scale of dislocation spacing, i. e. $|\nabla\rho| \ll \rho^{3/2}$, it does not make a difference which point is taken. Moreover, we also have to assume that the GND density is much smaller than the total one ($\kappa \ll \rho$) because in general the correlation function can also depend on the GND density too (Groma et al. (2003, 2016)). Similar approximation is used successfully for many other systems like for example in first principle quantum mechanics calculations to estimate the exchange energy. It is called "local density approximation" (see also Zaiser (2015)).

With the two approximations mentioned above the ρ dependence of the correlation function can be directly given from dimensionality argument. Namely, since $d_{ss'}$ cannot directly depend on $\vec{r} = \vec{r}_1 - \vec{r}_2$, a variable with length dimension, it should be normalized by a characteristic length scale of the problem. Since, if the two approximations mentioned above hold there is no other length scale in the problem but the dislocation spacing one concludes that

$$d_{ss'}(\vec{r}, \rho) = d_{ss'}(\sqrt{\rho}\vec{r}). \tag{134}$$

By substituting Eq. (132) into Eqs. (112, 113) one arrives at

$$\partial_t \rho_+(\vec{r}, t) + M_0 b \partial_x \{\rho_+ [\tau_{ext} + \tau_{sc} + \tau_+]\} = 0 \tag{135}$$

$$\partial_t \rho_-(\vec{r}, t) - M_0 b \partial_x \{\rho_- [\tau_{ext} + \tau_{sc} + \tau_-]\} = 0, \tag{136}$$

where $\tau_{sc}(\vec{r})$, given by Eq. (129), is the "self consistent fiels stress" generated by the GND density,

$$\tau_+(\vec{r}) = \int [\rho_+(\vec{r}')d_{++}(\vec{r} - \vec{r}') - \rho_-(\vec{r}')d_{+-}(\vec{r} - \vec{r}')] \, \tau_{ind}(\vec{r} - \vec{r}')d^2r', \tag{137}$$

and

$$\tau_-(\vec{r}) = -\int [\rho_-(\vec{r}')d_{--}(\vec{r} - \vec{r}') - \rho_+(\vec{r}')d_{-+}(\vec{r} - \vec{r}')] \, \tau_{ind}(\vec{r} - \vec{r}')d^2r' \tag{138}$$

are stresses depending on dislocation-dislocation correlations. In these expressions, the first terms in the integrals express the stress contribution due to correlated arrangements of dislocations of the same sign in pile-ups or walls, whereas the second terms express the stress contribution due to the interaction of dislocations of opposite signs forming correlated, dipolar configurations.

For the further considerations let us introduce the quantities

$$\tau_v = \frac{\tau_+ + \tau_-}{2}, \tag{139}$$

$$\tau_a = \frac{\tau_+ - \tau_-}{2}. \tag{140}$$

With these quantities Eqs. (135, 136) read (Groma et al. (2016); Valdenaire et al. (2016))

$$\partial_t \rho_+(\vec{r}, t) + M_0 b \partial_x \{\rho_+ [\tau_{ext} + \tau_{sc} + \tau_v + \tau_a]\} = 0, \tag{141}$$

$$\partial_t \rho_-(\vec{r}, t) - M_0 b \partial_x \{\rho_- [\tau_{ext} + \tau_{sc} + \tau_v - \tau_a]\} = 0. \tag{142}$$

In explicit form τ_v and τ_a are

$$\tau_v(\vec{r}) = \int [\rho(\vec{r}')d_a(\vec{r} - \vec{r}') + \kappa(\vec{r}')d_s(\vec{r} - \vec{r}')] * \tau_{ind}(\vec{r} - \vec{r}')d^2r', \tag{143}$$

$$\tau_a(\vec{r}) = \int [\rho(\vec{r}')d_p(\vec{r} - \vec{r}') + \kappa(\vec{r}')d_{a'}(\vec{r} - \vec{r}')] * \tau_{ind}(\vec{r} - \vec{r}')d^2r', \tag{144}$$

with

$$d_s = \tfrac{1}{2}(d_{++} + d_{--} + d_{+-} + d_{-+}), \tag{145}$$
$$d_p = \tfrac{1}{2}(d_{++} + d_{--} - d_{+-} - d_{-+}), \tag{146}$$
$$d_a = \tfrac{1}{2}(d_{++} - d_{--} - d_{+-} + d_{-+}), \tag{147}$$
$$d_{a'} = \tfrac{1}{2}(d_{++} - d_{--} + d_{+-} - d_{-+}). \tag{148}$$

It is important to summarize some symmetry properties of the pair correlation functions:

- the functions d_{++} and d_{--} must be invariant under a swap of the two dislocations resulting that they are even functions of $\vec{r}$.
- For dislocations with different signs one gets from the definition of correlation functions that $d_{+-}(\vec{r})$=$d_{-+}(-\vec{r})$.
- Hence $d_s(\vec{r})$ and $d_p(\vec{r})$ are even functions, while the difference $d_{+-} - d_{-+}$ appearing in d_a and $d_{a'}$ is an odd function.

It is useful to introduce the notations

$$\tau_f(\vec{r}) = -\int \rho(\vec{r}')d_a(\vec{r}-\vec{r}')\tau_{ind}(\vec{r}-\vec{r}')d^2r' \tag{149}$$

referred to "friction stress" hereafter,

$$\tau_b(\vec{r}) = \int \kappa(\vec{r}')d_s(\vec{r}-\vec{r}')\tau_{ind}(\vec{r}-\vec{r}')d^2r' \tag{150}$$

commonly called "back stress",

$$\tilde{\tau}_b(\vec{r}) = \int \rho(\vec{r}')d_p(\vec{r}-\vec{r}')\tau_{ind}(\vec{r}-\vec{r}')d^2r' \tag{151}$$

called "diffusion stress", and

$$\tilde{\tau}_f(\vec{r}) = \int \kappa(\vec{r}')d_{a'}(\vec{r}-\vec{r}')\tau_{ind}(\vec{r}-\vec{r}')d^2r'. \tag{152}$$

The physical meaning and so the origin of the names of the stress like expressions introduced are discussed later.

Since d_{++} and d_{--} are even functions in Eqs. (149, 152) for nearly homogeneous systems the contribution of the difference $d_{++} - d_{--}$ to $\tau_f(\vec{r})$ and $\tilde{\tau}_f(\vec{r})$ can be neglected resulting in

$$\tilde{\tau}_f(\vec{r}) = \frac{\kappa(\vec{r})}{\rho(\vec{r})}\tau_f(\vec{r}). \tag{153}$$

From Eqs. (143, 144, 153) one obtains

$$\tau_v = -\tau_f + \tau_b \tag{154}$$

and

$$\tau_a = \frac{\kappa}{\rho}\tau_f + \tilde{\tau}_b. \tag{155}$$

After substituting Eqs. (154, 144) into Eqs. (141, 142) we conclude

$$\partial_t \rho_+(\vec{r}, t) = \\ -M_0 b \partial_x \left\{ \rho_+ \left[\tau_{mf} + \tau_b - \left(1 - \frac{\kappa}{\rho}\right) \tau_f + \tilde{\tau}_b \right] \right\} \tag{156}$$

$$\partial_t \rho_-(\vec{r}, t) = \\ +M_0 b \partial_x \left\{ \rho_- \left[\tau_{mf} + \tau_b - \left(1 + \frac{\kappa}{\rho}\right) \tau_f - \tilde{\tau}_b \right] \right\} \tag{157}$$

with $\tau_{mf} = \tau_{ext} + \tau_{sc}$.

By adding and subtracting the above equations one gets

$$\partial_t \rho(\vec{r}, t) = \\ -M_0 b \partial_x \left[\kappa \tau_{mf} + \kappa \tau_b + \rho \tilde{\tau}_b \right] \tag{158}$$

$$\partial_t \kappa(\vec{r}, t) = \\ -M_0 b \partial_x \left[\rho \tau_{mf} + \rho \tau_b - \rho \tau_f + \frac{\kappa^2}{\rho} \tau_f + \kappa \tilde{\tau}_b \right]. \tag{159}$$

As it was discussed above, according to numerical simulations the correlation functions decay to zero within a few dislocation spacing $1/\sqrt{\rho}$. So, in the above expressions for τ_v and τ_a the densities $\rho(\vec{r}')$ and $\kappa(\vec{r}')$ can be approximated by their Taylor expansion around the point $\vec{r}$. For slowly varying dislocation density field we can retain only the lowest-order nonvanishing terms. Since $\tau_{ind}(x, y) = -\tau_{ind}(-x, y)$ and $\tau_{ind}(x, y) = \tau_{ind}(x, -y)$, from the symmetry properties of the correlation functions mentioned above one concludes that up to second order

$$\begin{aligned} \tau_f(\vec{r}) &= -\mu b C \sqrt{\rho(\vec{r})}, \\ C(\tau_{mf}) &= \int d_a^*(\vec{\tilde{r}}) \tau_{ind}^*(\vec{\tilde{r}}) d^2\tilde{r}, \end{aligned} \tag{160}$$

$$\begin{aligned} \tau_b(\vec{r}) &= -Gb \frac{D}{\rho} \partial_x \kappa(\vec{r}), \\ D &= \int \tilde{x} d_s^*(\vec{\tilde{r}}) \tau_{ind}^*(\vec{\tilde{r}}) d^2\tilde{r}, \end{aligned} \tag{161}$$

and

$$
\begin{aligned}
\tilde{\tau}_b(\vec{r}) &= -Gb\frac{A}{\rho}\partial_x\rho(\vec{r}), \\
A &= \int \tilde{x} d_p^*(\vec{\tilde{r}})\tau_{ind}^*(\vec{\tilde{r}})d^2\tilde{r}, \qquad (162)
\end{aligned}
$$

where $\vec{\tilde{r}} = \sqrt{\rho}\vec{r}$, $\tilde{x} = \sqrt{\rho}x$, $d_a^* = \rho d_a$, $d_s^* = \rho d_s$, $d_p^* = \rho d_p$, and $\tau_{ind}^* = \tau_{ind}^*/(\mu b\sqrt{\rho})$ are dimensionless quantities, and $G = \mu/(2\pi(1-\nu))$.

It should be pointed out that in general the correlation functions are stress dependent. As a consequence, the parameters C, D, and A introduced above can depend on the long-range stress τ_{mf}. More precisely, due to dimensionality reasons, parameters may depend on the dimensionless parameter $\tau_{mf}/(\mu b\sqrt{\rho})$. From the symmetry properties of the correlation function we can see that C is an odd, D, and A are even functions of τ_{mf}. As a consequence, at $\tau_{mf} = 0$, C vanishes, while D, and A have finite values and so they can be approximated up to second order in τ_{mf} by constants.

By substituting Eqs. (161, 162) into the evolution equations (158, 158) we arrive at (Groma et al. (2016))

$$
\begin{aligned}
\partial_t\rho &= -M_0 b\partial_x\left\{\kappa\tau_{mf} - GbD\frac{\kappa}{\rho}\partial_x\kappa - GbA\partial_x\rho\right\}, \\
\partial_t\kappa &= -M_0 b\partial_x\left\{\rho\left[\tau_{mf} - \left(1-\frac{\kappa^2}{\rho^2}\right)\tau_f\right]\right. \\
&\qquad \left. -GbD\partial_x\kappa - GbA\frac{\kappa}{\rho}\partial_x\rho\right\}. \qquad (163)
\end{aligned}
$$

To establish the stress dependence of the parameter C we note that from Eqs. (125, 163) an explicit expression for the plastic shear rate in a homogeneous system is given by

$$
\dot{\gamma} = \rho b M_0\left[\tau_{mf} - \left(1-\frac{\kappa^2}{\rho^2}\right)\tau_f\right]. \qquad (164)
$$

If we consider a system without excess dislocations ($\kappa = 0$), such a system exhibits a finite flow stress due to formation of dislocation dipoles or multipoles. For stresses below the flow stress, the strain rate is zero. It must therefore be that

$$
C = \begin{cases} \frac{\alpha}{\mu b\sqrt{\rho}}\tau_{mf}, & |\tau_{mf}| < \tau_{flow} \\ \alpha, & |\tau_{mf}| \geq \tau_{flow}, \end{cases} \qquad (165)
$$

where $\tau_{flow} = \alpha\mu b\sqrt{\rho}$ is the flow stress. In a system where excess dislocations are present, the excess dislocations cannot be pinned by dipole/multipole formation but their effective mobility is strongly reduced. The above argument explains why τ_f is called "friction stress". Below a certain stress level it prevents plastic shear, while above it, τ_f is a stress independent constant with a value of the flow stress.

Concerning τ_b, according to Eq. (161), it is proportional to the gradient of the GND density. Such a term is commonly introduced in phenomenological strain gradient plasticity (SGP) theories to account for size effects and it is termed as "back stress" (Aifantis (1984, 1987, 1994); Fleck and Hutchinson (2001); Gurtin (2002); Svendsen (2002)). There is, however, a major difference between τ_b obtained here and the "back stress" introduced in SGP theories. In SGP theories a length scale considered as material parameter is always introduced to "compensate" the length dimension related to the derivation in the back stress. Here the length scale is the dislocation spacing $1/\sqrt{\rho}$ that is an evolving quantity, and so, it is not a material parameter.

The third stress like quantity related to dislocation-dislocation correlation is $\tilde{\tau}_b$. It acts a diffusion term because it is proportional to the gradient of the total dislocation density. For the first sight its rather unusual feature is that it moves both the positive and negative dislocations in the same direction (see the different signs in Eqs. (156) and (157)), but it simple means, it moves the dislocation dipoles.

4 Phase field approach

In this subsection we show that the evolution equations for the two densities of positive and negative dislocations can be cast into the framework of phase field theories (Groma et al. (2006, 2007, 2010, 2015); Zaiser (2015); Groma et al. (2016)). It should be stressed that the phase field formalism introduced is established on a phenomenological ground, but it leads to the same evolution equations obtained by coarse-graining, so it is justified by that.

For a system of straight parallel edge dislocations with Burgers vectors parallel to the x axis the evolution of dislocation densities ρ_+ and ρ_- is described by the balance equations (Groma et al. (2007, 2015); Dogge et al. (2015))

$$\partial_t \rho_\pm + \partial_x[\rho_\pm v_\pm] = \pm f(\rho_+, \rho_-), \tag{166}$$

in which we consider only dislocation glide. Here $v\pm$ is the glide velocity of positive or negative signed dislocations, and $f(\rho_+, \rho_-)$ is a term accounting for dislocation multiplication or annihilation. Since multiplication terms cannot be derived for 2D systems (straight dislocations cannot multiply) they need to be introduced via ad-hoc assumptions, we assume that the number of dislocations is conserved, i.e., we consider the limit $f(\rho_+, \rho_-) = 0$. In the following we focus on the $\rho_\pm$ dependence of the velocities v_+ and v_-.

In the previous subsections over-damped dislocation motion was considered, i.e. the velocity of the dislocations are proportional to the stress. Keeping this in mind we can assume that $v_\pm$ is also proportional to the stress defined as the functional derivative of P with respect to the elastic deformation

$$\tau = \frac{\delta P}{\delta \gamma^e}. \tag{167}$$

However, as it is discussed above, the dislocation configuration itself does not uniquely define the elastic and plastic distortions while the stress is determined if the dislocation density is given. It follows that P should depend only on the dislocation density. Taking into account that $b\kappa = \partial_x \gamma^e$

$$P[\kappa] = P[\partial_x \gamma^e / b]. \tag{168}$$

From this one find that

$$\tau = \frac{\delta P}{\delta \gamma^e} = -\partial_x \frac{\delta P}{\delta \kappa} \frac{1}{b}. \tag{169}$$

From thermodynamical analogy $\nu_c = \delta P / \delta \kappa$ can be considered as the chemical potential of the dislocation system. So, assuming that $v_\pm \propto \tau$ one gets from Eq. (169)

$$v_\pm \propto -\partial_x \frac{\delta P}{\delta \kappa}, \tag{170}$$

i.e. it is proportional to the negative gradient of the chemical potential. It should be noted, however, that the analogy is somewhat formal because as it is seen above the thermal fluctuation does not play a role in the evolution of the dislocation system.

Since in the system considered there are two types of dislocations the above result has to be generalized (Groma et al. (2016)):

$$v_+ = -M_0 \left\{ \partial_x \left[\frac{1+\zeta}{2} \frac{\delta P}{\delta \rho_+} - \frac{1-\zeta}{2} \frac{\delta P}{\delta \rho_-} \right] \right\}, \tag{171}$$

$$v_- = -M_0 \left\{ \partial_x \left[\frac{1+\zeta}{2} \frac{\delta P}{\delta \rho_-} - \frac{1-\zeta}{2} \frac{\delta P}{\delta \rho_+} \right] \right\}, \tag{172}$$

where $P[\rho_+, \rho_-]$ is the phase field functional and ζ is a parameter. It should be noted that the above form fulfill the symmetry properties that swapping the + and - indexes must not influence the equations. This is expected because it is up to us to define which type of dislocation is considered as positive or negative.

From Eqs. (166, 171, 172) the evolution equations for the dislocation densities derive as

$$\partial_t \rho_+ - \partial_x \left\{ \rho_+ M_0 \left[\partial_x \frac{\delta P}{\delta \kappa} + \zeta \partial_x \frac{\delta P}{\delta \rho} \right] \right\} = 0, \tag{173}$$

$$\partial_t \rho_- + \partial_x \left\{ \rho_- M_0 \left[\partial_x \frac{\delta P}{\delta \kappa} - \zeta \partial_x \frac{\delta P}{\delta \rho} \right] \right\} = 0. \tag{174}$$

Accordingly we find

$$\partial_t \rho = \partial_x \left\{ \kappa M_0 \partial_x \frac{\delta P}{\delta \kappa} + \zeta \rho M_0 \partial_x \frac{\delta P}{\delta \rho} \right\}, \tag{175}$$

$$\partial_t \kappa = \partial_x \left\{ \rho M_0 \partial_x \frac{\delta P}{\delta \kappa} + \zeta \kappa M_0 \partial_x \frac{\delta P}{\delta \rho} \right\}. \tag{176}$$

Concerning the actual form of $P[\rho_+, \rho_-]$ it is useful to split it into two parts, a "mean field" or "self consistent" part P_{sc} and a "correlation" part P_c defined below.

According to Eqs. (43, 51) the equation for the mean field stress τ_{mf} can be obtained from a variational principle. By taking $P_{sc}[\chi, \rho_+, \rho_-]$ in the form

$$P_{sc}[\chi, \rho_+, \rho_-] = \int \left[-\frac{1-\nu}{4\mu} (\triangle \chi)^2 + b \chi \partial_y \kappa \right] d^2 r, \tag{177}$$

the minimum condition

$$\frac{\delta P_{sc}}{\delta \chi} = 0 \tag{178}$$

leads to the equation

$$\frac{1-\nu}{2\mu} \triangle^2 \chi = b \partial_y \kappa, \tag{179}$$

and $\tau_{mf} = \partial_x \partial_y \chi$. The general solution of Eq. (179) is τ_{mf} given by Eq. (129) plus the external stress.

Let us first see what one obtains by substituting Eq. (177) into (172) and (171). After a straightforward calculation one gets

$$\partial_t \rho_+(\vec{r}, t) + M_0 b \partial_x (\rho_+ \tau_{mf}) = 0, \tag{180}$$

$$\partial_t \rho_-(\vec{r}, t) - M_0 b \partial_x (\rho_- \tau_{mf}) = 0. \tag{181}$$

As it is seen P_{sc} recovers the mean field equations (127, 128) but not the terms which are related to dislocation-dislocation correlations. It thus needs to be complemented by a "correlation" part that is in close analogy with the "energy error" introduced by Mesarovic et al. (2010) (see details in Chapter I).

From coarse-graining of the energy of the discrete system one can have some indication how the correlation part should look like (Zaiser (2015)). but the one suggested here for the present dislocation system is rather an educated guess (Groma et al. (2007, 2016)):

$$P_{corr} = \int \left[Gb^2 A\rho \ln\left(\frac{\rho}{\rho_0}\right) + \frac{Gb^2 D}{2}\frac{\kappa^2}{\rho} \right] d^2 r. \tag{182}$$

It is justified by the evolution equations obtained from it.

Since we consider only weakly polarized dislocation arrangements, terms of higher than first order in κ/ρ and $\partial_x \rho/\rho^{3/2}$ can be neglected. With these we find that

$$\partial_t \rho_+ =$$
$$-\partial_x \left[\rho_+ M_0 b \left(\tau_{mf} - Gb\frac{D}{\rho}\partial_x \kappa - Gb\zeta\frac{A}{\rho}\partial_x \rho \right) \right], \tag{183}$$
$$\partial_t \rho_- =$$
$$+\partial_x \left[\rho_- M_0 b \left(\tau_{mf} - Gb\frac{D}{\rho}\partial_x \kappa + Gb\zeta\frac{A}{\rho}\partial_x \rho \right) \right]. \tag{184}$$

From the above equations the evolution equations for κ and ρ read

$$\partial_t \rho = -M_0 b \partial_x \left\{ \kappa\tau_{mf} - GbD\frac{\kappa}{\rho}\partial_x \kappa - GbA\partial_x \rho \right\}, \tag{185}$$

$$\partial_t \kappa = -M_0 b \partial_x \left\{ \rho\tau_{mf} - GbD\partial_x \kappa - GbA\frac{\kappa}{\rho}\partial_x \rho \right\}. \tag{186}$$

With $\zeta = 1$, apart from the term containing the "friction" stress τ_f, Eqs. (185, 186) are equivalent to Eqs. (163, 163). So, by applying the standard formalism of phase field theories, with the appropriate form of the correlation term in the phase field functional, we recover the evolution equations of the dislocation densities derived by ensemble averaging the equations of motion of individual dislocations. However, the friction stress τ_f playing a crucial role in the plastic deformation of any material can not be directly derived from the coarse-grained energy functional.

For resolving this issue we modify Eq. (176) by allowing a non-linear dependency on the driving force $\delta P/\delta\kappa$ (Groma et al. (2016)). The modified equation is given by

$$\partial_t \kappa \quad = \quad \partial_x \left\{ \rho M \left(\partial_x \frac{\delta P}{\delta \kappa} \right) + \kappa M_0 \partial_x \frac{\delta P}{\delta \rho} \right\}, \tag{187}$$

were $M(x)$ is a nontrivial mobility function defined as

$$M(x) = M_0 \begin{cases} \frac{\kappa^2}{\rho^2} x & \text{if } \ |x| < x_0 \\ sgn(x) \left[|x| - x_0 \left(1 - \frac{\kappa^2}{\rho^2} \right) \right] & \text{if } \ |x| \geqq x_0 \end{cases} \tag{188}$$

with $x_0 = \alpha \mu b^2 \sqrt{\rho}$ (see fig.5). It is easy to see that this mobility function

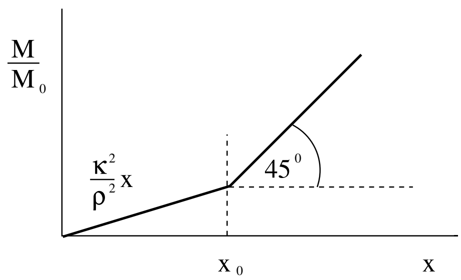


Figure 5. The $M(x)$ mobility function

recovers Eq. (163).

To sum up, it is obtained that the continuum theory of dislocations can be cast into the general framework of a phase field theory. Nevertheless, the phase field theory is different from the ones commonly applied for other problems. Due to the nontrivial on/off type mobility function there are infinite different stationary dislocation states. As the system enters into a state where the total stress (including the back and diffusion stresses) is everywhere below the local flow stress, resulting that the dislocation mobility is zero everywhere, the system stops evolving.

The most important advantage of the phase field formalism explained is that it opens the possibility of a systematic generalization of the theory. Without going into the details we mention that extending the continuum theory into 2D multiple slip is quite straightforward. For the mean field part of the phase field functional one have to replace P_{sc} given by Eq. (177) with the more general form of Eq. (51) with α_{ij} corresponding to the GNDs in the different slip systems. For the P_{corr} correlation part one simple can take the sum of the ones corresponding to each slip systems. It can be generalized by adding appropriate cross terms too. Generalization to 3D is much more difficult. Although there are some promising attempts (see below), there is not a generally accepted one.

5 Dislocation patterning

The continuum theory of dislocations presented can be validated by comparing its predictions with the results of 2D discrete dislocation dynamics simulations. Many direct comparisons indicate that the theory is able to reproduce the most important features of the collective evolution of the 2D dislocation system. For details the reader is refereed to the papers Yefimov et al. (2004); Groma et al. (2006); Dogge et al. (2015). In this paper we discuss a rather important issue only, namely if the continuum theory is able to predict dislocation patterning (Groma et al. (2016)). It is known

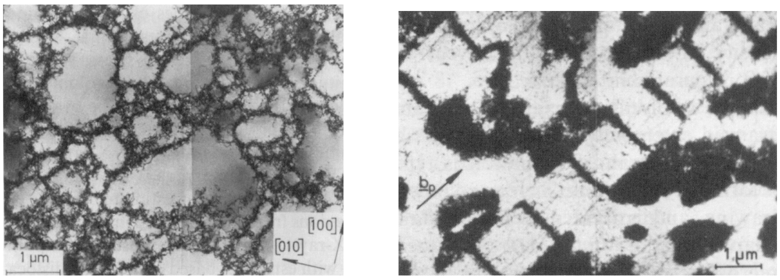


Figure 6. Fractal like cell structure obtained on Cu single crystal deformed by uniaxial tension (left box). The ladder structure developing in fatigued Cu single crystal.

for a long time that the arrangement of dislocations in deformed crystals is practically never homogeneous. During the deformation dislocations arrange themselves into heterogeneous patterns. Two beautiful patterns can be seen on Fig. 6.

There are many different models proposed to predict the pattern formation. Most of them, however, are based on analogies with pattern formation in other physical systems. Thus, it has been suggested that dislocation patterns can be understood as minimizers of some kind of energy functional, because the dislocations try to minimize elastic energy (Hansen and Kuhlmann-Wilsdorf (1986)). On the same line, in analogy with the Cahn Hilliard models of spinodal decomposition, Holt (1970) proposed a theory but some of the predictions of his model have never been observed experimentally. Another idea is that dislocations in a deforming crystal constitute a driven system far from equilibrium where patterns may form as dissipative structures. This has led to the formulation of nonlinear sets of partial differential equations for dislocation densities (Walgraef and Aifantis (1985); Pontes et al. (2006)) giving rise to a variety of different dislocation patterns.

The most important shortcoming of these theories is that it is not clear how they are related to the properties of individual dislocations. So, they are completely phenomenological ones. In the following we show that although it is a rather simplified system the continuum theory derived for 2D single slip is able to predict pattern formation.

5.1 Theory of pattern formation

In the following we discuss under what conditions the evolution equations derived above can lead to instability resulting in dislocation pattern formation (Groma et al. (2016)). One can easily see that the trivial homogeneous solution $\rho = \rho_0$, $\kappa = 0$ and $\tau_{mf} = \tau_0$ satisfies Eqs. (163, 163, 179), where ρ_0 and τ_0 are constants representing the initial dislocation density and the external shear stress, respectively. The stability of the trivial solution can be analyzed by applying the standard method of linear stability analysis. One can easily see that nontrivial behavior can happen only in the flowing regime i.e. if $|\tau_0| > \alpha\mu b\sqrt{\rho_0}$, so we consider only this case.

By adding small perturbations to the dislocation densities and the Airy stress function in the form

$$\begin{aligned} \rho(\vec{r},t) &= \rho + \delta\rho(\vec{r},t) \\ \kappa(\vec{r},t) &= \delta\kappa(\vec{r},t) \\ \chi(\vec{r},t) &= \tau_0 xy + \delta\chi(\vec{r},t) \end{aligned} \tag{189}$$

and keeping only the leading terms in the perturbations, equations (163, 163, 179) become

$$\partial_t \delta\rho = M_0 \partial_x \left[GbA\partial_x \delta\rho - \tau_0 \delta\kappa \right], \tag{190}$$

$$\begin{aligned} \partial_t \delta\kappa = & -M_0 \Theta_f \partial_x \left[\rho_0 \partial_x \partial_y \delta\chi - GbD\partial_x \delta\kappa \right] \\ & -M_0 \Theta_f \left[\tau^* - \alpha\mu b \frac{\sqrt{\rho_0}}{2} \right] \partial_x \delta\rho, \end{aligned} \tag{191}$$

$$\triangle^2 \delta\chi = 4\pi Gb \partial_y \delta\kappa. \tag{192}$$

In these expressions, $\tau^* = \tau_0 - \alpha\mu b\sqrt{\rho_0}$, and the step function $\Theta_f = \Theta(\tau^*)$ is zero if the applied stress is below the flow stress in the homogeneous reference state, and 1 otherwise. To obtain the above equations it was taken into account that the first-order variation of the flow stress is given by

$$\delta\tau_f = \frac{\alpha\mu b\sqrt{\rho_0}}{2}\frac{\delta\rho}{\rho_0}. \tag{193}$$

The solution of Eqs. (192, 190, 191) can be found in the form

$$\begin{pmatrix} \delta\rho \\ \delta\kappa \\ \delta\chi \end{pmatrix} = \begin{pmatrix} \delta\rho_0 \\ \delta\kappa_0 \\ \delta\chi_0 \end{pmatrix} \exp\left(\frac{\lambda}{t_0}t + i\sqrt{\rho_0}\vec{k}\vec{r}\right), \tag{194}$$

were $\vec{k}$ is a dimensionless quantity. After substituting the above form into Eqs. (192, 190, 191) in the flowing regime ($\Theta_f = 1$) one obtains

$$\begin{pmatrix} \lambda + Ak_x^2, & i(\dot{\gamma}' + 2\alpha')k_x \\ i(\dot{\gamma}' - \alpha')k_x, & \lambda + Dk_x^2 + T(\vec{k}) \end{pmatrix} \begin{pmatrix} \delta\rho \\ \delta\kappa \end{pmatrix} = 0, \tag{195}$$

where the notations $t_0 = b^2 G\rho_0/B$, $T(\vec{k}) = 4\pi k_x^2 k_y^2/|\vec{k}|^4$, $\dot{\gamma}' = \tau_*/(Gb\sqrt{\rho_0})$, and $\alpha' = \pi(1-\nu)\alpha$ were introduced. Note that in the above equations each of the parameters are dimensionless and $\dot{\gamma}'$ is proportional to the average shear rate $\dot{\gamma} = M_0 b^2 \rho_0 \tau^*$.

Eq. (195) has nontrivial solutions if

$$(\lambda + Ak_x^2)(\lambda + Dk_x^2 + T(\vec{k})) + k_x^2\beta = 0 \tag{196}$$

with $\beta = (\dot{\gamma}' + 2\alpha')(\dot{\gamma}' - \alpha')$. This leads to

$$\lambda_\pm = -\frac{(A+D)k_x^2 + T(\vec{k})}{2} \pm \frac{\sqrt{[(D+A)k_x^2 + T(\vec{k})]^2 - 4k_x^2[\beta + A(Dk_x^2 + T(\vec{k}))]}}{2}. \tag{197}$$

It follows that the condition for the existence of growing perturbations ($\lambda > 0$) is

$$[\beta + AT(\vec{k}) + ADk_x^2] < 0. \tag{198}$$

$T(\vec{k})$ cannot be negative and it vanishes if $\vec{k}$ is parallel to either the x or to the y axis. Thus, $\beta < 0$ is a necessary and sufficient condition for instability. This condition requires that

- the system is in the flowing phase,
- $\dot{\gamma}'$ must be smaller than α'. In this case there exists a region in the $\vec{k}$ space in which perturbations grow.

Perturbations with wave vectors outside this region decay in time (see figs. 7 and 8).

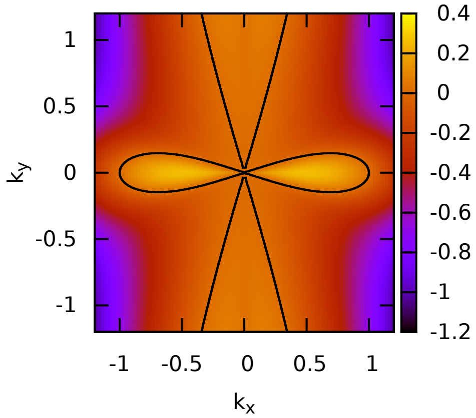


Figure 7. The $\lambda_+(k_x, k_y)$ function at $A = 1$, $D = 1$ and $\beta = -1$. The function is positive within the region marked by the contour line $\lambda_+(k_x, k_y) = 0$.

This results in a length scale selection corresponding to the fastest growing periodic perturbation $\vec{k}_{max}$ defined by the condition

$$\left.\frac{d\lambda_+(\vec{k})}{d\vec{k}}\right|_{\vec{k}_{max}} = 0. \tag{199}$$

For negative β, the $\lambda_+(k_x, k_y)$ function has two equal maxima along the x axis located at

$$k_x^2 = -2\beta\frac{-1 + \sqrt{1 + \frac{(A-D)^2}{4AD}}}{(A-D)^2}.$$

It should be stressed that according to Eq. (194) the actual wave vector of the fastest growing perturbation is $\sqrt{\rho_0}\vec{k}_{max}$. So, in agreement with the

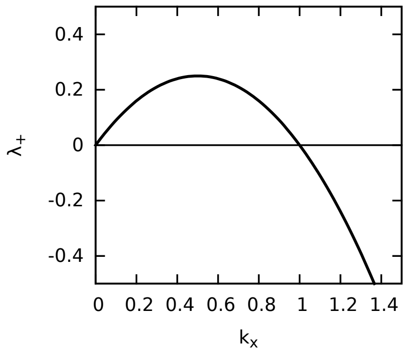


Figure 8. The $\lambda_+(k_x, 0)$ function at $A = 1$, $D = 1$ and $\beta = -1$.

principle of similitude observed experimentally the characteristic pattern wavelength scales with the dislocation spacing $1/\sqrt{\rho_0}$. It is important to note at this point that both the back-stress τ_b and the diffusion-like $\tilde{\tau}_b$ term introduced here play a crucial role in characteristic wavelength selection. If either $A = 0$ or $D = 0$ perturbations of all wave vectors would grow and there would be no mode of maximum growth rate (see Eq. (162)). So we can say that the primary source of instability is the flow stress being proportional to $\sqrt{\rho}$, but for length scale selection observed experimentally we need both the back and the diffusion-like stresses. It should be stressed that in contrast to several earlier models which relate patterning to a particular elementary dislocation mechanism, like cross slip (Xia and El-Azab (2015)), sweeping of dipoles with a moving curved dislocation (Kratochvil and Sedlacek (2003)), etc., the continuum theory predict patterning under rather general conditions. The particular form of dislocation-dislocation correlations are not really important.

6 3D continuum theory

The generalization of the 2D continuum theory to 3D is far from straightforward. The key issue is that a dislocation loop is an extended object in space while a continuum theory operates with local fields. So, first we have to find the appropriate quantities the continuum theory should operate with.

A dislocation loop can be given by the parametric equation $\vec{r}(s)$, where s is a scalar varying in a given interval. Since $\vec{r}(s)$ is extended in space, it is difficult to work with it in statistical sense. An equivalent description of the loop is the Taylor expansion of $\vec{r}(s)$ around a point s_o

$$\vec{r}(s) = \vec{r}(s_0) + \left.\frac{d\vec{r}}{ds}\right|_{s_0}(s - s_o) + \frac{1}{2}\left.\frac{d^2\vec{r}}{ds^2}\right|_{s_0}(s - s_o)^2 + ..., \tag{200}$$

where derivatives are local quantities. Since, however they depend on the actual form of parametrization of the loop, one should use quantities related to the derivatives but independent of the parametrization. These are the tangent $\vec{l}$, the curvature k (for simplicity we consider only planar loops), and quantities corresponding to higher derivatives (denoted by $\{\zeta_i\}$). With these, the p probability density of finding the dislocation network in a give state can be given as a function of $\vec{r}$, $\vec{l}$, k, and $\{\zeta_i\}$. The probability $p(\vec{r}, \vec{l}, k, \{\zeta_i\})$ is a "local" function. In this section 3 different approaches operating with certain mean values of $p(\vec{r}, \vec{l}, k, \{\zeta_i\})$ are shortly summarized.

6.1 Mean field theory

Recently Xia and El-Azab (2015) have suggested a mean field approach for the time evolution of the the vector field $\vec{\rho}(\vec{r}) = \rho_a(\vec{r})\vec{l}_a(\vec{r})$ where

$$\rho_a(\vec{r}) = N\int p(\vec{r}, \vec{l}, k, \{\zeta_i\})d\vec{l}dkd\zeta_i, \tag{201}$$

and

$$\vec{l}_a(\vec{r}) = \int \vec{l}p(\vec{r}, \vec{l}, k, \{\zeta_i\})d\vec{l}dkd\zeta_i, \tag{202}$$

with N denoting the number of dislocation loops.

According to Eq. (9) in this case the dislocation density tensor is

$$\alpha_{ij} = \rho_i b_j. \tag{203}$$

If we neglect the correlation between dislocation loops (mean field approximation) according to Eqs. (76, 78)

$$\dot{\alpha}_{ij} = -e_{ikl}\partial_k\dot{\beta}^p_{lj}, \tag{204}$$

and

$$\dot{\beta}^p_{ij} = -e_{ikl}u_k\alpha_{lj}, \tag{205}$$

where $\vec{u}(\vec{r})$ is the mean velocity of the dislocations at point $\vec{r}$. It has to be noted here that in general for a discrete dislocation system the mean value of $u_l\alpha_{ij}$ is not the product of the mean value of u_l and α_{ij}. In order to get Eq. (205) the dislocation-dislocation correlations have to be neglected. By combining Eqs. (203,204,205) one arrives at the evolution equation

$$\dot{\rho}_i b_j = e_{ipn}\partial_p(e_{nmk}u_m\rho_k b_j). \tag{206}$$

For getting a closed set of equation Xia and El-Azab (2015) assumed an over-damped dislocation motion with dislocation velocity proportional to the local shear stress generated by α_{ij}.

By the numerical solution of the evolution equation given above Xia and El-Azab (2015) have obtained a modulation on the dislocation density field. Interestingly by allowing dislocation cross slip introduced by a probabilistic rule they have found a clear tendency for dislocation cell formation.

6.2 Hydrodynamics approach

In the approach proposed by Kratochvil and Sedlacek (2003) the state of the material is also described by the density $\rho_a(\vec{r},t)$, $\vec{l}_a$, and the velocity $\vec{u}(\vec{r},t)$ fields, but $\rho_a(\vec{r},t)$ and $\vec{l}_a$ are assumed to evolve separately. Since $\vec{l}_a$ is a unite vector the angle β defined by the relation $\vec{l}_a = (\cos(\beta), \sin(\beta))$ is convenient to introduced.

For the sake of simplicity we assumed that all dislocation loops have the same Burgers vector and their slip planes are parallel.Taking the z axis perpendicular to the slip plane of the loops, the two nonvanishing components of the dislocation density tensor are

$$\alpha_{11} = b\rho\cos(\beta), \qquad \alpha_{21} = b\rho\sin(\beta). \tag{207}$$

Since the dislocation density tensor is the curl of the plastic distortion, it has to be div free:

$$\frac{\partial \alpha_{ij}}{\partial r_i} = 0. \tag{208}$$

One can find from Eqs(207,208) that ρ and β have to satisfy the conservation law

$$\frac{\partial \rho\cos(\beta)}{\partial x} + \frac{\partial \rho\sin(\beta)}{\partial y} = 0. \tag{209}$$

On the other hand, from the general expression of the evolution of the dislocation density tensor given by Eq. (75),the following evolution equations can be deduced for α and β fields(for details see Kratochvil and Sedlacek

(2003))

$$\rho\dot{\beta} = \cos(\beta)\frac{\partial \rho u}{\partial x} + \sin(\beta)\frac{\partial \rho u}{\partial y},$$
$$\dot{\rho} = \sin(\beta)\frac{\partial \rho u}{\partial x} - \cos(\beta)\frac{\partial \rho u}{\partial y}, \tag{210}$$

where $u = |\vec{u}|$.

To have a closed theory a constitutive relation is needed between the three fields $\rho(\vec{r},t)$, $\beta(\vec{r},t)$ and $u(\vec{r},t)$. Kratochvil and Sedlacek (2003) suggested the following constitutive relation for the velocity field :

$$Bu = \begin{cases} b\sigma_{13} + C\kappa_s - b\tau_0 - b\tau & if \quad b\sigma_{13} + C\kappa_s > b\tau_0 + b\tau \\ 0 & if \quad |b\sigma_{13} + C\kappa_s| < b\tau_0 + b\tau \\ b\sigma_{13} + C\kappa_s + b\tau_0 + b\tau & if \quad b\sigma_{13} + C\kappa_s < -b\tau_0 - b\tau \end{cases} \tag{211}$$

where $b\sigma_{13}$ is the Peach-Koehler force due to the local shear stress, $C\kappa_s$ is the self-force, $b\tau_0$ is the friction force, and $b\tau$ represents the interaction between the gliding dislocations an the dislocation loops.

The self-force $C\kappa_s$ is considered in the line tension approximation, where κ_s is the dislocation line tension. The curvature of a dislocation segment $C(\vec{r},\beta,t) = -\ \mathrm{div}\vec{n}$, where $\vec{n}$ is the unit normal to the dislocation segment. As it is explained in details in Kratochvil and Sedlacek (2003) C can be approximated by the expression

$$C = \cos(\beta)\frac{\partial \beta}{\partial x} + \sin(\beta)\frac{\partial \beta}{\partial y} \tag{212}$$

The most difficult problem is to set up an appropriate expression for $b\tau$. For this Kratochvil and Sedlacek (2003) suggested that

$$b\tau = Fc^{1/3} \tag{213}$$

were c is the loop density, and F is a constant.

According to detailed analytical and numerical investigations Kratochvil and Sedlacek (2003) the model explained above is able to predict both dislocation patterning and size effect. Nevertheless, the justification of the assumptions used requires further investigation.

6.3 General continuum theory in 3D

Hochrainer et al. (2007, 2014) have taken a more generalized approach. They have considered the quantities

$$\rho_a(\vec{r},\vec{l}) = N\int p(\vec{r},\vec{l},k,\{\zeta_i\})dkd\zeta_i, \tag{214}$$

and mean value of the local curvature

$$k_a(\vec{r}, \vec{l}) = \int kp(\vec{r}, \vec{l}, k, \{\zeta_i\}) dk d\zeta_i, \tag{215}$$

depending on the position $\vec{r}$ and the local tangent $\vec{l}$. With these they have moved to a higher, 3+2 dimension $(\vec{r}, \varphi, \theta)$ where φ and θ are the polar and azimuthal angles of $\vec{l}$. For plane problems (corresponding to $\theta = 0$) they have introduced the generalized nabla operator

$$\hat{\bigtriangledown} = \rho_a(\vec{r}, \varphi) + \partial_\varphi, \tag{216}$$

the 5D line direction

$$L(\vec{r}, \varphi) = (\cos(\varphi), \sin(\varphi), 0, k_a(\vec{r}, \varphi)) \tag{217}$$

and the 5D velocity vector

$$V(\vec{r}, \varphi) = (v_1, v_2, 0, - \bigtriangledown_L v) \tag{218}$$

with the 3D vector field perpendicular to the line direction

$$\vec{v} = (v_1, v_2, 0) = v(\vec{r}, \varphi)(\sin(\varphi), -\cos(\varphi), 0) \tag{219}$$

From the continuity of the dislocation line they derived the evolution equations for ρ_a and $q = \rho_a k_a$

$$\partial_t \rho_a = -\hat{\bigtriangledown}(\rho_a V) + qv \tag{220}$$

$$\partial_t q = -\hat{\bigtriangledown}(q_a V) - \rho \hat{\bigtriangledown}_L \hat{\bigtriangledown}_L v \tag{221}$$

The two equations, given above, however, do not form a closed set of equations, because they depend on the unknown velocity v. They represent only the "kinematics" of the dislocation evolution. In spite of some promising attempts (Hochrainer (2016)) at the moment it is not really developed how v should depend on the ρ_a and q fields. The issue require further investigations.

In summary it can be stated that, in spite of the large amount of excellent works carried out on the problem, the 3D continuum theory of dislocations is not completely developed. It still remains a challenge to establish it.

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