

## Link between the microscopic and mesoscopic length-scale description of the collective behavior of dislocations

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For describing the dislocation pattern formation, two different approaches are applied. In one of them the collective behavior of many individual dislocations is investigated by analytical or numerical methods, in the other one the dislocation system is described by continuous functions of the space coordinates. A method is proposed for establishing the link between the two length scales. Starting from the exact evaluation equation of the  $N$ -dislocation distribution function, a hierarchy of equations is derived for the one-, two-, three-, etc., particle distribution functions. Although the dislocations form a nonconservative system, the applied method is similar to the derivation of the so called BBGKY hierarchy which is frequently used in plasma physics. By assuming that the three-particle correlation function is negligible a closed set of equations can be obtained for the dislocation density and the two-particle correlation functions. The possible origin of appearance of dislocation patterns is also investigated. [S0163-1829(97)04134-9]

### INTRODUCTION

Currently one of the biggest challenges in dislocation theory is the understanding of the dislocation pattern formation. Although a huge amount of experimental results has been collected since the first dislocation was observed in an electron microscope more than 40 years ago, and there are several promising theoretical models of this typically self-organizational phenomena (for a broad overview of the field see Refs. 1 and 2), we are still far from its complete understanding. It is still not clear what the necessary input is which has to be introduced into a model for observing the occurrence of inhomogeneous dislocation distribution. The models developed so far can be sorted into two groups, the individual dislocation, and the continuum descriptions. In the first one the properties of individual dislocations are considered and the collective behavior of this assembly is investigated. Beside the analytical ones, this group includes the two-dimensional (2D) (Refs. 3–14) and 3D (Refs. 15–17) computer simulations.

Due to the long-range interaction of dislocations only a few thousand dislocations<sup>12</sup> can be modeled in 2D computer simulations, in 3D Cellular Automata models a few tens of thousand of short (about 100 nm) (Refs. 15 and 16) dislocation segments can be allowed, so the macroscopic properties can be investigated in a very limited way. In spite of this limitation the simulations are able to reproduce several important features of crystal plasticity.

Another possible approach is when the system is described by a few continuous variables, like the dislocation density, internal stress, etc. These models are often referred to as continuum models. Their common feature is that the dynamics of the system is determined by coupled balance equations of the introduced variables.

The existing continuum models can be summarized as follows: the so-called low-energy dislocation structure<sup>18–20</sup> (LEDS) approach proposed by Kulhman-Wilsdorf applies thermodynamical analogy by searching for dislocation con-

figuration of minimal elastic energy under given constraints. According to this concept dislocation pattern formation, like the development of cellular structure in unidirectional deformation or persistent slip band forming under periodical loading is driven by the reduction of the system energy. This essentially static description was improved by Holt<sup>21</sup> by introducing dynamics into the model. He adopted the method applied for the equilibrium thermodynamical description of nonuniform systems by setting up the following conservation law for the dislocation density,  $\rho$ :

$$\frac{\partial \rho}{\partial t} - \text{div} B \Delta \delta E_{\text{int}}(\rho) = 0, \quad (1)$$

where  $\delta E_{\text{int}}(\delta \rho)$  is the elastic energy change due to the dislocation density fluctuation  $\delta \rho$ , and  $B$  the dislocation mobility. In a similar way as is done in the theory of spinodal decomposition, he approximated the  $\delta E_{\text{int}}(\delta \rho)$  functional by a second-order Taylor expansion. Because of the appearance of the space derivative in this approximation a length parameter is automatically introduced which in Holt's model is taken proportional to the average dislocation distance,  $l = 1/\sqrt{\rho}$ . This leads to the appearance of dislocation density modulation with a wavelength which is also proportional to  $l$ .

The continuum model developed by Walgreaf and Aifantis<sup>22–27</sup> adopts the concept of the theory of oscillatory chemical reactions which is a strongly nonequilibrium approach. It describes the system with two variables, the mobile and the immobile dislocation density. The dynamics of the system is determined by diffusion terms and reaction terms. The latter include mobile dislocation generation from immobile ones, mobile dislocation trapping, immobile dislocation formation from sources, annihilation, and in some cases local interaction with other fields like solute atom concentration. The actual form of these terms depends on the deformation mode and geometry. In a certain range of the input parameters the model predicts the appearance of pat-

tern formation. Numerical investigation of the properties of this model have been carried out by Schiller *et al.*<sup>28</sup> and Glazov *et al.*<sup>29</sup>

The model proposed by Kratochvil and his co-workers<sup>30–36</sup> has a number of similarities with the reaction-diffusion model. It considers the interaction between gliding dislocation and dislocation dipoles. The interaction is created through the inhomogeneous stress field of the curved gliding dislocations, the curvature is due to the blocking of the gliding dislocations at dipole branches. Besides this, terms accounting for dislocation creation and annihilation are added. These also lead to inhomogeneous dislocation distribution.

In a series of recent papers Hähner<sup>37–39</sup> introduced the stochastic dislocation dynamics. It takes into account the stress field created by the dislocations as a random background. This is coupled to the fluctuating strain rate with relation similar to the ones known from the fluctuation dissipation theory of statistical mechanics. From the analysis of the corresponding Fokker-Planck equation he arrives at the possibility of structural transition in the dislocation system.

Although each model outlined above has its merit, their major common disadvantage is that the actual forms of the terms in the equations are based on several *ad hoc* assumptions which are difficult to prove from the properties of individual dislocations. On the other hand, none of them really takes into account the long-range natures and the spatial angular dependence of the interaction force between dislocations. The aim of this paper is to investigate the consequences of the precise form of dislocation interaction. Starting from the equations of motion of individual dislocations a continuum description is constructed. On the basis of this in the simplest so-called self-consistent field approximation the stability of the homogeneous dislocation distribution is investigated.

### CONSTRUCTION OF THE HIERARCHY OF EQUATIONS OF DIFFERENT ORDER DISTRIBUTION FUNCTIONS

Let us consider a system of  $N$  parallel straight edge dislocations. This is obviously a strong simplification of the real 3D dislocation networks which develop during the plastic deformation of the crystals, but in single slip configuration and in the regime of small strain it is a reasonable approximation. It reduces the 3D problem to 2D, which is certainly much easier to deal with. For obtaining the general structure of the equations which describe the behavior of the system, in the first part of the paper we suppose that each dislocation has the same Burgers vector  $\vec{b}$ . This is just for reducing the complexity of the expressions, later on we will allow for dislocations having opposite Burgers vectors in the system. Also for the sake of simplicity, in the first part dislocation creation and annihilation are excluded, i.e., the number of dislocations is conserved.

Because of the dissipative nature of dislocation motion, for setting up the equations of motion of dislocations, besides the force acting on a dislocation due to the elastic field, a friction force has to be taken into account. A frequently applied approximation is that the friction force is proportional to the velocity of a dislocation.<sup>11</sup> Since, in the case of a low deformation rate the inertia term can be neglected be-

sides the friction force, the equation of motion of a dislocation is only a first-order differential equation.

Let us denote the positions of dislocations in the  $xy$  plane by  $\{\vec{r}_i, i = 1 \cdot N\}$ . With the above approximations the velocity of the  $i$ th dislocation,  $\vec{v}_i$  can be given as

$$\vec{v}_i = B \left( \sum_{j \neq i}^N \vec{F}(\vec{r}_i - \vec{r}_j) + F_{\text{ext}} \right), \quad (2)$$

where  $\vec{F}$  is the elastic interaction force between two dislocations,  $\vec{F}_{\text{ext}}$  is the external force, and  $B$  is the dislocation mobility. This is the system of equations which is solved numerically in most of the 2D computer simulations.<sup>3–6,8,9,11–14</sup>

As it is well known, in statistical mechanics instead of describing the system with the coordinates of the  $N$  particles in the phase space, one can obtain precisely the same information from the  $N$  particle distribution function  $f_N$ . Although the dislocations form a nonconservative system, the method applied in statistical mechanics can be generalized for straight parallel dislocations. Since Eq. (2) is a first-order equation and the problem is two dimensional, the  $N$ -particle distribution function,  $f_N$ , is a  $2N$ -dimensional function of the space coordinates. According to the usual definition of  $f_N$  the probability of finding the  $N$  dislocations in the  $d\vec{r}_1, d\vec{r}_2, \dots, d\vec{r}_N$  vicinity of the points  $\vec{r}_1, \vec{r}_2 \dots \vec{r}_N$  at the moment  $t$  is  $f_N(t, \vec{r}_1, \vec{r}_2 \dots \vec{r}_N) d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_N$ . Due to the assumed conservation of the dislocation number,  $f_N$  has to fulfill the relation

$$\begin{aligned} f_N(t, \vec{r}_1, \vec{r}_2 \dots \vec{r}_N) d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_N \\ = f_N(t + \Delta t, \vec{r}_1 + \vec{v}_1 \Delta t, \vec{r}_2 + \vec{v}_2 \Delta t \dots \vec{r}_N + \vec{v}_N \Delta t) \\ \times d(\vec{r}_1 + \vec{v}_1 \Delta t) d(\vec{r}_2 + \vec{v}_2 \Delta t) \dots d(\vec{r}_N + \vec{v}_N \Delta t). \end{aligned} \quad (3)$$

It is interesting to note that in contrast with conservative systems

$$\begin{aligned} f_N(t, \vec{r}_1, \vec{r}_2 \dots \vec{r}_N) \\ \neq f_N(t + \Delta t, \vec{r}_1 + \vec{v}_1 \Delta t, \vec{r}_2 + \vec{v}_2 \Delta t \dots \vec{r}_N + \vec{v}_N \Delta t) \end{aligned} \quad (4)$$

because the volume  $d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_N$  is not conserved during the motion of dislocations. From Eq. (3) one gets that

$$\frac{\partial f_N}{\partial t} + \sum_{i=1}^N \frac{\partial}{\partial \vec{r}_i} \{f_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \vec{v}_i\} = 0. \quad (5)$$

Replacing  $\vec{v}_i$  by expression (2) in Eq. (5) we obtain that

$$\frac{\partial f_N}{\partial t} + \sum_{i \neq j}^N \frac{\partial}{\partial \vec{r}_i} \{f_N \vec{F}(\vec{r}_i - \vec{r}_j)\} = 0. \quad (6)$$

$B$  is eliminated from the above equation by a  $t \rightarrow Bt$  variable substitution, and for the sake of simplicity the external force  $\vec{F}_{\text{ext}}$  is taken to be zero.

Since Eqs. (2) and (6) are equivalent descriptions of the dislocation system, finding the solution of Eq. (6) is equally difficult as getting the solution of Eq. (2). However, in most cases in order to obtain the average properties of the dislocation assembly we do not need such a detailed picture about its evolution. A less detailed description of the system may be given by introducing the  $k$  order distribution function

$$f_k(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_k) = \int \int \dots \int f_N(t, \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \times d\vec{r}_{k+1} d\vec{r}_{k+2} \dots d\vec{r}_N. \quad (7)$$

By integrating Eq. (6) over the  $\vec{r}_{k+1}, \vec{r}_{k+2}, \dots, \vec{r}_N$  subspace and using definition (7) of  $f_k$ , one finds that

$$\frac{\partial f_k}{\partial t} = - \sum_{i=1}^N \sum_{j=1, j \neq i}^N \int \frac{\partial}{\partial \vec{r}_i} \{f_N \vec{F}(\vec{r}_i - \vec{r}_j)\} \times d\vec{r}_{k+1} d\vec{r}_{k+2} \dots d\vec{r}_N. \quad (8)$$

The double sum on the right-hand side of Eq. (8) can be split into three sums:

$$\begin{aligned} \sum_{i=1}^N \sum_{j=1, j \neq i}^N \int \frac{\partial}{\partial \vec{r}_i} \{f_N \vec{F}(\vec{r}_i - \vec{r}_j)\} d\vec{r}_{k+1} d\vec{r}_{k+2} \dots d\vec{r}_N &= \sum_{i=1}^k \sum_{j=1, j \neq i}^k \int \frac{\partial}{\partial \vec{r}_i} \{f_k \vec{F}(\vec{r}_i - \vec{r}_j)\} \\ &+ \sum_{i=1}^k \sum_{j=k+1}^N \int \frac{\partial}{\partial \vec{r}_i} \{f_N \vec{F}(\vec{r}_i - \vec{r}_j)\} d\vec{r}_{k+1} d\vec{r}_{k+2} \dots d\vec{r}_N \\ &+ \sum_{i=k+1}^N \sum_{j=1, j \neq i}^N \int \frac{\partial}{\partial \vec{r}_i} \{f_N \vec{F}(\vec{r}_i - \vec{r}_j)\} d\vec{r}_{k+1} d\vec{r}_{k+2} \dots d\vec{r}_N. \end{aligned} \quad (9)$$

The last term is an integral of a divergence, so it can be substituted by an integral over the system surface, which gives zero because the distribution functions are supposed to go to zero fast enough at infinity. Taking into account that  $f_N$  has to be invariant for swapping two dislocation coordinates we get that the  $k$ th-order distribution function fulfills the relation

$$\frac{\partial f_k}{\partial t} + \sum_{i=1}^k \sum_{j=1, j \neq i}^k \int \frac{\partial}{\partial \vec{r}_i} \{f_k \vec{F}(\vec{r}_i - \vec{r}_j)\} + (N-k) \int \frac{\partial}{\partial \vec{r}_i} \{f_{k+1} \vec{F}(\vec{r}_i - \vec{r}_{k+1})\} d\vec{r}_{k+1} = 0. \quad (10)$$

As it can be seen from Eq. (10), the equation of the  $k$ th-order distribution function contains an integral of the one order higher distribution function. So, the applied reduction gives a hierarchy for the reduced distribution functions, where each function is coupled to the one above it in the series. This is a similar construction to what is called BBGKY hierarchy in hydrodynamics and plasma physics.<sup>40</sup>

Since most measurable quantities can be expressed in terms of functions  $f_1$  and  $f_2$  let us write down the equations for the first two distribution functions:

$$\frac{\partial \rho_1(\vec{r}_1, t)}{\partial t} + \int \frac{\partial}{\partial \vec{r}_1} \{\rho_2(\vec{r}_1, \vec{r}_2, t) \vec{F}(\vec{r}_1 - \vec{r}_2)\} d\vec{r}_2 = 0 \quad (11)$$

and

$$\frac{\partial \rho_2(\vec{r}_1, \vec{r}_2, t)}{\partial t} + \left( \frac{\partial}{\partial \vec{r}_1} - \frac{\partial}{\partial \vec{r}_2} \right) \rho_2(\vec{r}_1, \vec{r}_2, t) \vec{F}(\vec{r}_1 - \vec{r}_2) + \frac{\partial}{\partial \vec{r}_1} \int \rho_3(\vec{r}_1, \vec{r}_2, \vec{r}_3, t) \vec{F}(\vec{r}_1 - \vec{r}_3) d\vec{r}_3 + 1 \leftrightarrow 2 = 0, \quad (12)$$

where for obtaining formulas independent from the system size the  $\rho_1 = N f_1, \rho_2 = N(N-1) f_2, \rho_3 = N(N-1)(N-2) f_3$  one-, two-, and three-particle density distribution functions were introduced. The symbol  $1 \leftrightarrow 2$  indicates a similar term as the previous one with swapped indexes.

As in statistical mechanics these density functions can be expressed by a form known as the Mayer cluster expansion:<sup>40</sup>

$$\rho_1(\vec{r}_1) = \rho_1(\vec{r}_1), \quad (13)$$

$$\rho_2(\vec{r}_1, \vec{r}_2) = \rho_1(\vec{r}_1) \rho_1(\vec{r}_2) + D(\vec{r}_1, \vec{r}_2), \quad (14)$$

$$\rho_3(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \rho_1(\vec{r}_1) \rho_1(\vec{r}_1) \rho_1(\vec{r}_1) + \rho_1(\vec{r}_1) D(\vec{r}_2, \vec{r}_3) + \rho_1(\vec{r}_2) D(\vec{r}_3, \vec{r}_1) + \rho_1(\vec{r}_3) D(\vec{r}_2, \vec{r}_1) + T(\vec{r}_1, \vec{r}_2, \vec{r}_3). \quad (15)$$

Clearly, the functions  $D(\vec{r}_1, \vec{r}_2)$  and  $T(\vec{r}_1, \vec{r}_2, \vec{r}_3)$  describe two- and three-particle correlations, respectively. With these notations Eqs. (11) and (12) have the forms

$$\frac{\partial \rho_1(\vec{r}_1, t)}{\partial t} + \frac{\partial}{\partial \vec{r}_1} \rho_1(\vec{r}_1, t) \int \rho_1(\vec{r}_2, t) \vec{F}(\vec{r}_1 - \vec{r}_2) d\vec{r}_2 + \int \frac{\partial}{\partial \vec{r}_1} D(\vec{r}_1, \vec{r}_2, t) \vec{F}(\vec{r}_1 - \vec{r}_2) d\vec{r}_2 = 0 \quad (16)$$

and

$$\begin{aligned} & \frac{\partial D(\vec{r}_1, \vec{r}_2, t)}{\partial t} + \left( \frac{\partial}{\partial \vec{r}_1} - \frac{\partial}{\partial \vec{r}_2} \right) \rho_1(\vec{r}_1, t) \rho_1(\vec{r}_2, t) \vec{F}(\vec{r}_1 - \vec{r}_2) + \left( \frac{\partial}{\partial \vec{r}_1} - \frac{\partial}{\partial \vec{r}_2} \right) D(\vec{r}_1, \vec{r}_2, t) \vec{F}(\vec{r}_1 - \vec{r}_2) \\ & + \frac{\partial}{\partial \vec{r}_1} \int \rho_1(\vec{r}_2, t) D(\vec{r}_3, \vec{r}_1, t) \vec{F}(\vec{r}_1 - \vec{r}_3) d\vec{r}_3 + 1 \leftrightarrow 2 + \frac{\partial}{\partial \vec{r}_1} \int \rho_1(\vec{r}_3, t) D(\vec{r}_2, \vec{r}_1, t) \vec{F}(\vec{r}_1 - \vec{r}_3) d\vec{r}_3 + 1 \leftrightarrow 2 \\ & + \frac{\partial \rho_1(\vec{r}_1)}{\partial \vec{r}_1} \int [\rho_1(\vec{r}_2) \rho_1(\vec{r}_3) + D(\vec{r}_2, \vec{r}_3, t)] \vec{F}(\vec{r}_1 - \vec{r}_3) d\vec{r}_3 + 1 \leftrightarrow 2 + \frac{\partial}{\partial \vec{r}_1} \int T(\vec{r}_1, \vec{r}_2, \vec{r}_3, t) \vec{F}(\vec{r}_1 - \vec{r}_3) d\vec{r}_3 + 1 \leftrightarrow 2 = 0. \end{aligned} \quad (17)$$

In order to get expression (17), Eq. (16) was used to eliminate some terms.

If the system is not far from the homogeneous one, i.e., the system is ‘‘dilute,’’ one may expect that  $D$  and  $T$  are considerably smaller than the other terms in the corresponding expressions (14) and (15). This cannot be proved directly, but as a first step one can close the equation chain (10) by neglecting  $D$  than as a second step by neglecting only  $T$ , and so on. In this way the influence of the different order correlations can be investigated. Since the equations are complicated integrodifferential equations this can be done only numerically. In this paper only the simplest case is discussed in detail, namely when  $D$  is already neglected. As it will be shown, this leads to a mean-field description of the problem.

In the assembly discussed so far each dislocation has the same Burgers vector. However, in a real system the net Burgers vector is approximately zero, so the above-developed formalism has to be extended for the case where dislocations both with positive and negative Burgers vectors are allowed in the system. It is easy to see that the equations for first-order density functions are

$$\begin{aligned} \frac{\partial \rho_+(\vec{r}_1, t)}{\partial t} = & \int \frac{\partial}{\partial \vec{r}_1} \{ \rho_{+-}(\vec{r}_1, \vec{r}_2, t) - \rho_{++}(\vec{r}_1, \vec{r}_2, t) \} \\ & \times \vec{F}(\vec{r}_1 - \vec{r}_2) d\vec{r}_2 \end{aligned} \quad (18)$$

and

$$\begin{aligned} \frac{\partial \rho_-(\vec{r}_1, t)}{\partial t} = & \int \frac{\partial}{\partial \vec{r}_1} \{ \rho_{-+}(\vec{r}_1, \vec{r}_2, t) - \rho_{--}(\vec{r}_1, \vec{r}_2, t) \} \\ & \times \vec{F}(\vec{r}_1 - \vec{r}_2) d\vec{r}_2, \end{aligned} \quad (19)$$

where  $\rho_+, \rho_-$  are the one-particle and  $\rho_{++}, \rho_{+-}, \rho_{-+}, \rho_{--}$  are the two-particle density functions with the corresponding signs, and  $\vec{F}(\vec{r}_1 - \vec{r}_2)$  stands for the interaction force between dislocations of equal signs. [The negative signs in front of  $\rho_{++}$  and  $\rho_{--}$  in Eqs. (18) and (19) come from the simple

fact that the interaction force between dislocations of equal signs has the opposite direction as it has between those with different signs.]

#### SELF-CONSISTENT FIELD APPROXIMATION

Equations (18) and (19) contain the second-order density functions, so they do not form a closed system of equations. As was explained earlier, in a first approximation the correlation function  $D$  can be neglected, so the two-particle density functions can be given as

$$\rho_{i,j}(\vec{r}_1, \vec{r}_2) = \rho_i(\vec{r}_1) \rho_j(\vec{r}_2), \quad i, j = +, -. \quad (20)$$

With this assumption from Eqs. (18) and (19) one gets

$$\begin{aligned} \frac{\partial \rho_+(\vec{r}_1, t)}{\partial t} = & + \frac{\partial}{\partial \vec{r}_1} \left\{ \rho_+(\vec{r}_1, t) \int [\rho_-(\vec{r}_2, t) - \rho_+(\vec{r}_2, t)] \right. \\ & \left. \times \vec{F}(\vec{r}_1 - \vec{r}_2) d\vec{r}_2 \right\} \end{aligned} \quad (21)$$

and

$$\begin{aligned} \frac{\partial \rho_-(\vec{r}_1, t)}{\partial t} = & + \frac{\partial}{\partial \vec{r}_1} \left\{ \rho_-(\vec{r}_1, t) \int [\rho_+(\vec{r}_2, t) - \rho_-(\vec{r}_2, t)] \right. \\ & \left. \times \vec{F}(\vec{r}_1 - \vec{r}_2) d\vec{r}_2 \right\}. \end{aligned} \quad (22)$$

By adding and subtracting Eqs. (21) and (22) one obtains

$$\begin{aligned} \frac{\partial \rho(\vec{r}_1, t)}{\partial t} + \frac{\partial}{\partial \vec{r}_1} \left\{ k(\vec{r}_1, t) \int k(\vec{r}_2, t) \vec{F}(\vec{r}_1 - \vec{r}_2) d\vec{r}_2 \right\} = 0 \end{aligned} \quad (23)$$

and

$$\begin{aligned} \frac{\partial k(\vec{r}_1, t)}{\partial t} + \frac{\partial}{\partial \vec{r}_1} \left\{ \rho(\vec{r}_1, t) \int k(\vec{r}_2, t) \vec{F}(\vec{r}_1 - \vec{r}_2) d\vec{r}_2 \right\} = 0, \end{aligned} \quad (24)$$

in which the total dislocation density  $\rho(\vec{r}) = \rho_+(\vec{r}) + \rho_-(\vec{r})$  and the sign dislocation density  $k(\vec{r}) = \rho_+(\vec{r}) - \rho_-(\vec{r})$  were introduced.

The interaction force between two dislocations is  $\vec{F}(\vec{r}) = \vec{b} \tau_{\text{sing}}(\vec{r})$  (see Ref. 41) where  $\tau_{\text{sing}}(\vec{r})$  is the shear stress field of one of the dislocations and  $\vec{b}$  is the Burgers vector. As a consequence of this

$$\int k(\vec{r}_1, t) \vec{F}(\vec{r} - \vec{r}_1) d\vec{r}_1 = \vec{b} \tau_{\text{int}}(\vec{r}). \quad (25)$$

Here  $\tau_{\text{int}}(\vec{r})$  is the shear stress at the point  $\vec{r}$  caused by all the dislocations, i.e., this is a self-consistent field created by the dislocation system. After substituting Eq. (25) into Eqs. (23) and (24) one arrives at

$$\frac{\partial \rho(\vec{r}, t)}{\partial t} + \frac{\partial}{\partial r} \{ \vec{b} k(\vec{r}, t) \tau_{\text{int}}(\vec{r}, t) \} = 0, \quad (26)$$

$$\frac{\partial k(\vec{r}, t)}{\partial t} + \frac{\partial}{\partial r} \{ \vec{b} \rho(\vec{r}, t) \tau_{\text{int}}(\vec{r}, t) \} = 0. \quad (27)$$

Instead of applying the integral formula (25) for the determination of  $\tau_{\text{int}}(\vec{r})$  one can use the field equations<sup>42</sup>

$$\Delta^2 \chi(\vec{r}) = \frac{\mu b}{1 - \nu} \frac{\partial}{\partial y} k(\vec{r}), \quad (28)$$

$$\tau_{\text{int}}(\vec{r}) = \frac{\partial \chi(\vec{r})}{\partial x \partial y}, \quad (29)$$

where  $\chi$  is the stress function,  $\mu$  is the shear modulus, and  $\nu$  is the Poisson ratio. For simplicity, in the above expression and in the following  $\vec{b}$  is taken parallel to the  $x$  axis.

In most cases the dislocation system is quasineutral, i.e., the number of dislocations with positive and negative signs are equal in an area large enough. So, in a similar way as with charge density in electrodynamics, the sign dislocation density  $k(\vec{r})$  can be given as a divergence of a polarization density field  $\vec{P}(\vec{r})$  (see Ref. 43)

$$k(\vec{r}) = - \frac{\partial}{\partial r} \vec{P}(\vec{r}). \quad (30)$$

$\vec{P}$  is a vector but in the following it is assumed that only its component parallel to the Burgers vector differs from zero. In the above consideration the external stress,  $\tau_0$ , was not introduced. Clearly, it has to be taken into account by adding it to the internal stress in Eqs. (26) and (27).

Summarizing the results, on the basis of Eqs. (23)–(30) in a self-consistent field approximation the behavior of a parallel edge dislocation system can be described by the following equations:

$$\frac{\partial \rho(\vec{r}, t)}{\partial t} - \frac{\partial}{\partial x} \left\{ \frac{\partial P(\vec{r}, t)}{\partial x} b [ \tau_0 + \tau_{\text{int}}(\vec{r}, t) ] \right\} = 0, \quad (31)$$

$$\frac{\partial}{\partial x} \left\{ \frac{\partial P(\vec{r}, t)}{\partial t} - \rho(\vec{r}, t) b [ \tau_0 + \tau_{\text{int}}(\vec{r}, t) ] \right\} = 0, \quad (32)$$

and

$$\Delta^2 \tau_{\text{int}}(\vec{r}) = - \frac{\mu b}{1 - \nu} \frac{\partial^4}{\partial x^2 \partial y^2} P(\vec{r}, t). \quad (33)$$

### STABILITY ANALYSIS OF THE HOMOGENEOUS SOLUTION

It is easy to see that if the external stress  $\tau_0$  is constant the homogeneous stationary solution  $\rho(\vec{r}, t) = \rho_0, P(\vec{r}, t) = 0$  satisfies Eqs. (31)–(33). It has to be investigated however, whether this trivial solution is a stable one. For this, the usual technique of linear stability analysis is applied.

Let us seek the solution of Eqs. (31)–(33) in the form  $\rho(\vec{r}, t) = \rho_0 + \delta \rho(\vec{r}, t), P(\vec{r}, t) = \delta P(\vec{r}, t)$ , where  $\delta \rho(\vec{r}, t)$  and  $\delta P(\vec{r}, t)$  are small perturbations, so their higher-order terms can be neglected in Eqs. (31)–(33). After the Fourier transformation of the linearized equations one finds that

$$\frac{\partial \delta \rho^*}{\partial t} + q_x^2 b \tau_0 \delta P^* = 0, \quad (34)$$

$$\frac{\partial \delta P^*}{\partial t} - b \tau_0 \delta \rho^* - \rho_0 b \tau_{\text{int}}^* = 0, \quad (35)$$

$$(q_x^2 + q_y^2)^2 \tau_{\text{int}}^* = - \frac{\mu b}{1 - \nu} q_x^2 q_y^2 \delta P^*, \quad (36)$$

where the symbols marked with \* indicate the Fourier transforms of the corresponding variables, and  $(q_x, q_y)$  is the wave number vector. Seeking the solution of Eqs. (34)–(36) in the form

$$\delta \rho^* = \delta \rho_0 \exp(\lambda t), \quad \delta P^* = \delta P_0 \exp(\lambda t), \quad (37)$$

leads to the following requirement for  $\lambda$ :

$$\begin{vmatrix} \lambda & q_x^2 b \tau_0 \\ -b \tau_0 & \lambda + \rho_0 b T(\phi) \end{vmatrix} = 0, \quad (38)$$

where

$$T(\phi) = \frac{\mu b}{1 - \nu} \frac{q_x^2 q_y^2}{(q_x^2 + q_y^2)^2} \quad (39)$$

and  $\phi$  is the angle between the wave number vector  $(q_x, q_y)$  and the  $x$  axis. From this

$$2\lambda_{1,2} = -\rho_0 b T(\phi) \pm \sqrt{\rho_0^2 b^2 T^2(\phi) - 4b^2 \tau_0^2 q_x^2}. \quad (40)$$

Due to the fact that the function  $T(\phi)$  is always positive, the real part of  $\lambda_1$  and  $\lambda_2$  cannot be positive. As a consequence of this, perturbation cannot grow in this system, i.e., the homogeneous dislocation distribution is a stable solution. However, it is important to notice, if the wave number vector  $(q_x, q_y)$  is parallel either to the  $x$  or to the  $y$  axis the real parts of  $\lambda_1$  and  $\lambda_2$  are zero, which means that these perturbations neither grow nor die out, they are stable.

### THE INFLUENCE OF DISLOCATION SOURCES

In the system which was investigated so far the number of dislocations was conserved. Clearly, for allowing dislocation creation or annihilation the balance equation (31) has to be modified by adding a source term  $g$  to the right-hand side of the equation:

$$\frac{\partial \rho(\vec{r}, t)}{\partial t} - \frac{\partial}{\partial x} \left\{ \frac{\partial P(\vec{r}, t)}{\partial x} b[\tau_0 + \tau_{\text{int}}(\vec{r}, t)] \right\} = g(\rho, \dots). \quad (41)$$

Equation (32) however has to remain unchanged because it expresses the conservation of the Burgers vector. In general, besides the dislocation density  $\rho$ ,  $g$  may depend on the polarization, the external stress and also on their functionals,

but for simplicity in the following only its  $\rho$  dependence is considered.

Although the homogeneous solution of Eqs. (32) and (41) is not necessarily time independent, for investigating its stability one still can seek the solution of the corresponding linearized equation in the exponential form (37) in a time interval shorter than the characteristic time of dislocation density changes. Applying the same method as above one gets the

$$\begin{vmatrix} \lambda - \frac{dg}{d\rho} & q_x^2 b \tau_0 \\ -b \tau_0 & \lambda + \rho_0 b T(\phi) \end{vmatrix} = 0 \quad (42)$$

requirement for  $\lambda$ . From this

$$2\lambda_{1,2} = \frac{dg}{d\rho} - \rho_0 b T(\phi) \pm \sqrt{[dg/d\rho - \rho_0 b T(\phi)]^2 - 4[b^2 \tau_0^2 q_x^2 - (dg/d\rho) \rho_0 b T(\phi)]}. \quad (43)$$

Since  $T(\phi)$  is zero along the  $x$  and  $y$  axes if  $dg/d\rho$  is positive there are growing perturbations in the system.

### CONCLUSIONS

The collective behavior of a system of parallel edge dislocations was investigated. Starting from the equations of motion of individual dislocations interacting with each other through their elastic fields, a hierarchy of the evaluation equations of different order density functions was derived. Since these are coupled to each other, to obtain a closed set of equations it has to be assumed that the density functions having higher order than a certain one can be built up from the lower order ones according to the Mayer cluster expansion (14) and (15).

It was shown that in the simplest case, when the two-particle correlation is already neglected, one obtains a self-consistent field (also often referred to as a mean-field) description. Although the self-consistent field equations could be set up in a speculative way, the advantage of the method outlined here is that it clearly points out the necessary assumptions. It should be emphasized however that at this stage of the work it is not possible to see the precise limits of the mean-field approximation. On the other hand, the obtained hierarchy of equations makes the investigation of the

influence of different order correlation possible. Due to the complexity of the equations for the correlation function, this can only be done numerically.

By analyzing the stability of the homogeneous solution within the framework of the self-consistent field approximation it was found that the elastic interaction alone is not enough to introduce growing instability, which is in agreement with experimental evidences. However, the elastic interaction already leads to the appearance of stable perturbations. Introduction of dislocation sources can lead to increasing perturbation even in the case of small production rates.

As a consequence of this, it is important to note that in a general theory of dislocation pattern formation the precise long-range stress field of the dislocations has to be taken into account, because the elastic interaction creates a background which alone is already "almost enough" to produce dislocation pattern formation.

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<sup>1</sup>L. Kubin, in *Material Science and Technology: A Comprehensive Treatment*, edited by R. W. Chan, P. Haasen, and E. J. Kramer (VHC, Weinheim, 1993), Vol. 6.

<sup>2</sup>L. Kubin, in *Dislocation Patterns: Experiment, Theory and Simulation*, NATO Advanced Study Institute on Stability of Materials, edited by A. Gonis and P. Turchi (Plenum, New York, 1996).

<sup>3</sup>A. Gullouglu, D. Srolovity, R. LeSar, and P. Lomdahl, *Scr. Metall.* **23**, 1347 (1989).

<sup>4</sup>N. M. Ghoniem and R. J. Amodeo, *Solid State Phen.* **3-4**, 377 (1988).

<sup>5</sup>R. J. Amodeo and N. M. Ghoniem, *Phys. Rev. B* **41**, 6958 (1989).

<sup>6</sup>R. J. Amodeo and N. M. Ghoniem, *Phys. Rev. B* **41**, 6968 (1989).

<sup>7</sup>V. A. Lubarda, J. A. Blume, and A. Needleman, *Acta Metall. Mater.* **41**, 625 (1993).

<sup>8</sup>A. N. Gullouglu and C. S. Hartley, *Modeling Simul. Mater. Sci. Eng.* **1**, 1 (1992).

- <sup>9</sup>A. N. Gullouglu and C. S. Hartley, *Modeling Simul. Mater. Sci. Eng.* **1**, 383 (1992).
- <sup>10</sup>X. F. Fang and W. Dahl, *Mater. Sci. Eng. A* **164**, 300 (1993).
- <sup>11</sup>I. Groma and G. S. Pawley, *Philos. Mag. A* **67**, 1459 (1993).
- <sup>12</sup>I. Groma and G. S. Pawley, *Mater. Sci. Eng. A* **164**, 306 (1993).
- <sup>13</sup>I. Groma and G. S. Pawley, *Solid State Phen.* **35-36**, 369 (1994).
- <sup>14</sup>R. Fournet and J. M. Salazar, *Phys. Rev. B* **53**, 6283 (1996).
- <sup>15</sup>L. P. Kubin and G. R. Canova, *Scr. Metall. Mater.* **27**, 957 (1992).
- <sup>16</sup>Y. J. Bréchet, G. R. Canova, and L. P. Kubin, *Scr. Metall. Mater.* **29**, 1165 (1993).
- <sup>17</sup>B. Devincre and M. Condat, *Acta Metall. Mater.* **40**, 2629 (1992).
- <sup>18</sup>D. Kuhlmann-Wilsdorf and J. H. van der Merve, *Mater. Sci. Eng.* **55**, 79 (1982).
- <sup>19</sup>M. N. Bassim, W. A. Jesser, D. Kuhlmann-Wilsdorf, and H. G. F. Wilsdorf, *Mater. Sci. Eng.* **81**, 122 (1986).
- <sup>20</sup>M. N. Bassim, W. A. Jesser, D. Kuhlmann-Wilsdorf, and G. J. Shiflet, *Mater. Sci. Eng. A* **113**, 22 (1989).
- <sup>21</sup>D. L. Holt, *J. Appl. Phys.* **41**, 3179 (1970).
- <sup>22</sup>D. Walgraef and E. C. Aifantis, *J. Appl. Phys.* **15**, 688 (1985).
- <sup>23</sup>D. Walgraef and E. C. Aifantis, *Int. J. Eng. Sci.* **23**, 1359 (1985).
- <sup>24</sup>D. Walgraef and E. C. Aifantis, *Int. J. Eng. Sci.* **23**, 1365 (1985).
- <sup>25</sup>E. C. Aifantis, *Mater. Sci. Eng.* **81**, 563 (1986).
- <sup>26</sup>E. C. Aifantis, *Int. J. Plasticity* **3**, 211 (1987).
- <sup>27</sup>E. C. Aifantis, in *Proceedings of an International Symposium on the Mechanics of Dislocation*, edited by E. C. Aifantis and J. P. Hirsh (Choise Book, Pennsylvania, 1993), p. 127.
- <sup>28</sup>C. Schiller and D. Walgraef, *Acta Metall. Mater.* **36**, 563 (1988).
- <sup>29</sup>M. V. Glazov and C. Laird, *Acta Metall. Mater.* **43**, 2849 (1995).
- <sup>30</sup>J. Kratochvil and S. Libovicky, *Scr. Metall.* **20**, 1625 (1986).
- <sup>31</sup>J. Kratochvil, *Rev. Phys. Appl.* **23**, 419 (1988).
- <sup>32</sup>J. Kratochvil and A. Orlova, *Philos. Mag. A* **61**, 281 (1990).
- <sup>33</sup>J. Kratochvil, *J. Mech. Behav. Met.* **2**, 353 (1990).
- <sup>34</sup>A. Franek, R. Kalus, and J. Kratochvil, *Philos. Mag. A* **64**, 497 (1991).
- <sup>35</sup>J. Kratochvil and M. Saxlova, *Scr. Metall. Mater.* **26**, 113 (1993).
- <sup>36</sup>J. Kratochvil, *Mater. Sci. Eng. A* **164**, 15 (1993).
- <sup>37</sup>P. Hähner, *Acta Mater.* **44**, 2345 (1996).
- <sup>38</sup>P. Hähner, *Appl. Phys. A* **62**, 473 (1996).
- <sup>39</sup>P. Hähner, in *Continuum Models and Discrete Systems 8*, edited by K. Z. Markov (World Scientific, Singapore, 1996), pp. 514–521.
- <sup>40</sup>C. N. Lashmore-Davis (unpublished).
- <sup>41</sup>I. Kovacs and L. Zsoldos, *Dislocations and Plastic Deformation* (Pergamon Press, London, 1973).
- <sup>42</sup>E. Kröner, in *Physics of Defects*, edited by R. Balian, M. Kléman, and J. P. Poirier (North-Holland, Amsterdam, 1981), p. 215.
- <sup>43</sup>L. D. Landau and E. M. Lifshitz, *Theory of Elasticity, Course of Theoretical Physics*, 3rd ed. (Pergamon, Oxford, 1986), Vol. 7.