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Stochastic approach for modeling dislocation patterning

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(Received 19 June 1998; revised manuscript received 26 January 1999)

The collective behavior of a system of straight parallel edge dislocations under cyclic plastic deformation is investigated. For describing the dislocation pattern formation two different stochastic approaches are considered and compared. In one of them the discrete dislocation system is described by coupled Langevin equations; in the other one a continuum approach is applied. Typical deformation patterns (''matrix structures'') are found by stochastic integration. [S0163-1829(99)08825-6]

I. INTRODUCTION

Many different dislocation structures are known to exist in deformed metals. It is well known, e.g., that a very heterogeneous dislocation distribution called persistent slip bands in a surrounding ''matrix'' may form upon cyclic deformation of single crystals. To understand how the collective motion of dislocations leads to such collective effects is presently one of the most fundamental challenges in dislocation theory. Several models have been proposed to describe these organized structures observed by transmission electron microscopy, but we are still far from the complete understanding of this typically self-ordering phenomena.

Due to the long-range nature of the dislocation-dislocation interaction and the high degree of freedom, the theoretical investigation of this problem is very difficult. Each analytical model developed so far (Kulhmann-Wilsdorf and van der Merve,[1] Holt,[2] Rickman and Vinals,[3] Walgreaf and Aifantis,[4] Aifantis,[5] Schiller and Walgreaf,[6] Kratochvil and co-worker,[7,8] Franek *et al.*,[9] and Hähner[10,11]) is able to predict the formation of inhomogeneous dislocation distribution; their common shortcoming is, however, that they are based on *ad hoc* assumptions.

Besides the theoretical models mentioned above, over the past few years several computer-simulation techniques were developed for studying the dislocation-patterning phenomenon. Both the two-dimensional[12–24] (2D) and the 3D (Refs. 25–27) simulations were limited to relatively small numbers of dislocations ($N \sim 10^3$–10^4 or less), owing to the computational complexity of the internal stress calculation. In order to study much larger systems, several $O(N)$ methods, such as the ''particle-particle–particle-mesh'' method,[28] multipole expansion,[29] or stochastic methods,[30] have been applied to treat the long-range dislocation-dislocation interaction forces.

Since the real systems consist of an enormous number of dislocations, the high degree of freedom makes the theoretical investigation very difficult. As it has been found by studying short-time evolution of discrete dislocation systems the internal stress created by the dislocations can be decomposed into the sum of two independent components,[30] namely, a mean-field force originated from the ''smoothed out'' dislocation distribution and a stochastic, fluctuating component. This is rigorously true only for systems with no correlations among the dislocations. However, if the correlations are weak, as is the case when the system is not far from homogeneous, the decomposition of the stress field mentioned above still applies. All the results presented in this paper are valid only under this assumption.

For describing the dislocation-pattern formation, two different stochastic approaches are applied. In one of them the discrete dislocation system is described by Langevin equations. The evolution of the system is studied by the stochastic $O(N)$ method proposed by Bakó and Groma.[30] In the other one, the dislocation system is described by the dislocation and the Burgers vector density that are continuous functions of the space coordinates and obey a Langevin-type equation. Then the two different stochastic approaches are compared.

II. MODEL EQUATIONS FOR DISCRETE 2D SYSTEMS

Let us consider a system of N interacting parallel straight edge dislocations with Burgers vectors of equal magnitudes and opposite directions. 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 a certain power of the dislocation velocity.[21] Since in the case of a low deformation rate the inertia term can be neglected besides the friction force, the equation of motion of a dislocation is only a first-order differential equation. For the sake of simplicity the Burgers vector of each dislocation is taken parallel to the x axis, and the dislocation lines are parallel to the z axis. The positions of dislocations in the xy plane are denoted by $\vec{r}_i = (x_i, y_i)$, $i = 1, \ldots, N$. With the assumptions outlined above the velocity of the ith dislocation, $\vec{v}_i$ can be given as[31]

$$\vec{v}_i = B\vec{b}_i[\tau^{\rm int}(\vec{r}) + \tau^{\rm ext}(\vec{r})]^{1/m}, \tag{1}$$

where B is the dislocation mobility, m is the velocity-stress exponent, $\tau^{\rm int}$ and $\tau^{\rm ext}$ represents the internal and external stresses, respectively. This is the system of equations that is solved numerically in most of the 2D computer

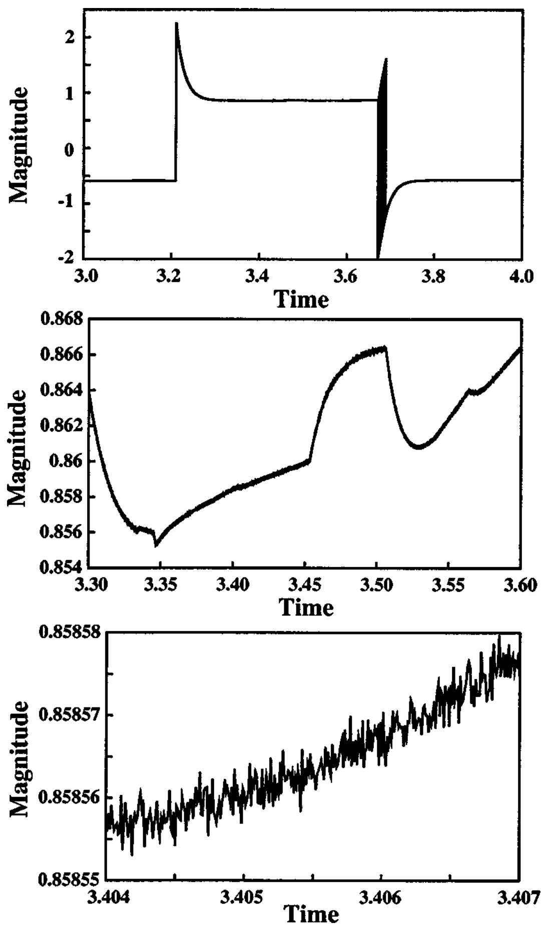

FIG. 1. A typical internal stress versus time curve (in three different magnifications) obtained by numerical integration of Eq. (1).

simulations.[12–17,21–24] The internal shear stress created by the dislocation system can be given as[32]

$$\tau^{\mathrm{int}}(\vec{r})=\sum_{j=1}^{N}\tau_{\mathrm{ind}}^{j}(x_j-x,y_j-y),\tag{2}$$

where

$$\tau_{\mathrm{ind}}^{j}(x,y)=\frac{\mu b_j}{2\pi(1-\nu)}\,\frac{x(x^2-y^2)}{(x^2+y^2)^2}\tag{3}$$

is the individual shear stress created by an edge dislocation with Burgers vector of magnitude b_j, in which μ is the shear modulus and ν represents the Poisson ratio.

Numerical integrations of Eq. (1) for short (shorter than the relaxation time) periods of time show that the internal stress $\tau^{\mathrm{int}}(\vec{r})$ created by the dislocations can be viewed as a sum of a slowly varying mean stress originating from the internal stress of the smoothed out dislocation distribution $\overline{\tau(\vec{r},t)}$ and a rapidly varying, highly irregular function with a zero mean value that satisfies the requirement of no correlation at different times or places and that represents the influence of the near neighbors (see Fig. 1). An important consequence of this numerical observation is that the computationally very expensive precise calculation of the internal stress created by the dislocation is not necessary.

According to the above finding, the internal stress can be considered as a stochastic variable, which can be described through the assignment of a stress-distribution function $P(\tau)$. $P(\tau_0)d\tau_0$ gives the probability of occurrence of τ at an arbitrary time in the range

$$\tau_0-\frac{d\tau_0}{2}\leqslant\tau(\vec{r})\leqslant\tau_0+\frac{d\tau_0}{2},\tag{4}$$

where τ_0 is a preassigned value for τ. Denoting the N particle dislocation density function by $w_N(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)$ the characteristic function $P(q)$ has the form[33]

$$\begin{aligned}P(q)={}&\int w_N(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\\&\times\prod_{j=1}^{N}\exp\{iq\tau_{\mathrm{ind}}^{j}(\vec{r}_i-\vec{r}_j)\}d\vec{r}_1d\vec{r}_2\cdots d\vec{r}_N\\&\approx\exp[Q(\vec{r},q)],\end{aligned}\tag{5}$$

where

$$\begin{aligned}Q(\vec{r},q)={}&-\int\rho(\vec{r}_1)B(\vec{r}-\vec{r}_1,q)d\vec{r}_1\\&+\frac{1}{2}\int g(\vec{r}_1,\vec{r}_2)B(\vec{r}-\vec{r}_1,q)\\&\times B(\vec{r}-\vec{r}_2,q)d\vec{r}_1d\vec{r}_2+\cdots,\end{aligned}\tag{6}$$

$$B(\vec{r},q)=1-\exp\{i\tau_{\mathrm{ind}}(\vec{r})q\}.\tag{7}$$

Here $\rho(\vec{r}_1)$ and $g(\vec{r}_1,\vec{r}_2)$ represent the dislocation density and dislocation-dislocation correlation functions, respectively.

Because of the strongly inhomogeneous distributions of the dislocations the analytical form of $P(\tau^{\mathrm{int}})$ cannot be determined. However, for small q values the characteristic function $P(q)$ can be given by an explicit expression (see Ref. 33),

$$P(q,\vec{r})\approx\exp[iq\overline{\tau(\vec{r})}+C\rho(\vec{r})q^2\ln(q\tau_{\mathrm{eff}})+\cdots],\tag{8}$$

which leads to the asymptotic form

$$P(\tau)|_{\tau\to\infty}\approx\frac{C\rho(\vec{r})}{\tau^3(\vec{r})},\tag{9}$$

where C is a constant determined by the angular anisotropy of the dislocation-dislocation interaction,[33]

$$C=b^2\int_0^{2\pi}K^2(\varphi)d\varphi.\tag{10}$$

$K(\varphi)$ describes the angular dependence of the individual stress field determined by the actual type of the dislocation under consideration. The effective stress τ_{eff} appearing in expression (8) is determined by the dislocation-dislocation correlation, namely, by the length parameter,

$$R_{\mathrm{eff}}=\frac{\mu b}{2\pi(1-\nu)}\,\frac{1}{\tau_{\mathrm{eff}}},\tag{11}$$

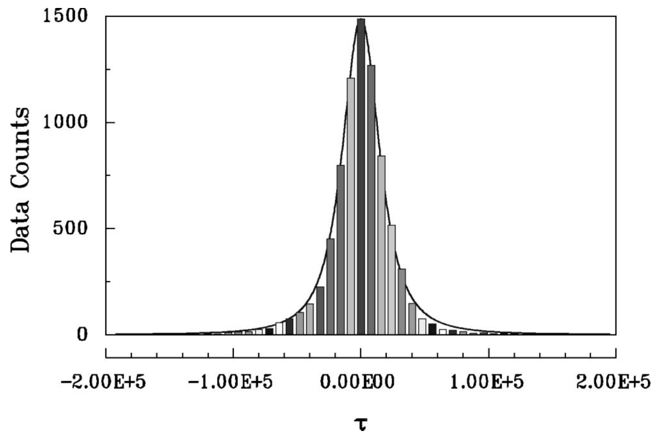

FIG. 2. Stress distribution function (lines) given by Eq. (14) versus distribution of internal stresses acting on 8000 dislocations in the center of a disk containing 4×10^8 randomly positioned, uniformly distributed dislocation dipoles with 0.14 dipole-width to dipole-distance ratio (boxes).

which is a characteristic length scale of the dislocation configuration (like, e.g., the dipole width).

An important characteristic value of the distribution function $P(\tau)$ is its first moment,

$$\overline{\tau}(\vec{r})=\frac{i}{P(0,\vec{r})}\frac{dP(q,\vec{r})}{dq}\bigg|_{q=0}=\int k(\vec{r}_1,t)\tau_{\mathrm{ind}}(\vec{r}_1-\vec{r})d\vec{r}_1, \tag{12}$$

which is the self-consistent field created by the dislocation system at the point $\vec{r}$ and $k(\vec{r},t)=\rho_+(\vec{r},t)-\rho_-(\vec{r},t)$ is the sign dislocation density, with ρ_+ and ρ_- representing the density of dislocations with positive and negative Burgers vectors, respectively. As it is shown in Ref. 34 for edge dislocations $\overline{\tau}(\vec{r})$ fulfill the field equation

$$\Delta^2\overline{\tau}(\vec{r})=-\frac{\mu b}{1-\nu}\frac{\partial^3}{\partial x\partial y^2}k(\vec{r}). \tag{13}$$

Since the explicit form of the stress-distribution function cannot be determined, one has to approximate it with an analytical function, which for small Fourier parameters fulfill condition (8). The form

$$P(\tau_{\mathrm{fluct}})=C\rho(\vec{r})[\tau^2_{\mathrm{fluct}}(\vec{r})+2C\rho(\vec{r})]^{-3/2}, \tag{14}$$

where $\tau_{\mathrm{fluct}}(\vec{r})=\tau_{\mathrm{int}}(\vec{r})-\overline{\tau_{\mathrm{int}}}(\vec{r})$ describes well the distribution of the fluctuations of the internal stress around its mean field value $\overline{\tau}_{\mathrm{int}}(\vec{r})$ for weakly correlated dislocation configurations (for numerical verification, see Fig. 2) and it is suitable for analytical and numerical computations.

Using Eq. (1) and taking into account the stochastic character of the internal stress, a system of coupled Langevin equations can be constructed for the dislocations. Consequently the ith dislocation obeys the Langevin equation

$$\vec{v}_i=B\vec{b}_i[\overline{\tau}(\vec{r}_i,t)+\tau_{\mathrm{fluct}}(\vec{r}_i,t)+\tau^{\mathrm{ext}}]^{1/m}. \tag{15}$$

III. 2D CONTINUUM DESCRIPTION FOR DISLOCATION SYSTEMS

In order to establish a link between the existing models and the stochastic approximation of the dynamical evolution of the interacting dislocation systems outlined in this paper instead of describing the system by the time variation of the coordinates of the N interacting dislocations, one has to use the N-particle distribution function f_N, which is a $2N$-dimensional function of the space coordinates. For the sake of simplicity let us consider only dislocations with the same Burgers vector $\vec{b}$ (this restriction will be lifted later).

According to the common definition, the quantity $f_N(t,\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)d\vec{r}_1d\vec{r}_2\cdots d\vec{r}_N$ gives the probability of finding the N dislocations in the volume $d\vec{r}_1d\vec{r}_2\cdots d\vec{r}_N$ vicinity of the points $\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N$ at the moment t. Due to the assumed conservation of the dislocation number, f_N has to fulfill the relation

$$\begin{aligned}f_N(t,\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)d\vec{r}_1d\vec{r}_2\cdots d\vec{r}_N=f_N(t+dt,\vec{r}_1\\+\vec{v}_1dt,\ldots,\vec{r}_N+\vec{v}_Ndt)d(\vec{r}_1+\vec{v}_1dt)\cdots d(\vec{r}_N+\vec{v}_Ndt),\end{aligned} \tag{16}$$

from which

$$\frac{\partial}{\partial t}f_N(t,\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)+\sum_{i=1}^{N}\nabla_{\vec{r}_i}[f_N(t,\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\vec{v}_i]=0. \tag{17}$$

Substituting the expression of $\vec{v}_i$ from Eq. (15) into Eq. (17) we obtain

$$\begin{aligned}\frac{\partial}{\partial t}f_N(t,\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)+B\sum_{i=1}^{N}(\vec{b}\nabla_{\vec{r}_i})\{f_N(t,\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\\ \times[\overline{\tau}(\vec{r}_i,t)+\tau_{\mathrm{fluct}}(\vec{r}_i,t)+\tau^{\mathrm{ext}}]^{1/m}\}=0.\end{aligned} \tag{18}$$

By allowing dislocations of both positive and negative Burgers vectors $\pm\vec{b}$ and by introducing the dislocation density functions $\rho_\pm(\vec{r},t)=Nf_1(t,\vec{r})$ of dislocations with positive and negative Burgers vectors, respectively, and integrating Eq. (17) over the $\vec{r}_2,\vec{r}_3,\ldots,\vec{r}_N$ subspace, one gets

$$\frac{\partial\rho_+(\vec{r},t)}{\partial t}=-(\vec{b}\nabla)\{B\rho_+(\vec{r},t)[\overline{\tau}(\vec{r},t)+\tau_{\mathrm{fluct}}(\vec{r},t)+\tau^{\mathrm{ext}}]^{1/m}\}, \tag{19}$$

$$\frac{\partial\rho_-(\vec{r},t)}{\partial t}=(\vec{b}\nabla)\{B\rho_-(\vec{r},t)[\overline{\tau}(\vec{r},t)+\tau_{\mathrm{fluct}}(\vec{r},t)+\tau^{\mathrm{ext}}]^{1/m}\}. \tag{20}$$

By adding and subtracting Eqs. (19) and (20), one concludes

$$\frac{\partial\rho(\vec{r},t)}{\partial t}+(\vec{b}\nabla)\{Bk(\vec{r},t)[\overline{\tau}(\vec{r},t)+\tau_{\mathrm{fluct}}(\vec{r},t)+\tau^{\mathrm{ext}}]^{1/m}\}=0, \tag{21}$$

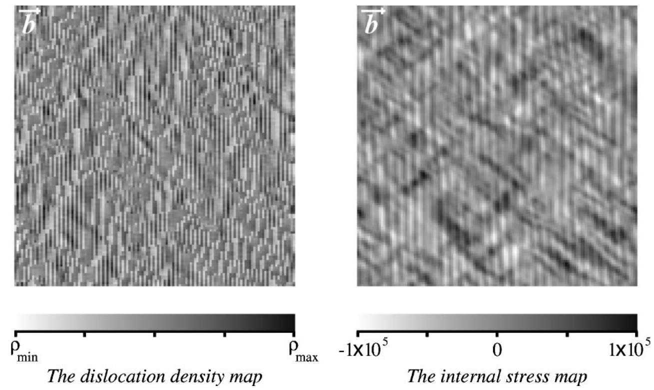

FIG. 3. Dislocation density map and the corresponding self-consistent mean field (12) in the case of a discrete dislocation system without sources after 70 fatigue cycles.

$$\frac{\partial k(\vec{r},t)}{\partial t}+(\vec{b}\nabla)\{B\rho(\vec{r},t)[\overline{\tau}(\vec{r},t)+\tau_{\text{fluct}}(\vec{r},t)+\tau^{\text{ext}}]^{1/m}\}=0, \tag{22}$$

where $\rho(\vec{r},t)=\rho_{+}(\vec{r},t)+\rho_{-}(\vec{r},t)$ is the total dislocation density.

The balance equation (21) represents the conservation of dislocation number, while Eq. (22) expresses the conservation of the net Burgers vector bk.

For allowing dislocation creation and annihilation, the balance equation (21) has to be modified by adding a source term to the right-hand side that may depend on ρ, $\overline{\tau}$, the external stress τ^{ext}, etc.,

$$\frac{\partial \rho(\vec{r},t)}{\partial t}+(\vec{b}\nabla)\{Bk(\vec{r},t)[\overline{\tau}(\vec{r},t)+\tau_{\text{fluct}}(\vec{r},t)+\tau^{\text{ext}}]^{1/m}\}$$
$$=f(\rho,\overline{\tau},\tau^{\text{ext}},\ldots). \tag{23}$$

IV. DISLOCATION STRUCTURES IN CYCLIC DEFORMATION

Let us consider an initially homogeneous system of 2^{20} parallel straight edge dislocations with Burgers vectors of equal magnitudes and opposite directions fatigued by a periodic external stress field. The number of dislocations is constrained only by the requirement that the system has overall neutrality, i.e., the Burgers vectors satisfy the neutrality condition $\Sigma_i\vec{b}_i=0$. For simplicity, for simulations we assume a constant value for the mobility B and a linear velocity-stress relationship (the same stress exponent $m=1$ was experimentally observed for the phonon-related friction in a copper-single crystal[35]); for other materials, however, the model equations can be used as well by replacing the linear velocity-stress dependence with the corresponding material specific power or exponential stress dependence of velocities in Eq. (1).

We start the simulations from an initially homogeneous dislocation dipole distribution, considering dipoles with a 0.14 mean dipole-width to dipole-distance ratio. A similar value was experimentally observed by Tippelt *et al.*[36] on cyclically deformed Ni single crystals oriented for single slip. From the homogeneous dislocation system with small fluctuations of the Burgers vector density field bk, the stochastic integration of the system of coupled stochastic differential equations (15) corresponding to the 2^{20} dislocations over a time interval of a few tens of periods of the external stress field leads to a dislocation configuration shown in Fig. 3. The figure shows the dislocation density field and the corresponding self-consistent mean stress field created by the dislocation system for one realization of the noise. The smoothed out dislocation density $\rho(\vec{r})$ is determined by counting the dislocations in 128×128 cells. The development of an ordered structure of the dislocation density and corresponding internal stress field can be observed. These results suggest that the $1/r$-type angularly anisotropic stress field acting between two dislocations is alone sufficient to lead to an arrangement of dislocations in which a highly organized global stress field is generated during the cyclic deformation. This field can act as a periodic background for the dislocation sources. By allowing a source term proportional to the local dislocation density and to the square of the local stress field [which is based on the assumption that in two dimensions a certain fraction of the local plastic energy that is proportional to $\rho(\vec{r})\tau^2(\vec{r})$ is spent for dislocation creation] formation of completely different dislocation structures can be obtained using the same initial configuration as before. The dislocation annihilation process is introduced in the model via a critical annihilation distance. Figure 4 shows snapshots of the growth of domains with high dislocation density. The dislocation density pictures show that the experimentally ob-

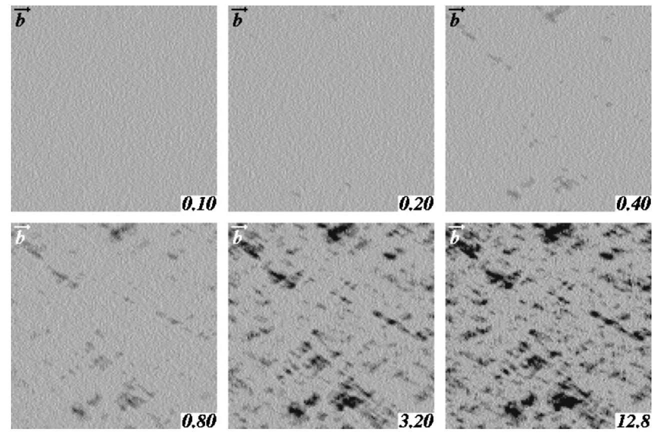

FIG. 4. Dislocation density maps showing the formation and the time evolution of domains in the discrete model in the presence of sources in the course of fatigue by an external stress field (the elapsed time is shown in each picture in units of the period of the external stress field).

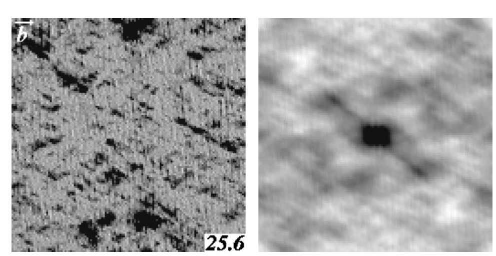

FIG. 5. The dislocation density map and the corresponding density correlation function in an advanced stage of the evolution of system shown in Fig. 4.

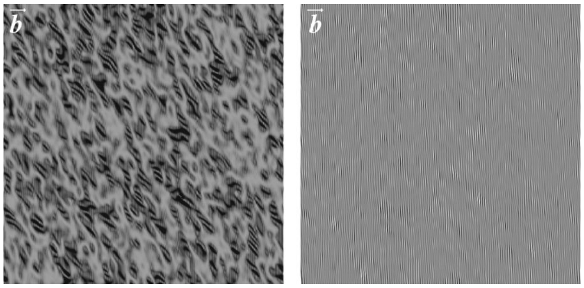

FIG. 6. Dislocation density map and the corresponding net Burgers vector density field for the case of the continuum model fatigued by an external stress field.

served ''matrix'' structure[37] is reproduced qualitatively by the model equations (15) if dislocation production and annihilation is allowed. The high dislocation density domains are aligned more or less along parallel lines at directions of about 35°–45° to the glide plane. Less correlated domains can be observed by a visual appreciation of the dislocation correlation $\langle\rho(\vec{r})\rho(\vec{r}-\vec{r}\,')\rangle$ shown in Fig. 5 at directions of about 65° and 27° to the glide plane. The same ordering tendencies were observed experimentally by Buchinger and Stanzl[37] in copper single crystals fatigued at low amplitudes.

The stochastic integration of the coupled equations (12), (22), and (23) with the same initial conditions as in the case of the discrete system, i.e., a quasineutral dislocation system with homogeneous dislocation distribution, small fluctuations of the Burgers vector density field, and a source term $f\sim\rho\tau^2$ leads to the ''matrix'' structure shown in Fig. 6. The figure shows an average of 30 histories.

Numerical experiments show that the model equations (22) and (23) allow the existence of local growing perturbations. This means that the solution becomes locally unstable, so that the continuum model can be integrated only for short intervals. The local instability observed in the continuum model does not occur in the discrete model because the dislocations form rapidly in the early stage of the evolution of the structure, then the dislocation annihilation becomes important due to the introduced dislocation annihilation distance. In this later stage there is a balance between dislocation creation and annihilation, the dislocation population reaches its steady state, the new dislocations contribute to the annihilation process.

The results of the two different methods show that, as it is well known, the elastic interaction alone is not enough for pattern formation. It however leads to the development of an inhomogeneous stress field. The introduction of dislocation sources with positive production rates in the presence of the external periodic stress field changes the dynamics essentially and allows pattern formation. In summary, it is believed that for dislocation patterning the particular form of the elastic interaction and the presence of the dislocation sources with a positive rate of dislocation production are needed for pattern formation. In the stochastic models presented here only these two factors are used to reproduce the ''matrix'' structure as an example of fatigue patterning.

V. SUMMARY

It was observed by numerical simulations performed on discreet dislocation assemblies, that the stress field created by the dislocations has a stochastic nature. On the basis of this numerical finding, a fully stochastic theory was formulated for describing the interaction of a system of weakly correlated straight parallel edge dislocations under cyclic plastic deformation. The collective behavior of the dislocation system was investigated numerically by two (a discrete and a continuum) variants of the stochastic theory.

The Langevin equations of individual dislocation motion were used to construct field equations for the dislocation and Burgers vector density fields. By a stochastic integration of the coupled Langevin equations (15) in the presence of a cyclic external stress field, the ''matrix'' structure observed in fatigued single crystals can be qualitatively reproduced. The ''matrix'' structure could be reproduced also by stochastic integration of the continuum equations (22) and (23).

In comparison with the models proposed earlier, the following needs to be stressed: The stochastic dislocation dynamics outlined in this paper differ strongly from the one proposed by Hähner,[10,11] where the dislocation system is described by a single variable (without direct spatial dependence), the dislocation density, time evolution of which is also governed by a Langevin-type equation.

In the model outlined above, due to the stochastic motion of the dislocations on time scales large enough the motion of the dislocations can be described as an effective diffusion process (the form of the appropriate diffusion term is not completely developed so far). For describing dislocation pattern formation Walgreaf and Aifantis,[4] Aifantis,[5] and Schiller and Walgreaf[6] adopt reaction-diffusion equations originally developed for oscillating chemical reactions. As a consequence of this, the expressions they propose for different dislocation processes are difficult to deduce from the theory of individual dislocation. Although the model developed by Kratochvil and co-worker[7,8] is based on a well-defined dislocation mechanism, it also contains several unknown parameters. In contrast, the model proposed in this paper uses the precise form of dislocation-dislocation interaction. Its further important feature is that if the correlations are negligible in the system, one arrives at the mean-field description elaborated by Groma[38] by a truncation of the Bogoliubov-Born-Green-Kirkwood-Yuon hierarchy of the dislocation distribution functions of different order.

Albeit this simple stochastic model, in which the evolution of the system of interacting dislocations can be viewed as a response to a self-consistently generated mean field and stochastic fluctuations extraordinarily successful, it cannot correctly handle the effects of strong correlations, the results remaining valid only in the regime not far from homogeneous.

In conclusion, it appears evident that the stochastic viewpoint outlined in this paper provides a useful approach for the analysis of the dynamical evolution of the interacting dislocation systems, although clearly unanswered questions remain, and they need further investigations.

ACKNOWLEDGMENTS

We are grateful to Professor T. Tél and Professor J. Lendvai for discussions. The financial support of OTKA under Contracts Nos. T 030791 and T 017609 is acknowledged.

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