Probability distribution of internal stresses in parallel straight dislocation systems

I. Groma and B. Bakó
Department of General Physics, Eötvös University Budapest, Budapest Múzeum krt. 6-8, POB 323, H-1445, Hungary
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The collective behavior of a system of straight parallel dislocations is investigated. It is found by numerical simulation that the internal stress τ created by the dislocation has a stochastic component. In order to describe this stochastic character the form of the probability distribution function of the internal stress is determined. It is shown that the mean value of the distribution function is the self-consistent field created by the dislocation and the distribution function decays with $1/\tau^3$. [S0163-1829(98)05230-8]

INTRODUCTION

It is well known that during plastic deformation of crystalline materials the dislocation distribution does not remain homogeneous. Because of the long-range character of the dislocation interaction the dislocations can form many different type patterns, such as dislocation walls and vein and ladder structures. In spite of the increasing experimental and theoretical activity in this field (for a broad overview see Refs. 1,2), we are far from understanding these typically self-organizatory phenomena.

A possible approach for the modeling of these pattern formation processes is the continuum approximation in which the system is described by continuous variable. In the models of Kulhman-Wilsdorf and van der Merve,[3] Holt,[4] and Ricman and Vinals [5] thermodynamical analogies are used, which lead to quasistatic descriptions. In contrast to these models, Walgreaf and Aifantis,[6] Aifantis,[7] and Schiller and Walgraef[8] adopt reaction-diffusion equations originally developed for oscillating chemical reactions. In the models of Kratochvil and Libovicky,[9,10] and Franek, Kalus, and Kratochvil[11] a dislocation-dipole, mobile-dislocation interaction mechanism is proposed to predict pattern formation. In a series of papers Hähner[12,13] introduced the concept of stochastic dislocation dynamics using a statistical mechanical analogy. Each model is able to predict the formation of inhomogeneous dislocation distribution, but their common shortcoming is that they are based on *ad hoc* assumptions.

Another possibility is to investigate the collective behavior of systems consisting of individual dislocations by computer simulation. During the past few years several two-dimensional (2D) (Refs. 14–23) and 3D (Refs. 24–26) simulations were carried out. In many of them evidence for pattern formation was reported, but due to the long-range nature of the dislocation-dislocation interaction macroscopic properties could be investigated only in a very limited way.

Recent investigations of Groma and Balogh[27,28] have shown that the individual and the continuum approaches can be linked through the construction of a hierarchy of evolution equations of the different order dislocation distribution functions. By neglecting the dislocation-dislocation correlations a self-consistent field description has been derived which can be considered as a zero order approximation. However, as was pointed out by Wilkens[29] the elastic energy of an uncorrelated dislocation system diverge logarithmically with the crystal size, therefore the dislocation-dislocation correlation cannot be completely neglected. The aim of the investigation presented in this paper is to obtain a method in which correlation effects are also take into account.

SHORT TIME BEHAVIOR OF A SYSTEM OF PARALLEL DISLOCATION INVESTIGATED BY NUMERICAL SIMULATION

In most of the 2D simulations performed earlier the behavior of dislocation systems has been investigated on a time scale longer than the relaxation time of the system. In order to determine further properties of the internal stress created by the dislocations short time (much shorter than the relaxation time) simulations were carried out. In the simulations a system of a few hundreds of parallel edge dislocations were considered. Each dislocation had the same Burgers vector $\vec{b}$ parallel to the x axis with equal number of positive and negative signs. As in the simulations reported in Refs. 21,22 overdumped dislocation motion was assumed, i.e., the velocity of the dislocations was proportional to the force acting on them. This leads to the system of equations of motions[21]

$$\frac{dx_i}{dt}=Bb_i\sum_{j\neq i}\tau_{\mathrm{ind}}^j(x_j-x_i,y_j-y_i)+Bb_i\tau_{\mathrm{ext}},\qquad j=\overline{1,N}, \tag{1}$$

where (x_i,y_i) denotes the position of the ith dislocation, B is the dislocation mobility, τ_{ext} is the external shear stress, and

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

is the shear stress created by an edge dislocation where the shear modulus μ and the Poisson ratio ν were introduced.

It was observed for several different dislocation configurations that besides an average value the stress created by the dislocations has a stochastic component. The Fourier spectra of the time evolution of the internal stress at a given point of the simulation area obtained on a system containing 500 randomly distributed dislocation dipoles is plotted on Fig. 1. Similar results were obtained for many other dislocation configurations too. In the figure each frequency appears with more or less the same amplitude (there is no characteristic

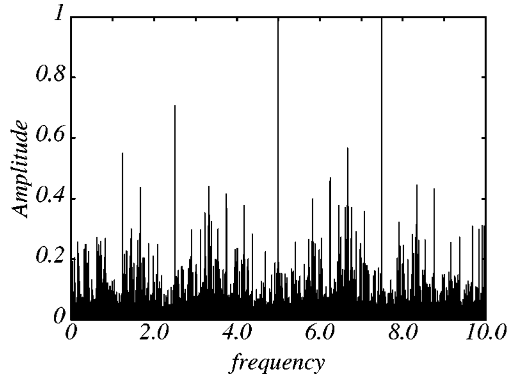

FIG. 1. Fourier spectrum of the time-evolution of the internal shear stress created by the dislocation system. (The units are arbitrary.)

decay or maximum), showing that the stochastic stress component has a white noise character.

GENERAL FORM OF THE PROBABILITY DISTRIBUTION OF THE INTERNAL SHEAR STRESS

For describing the properties of the stochastic component of the internal stress observed in computer simulations its probability distribution function has to be determined. Let us consider a system of N parallel straight edge dislocations positioned at the points $\vec{r}_i$, $i=\overline{1,N}$ in the xy plane perpendicular to the dislocation lines. For the sake of simplicity, we assume that each dislocation has the same Burgers vector $\vec{b}$. As it will be shown later, the generalization of the results for systems consisting of dislocations with different Burgers vectors is straightforward. The internal shear stress at the point $\vec{r}$ is the sum of the stress fields of the individual dislocations

$$\tau(\vec{r})=\sum_{i=1}^{N} \tau_{\rm ind}(\vec{r}-\vec{r}_i). \tag{3}$$

[Since in the following only one type of dislocation is considered for the sake of simplicity the upper index in $\tau_{\rm ind}(\vec{r})$ is omitted.]

The problem addressed in this paper is to determine the $P(\tau_0)d\tau_0$ probability of occurrence of τ 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. $P(\tau_0)$ can be obtained as a direct application of Markoff's method[30] applied for several problems, such as the problem of random flights or for the determination of the distribution of forces in gravitationally interacting random systems. In contrast with the two problems mentioned, in case of dislocation the N particle distribution function cannot be built up from the one particle distribution functions since as it will be shown later it would lead to system size dependent internal stress distribution function $P(\tau_0)$. To avoid this the dislocation-dislocation correlation must be taken into account.

Denoting the N particle dislocation density function by $w_N(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)$ the internal stress distribution can be expressed as

$$P(\tau_0)d\tau_0=\int\cdots\int w_N(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)d\vec{r}_1d\vec{r}_2\cdots d\vec{r}_N, \tag{5}$$

where the integration is effected only over that part of configuration space for which the inequalities (4) are satisfied. By the introduction of the factor

$$\Delta(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)=\begin{cases}1 & \text{whenever}\quad \tau_0-\frac{d\tau_0}{2}\leqslant\tau\leqslant\tau_0+\frac{d\tau_0}{2},\\ 0 & \text{otherwise,}\end{cases} \tag{6}$$

the integral in Eq. (5) can be extended over $2N$-dimensional space $\mathfrak{R}^{2N}$:

$$P(\tau_0)d\tau_0=\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\Delta(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\times w_N(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)d\vec{r}_1d\vec{r}_2\cdots d\vec{r}_N. \tag{7}$$

For the determination on the structure of expression (7) one has to consider the integral

$$\delta=\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\sin(\alpha n)}{n}\exp[\mathrm{i}\gamma n]dn, \tag{8}$$

which is the well-known discontinuous integral of the Dirichlet function with the properties

$$\delta=\begin{cases}1 & \text{whenever}\quad -\alpha<\gamma<\alpha,\\ 0 & \text{otherwise.}\end{cases} \tag{9}$$

By taking

$$\alpha=\frac{d\tau_0}{2}\quad\text{and}\quad\gamma=\sum_{i=1}^{N}\tau_{\rm ind}(\vec{r}-\vec{r}_i)-\tau_0 \tag{10}$$

from Eq. (6) one gets that $\Delta=\delta$. With the substitution of the Eq. (8) form of δ into Eq. (7), we obtain that

$$P(\tau_0)d\tau_0=\frac{1}{\pi}\int_{\mathfrak{R}}dn\int_{\mathfrak{R}^{2N}}d\vec{r}_1d\vec{r}_2\cdots d\vec{r}_Nw_N\times(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\frac{\sin[(1/2)d\tau_0n]}{n}\times\exp\left\{i\left[\sum_{i=1}^{N}\tau_{\rm ind}(\vec{r}-\vec{r}_i)n-\tau_0n\right]\right\}. \tag{11}$$

It can be seen from the structure of the above expression that the Fourier transform of the internal stress distribution

$$A_N(\vec{r},n)=\mathcal{F}P(\tau_0) \tag{12}$$

has the form

$$A_N(\vec{r},n)=\int w_N(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\times\prod_{j=1}^{N}\exp\{in\tau(\vec{r}-\vec{r}_j)\}d\vec{r}_1d\vec{r}_2\cdots d\vec{r}_N. \quad (13)$$

If we introduce the function

$$B(\vec{r},n)=1-\exp\{i\tau_{\mathrm{ind}}(\vec{r})n\} \quad (14)$$

expression (13) can be rewritten into a power series of $B(\vec{r},n)$

$$\begin{aligned}A_N(\vec{r},n)&=\int d\vec{r}_1d\vec{r}_2\cdots d\vec{r}_Nw_N(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\times\prod_{j=1}^{N}[1-B(\vec{r}-\vec{r}_j,n)]\\&=1-\int\rho_1(\vec{r}_1)B(\vec{r}-\vec{r}_1,n)d\vec{r}_1+\frac{1}{2}\int\rho_2(\vec{r}_1,\vec{r}_2)\\&\quad\times B(\vec{r}-\vec{r}_1,n)B(\vec{r}-\vec{r}_2,n)d\vec{r}_1d\vec{r}_2+\cdots, \quad (15)\end{aligned}$$

where

$$\rho_k(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_k)=N(N-1)\cdots(N-k+1)\times\int w_N(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\times d\vec{r}_{k+1}d\vec{r}_{k+2}\cdots d\vec{r}_N \quad (16)$$

is the kth order dislocation-density function. Equation (15) can be transformed into an exponential form

$$A_N(\vec{r},n)=\exp\{E(n,\vec{r})\}, \quad (17)$$

where

$$\begin{aligned}E(n,\vec{r})=&-\int\rho_1(\vec{r}_1)B(\vec{r}-\vec{r}_1,n)d\vec{r}_1\\&+\frac{1}{2}\int D_2(\vec{r}_1,\vec{r}_2)B(\vec{r}-\vec{r}_1,n)B(\vec{r}-\vec{r}_2,n)d\vec{r}_1d\vec{r}_2\\&+\cdots \quad (18)\end{aligned}$$

in which

$$D_2(\vec{r}_1,\vec{r}_2)=\rho_2(\vec{r}_1,\vec{r}_2)-\rho_1(\vec{r}_1)\rho_1(\vec{r}_2) \quad (19)$$

is the dislocation-dislocation correlation function.

THE MOMENTS AND THE ASYMPTOTIC BEHAVIOR OF $P(\tau)$

Since dislocations form strongly inhomogeneous distributions the explicit form of $P(\tau)$ cannot be determined analytically. Nevertheless, analytical results can be obtained for some of its properties. An important characteristic value of the distribution function $P(\tau)$ is its first moment $\langle\tau(\vec{r})\rangle$. By applying the relation

$$\langle\tau(\vec{r})\rangle=\frac{i}{A(\vec{r},0)}\left.\frac{dA(\vec{r},n)}{dn}\right|_{n=0} \quad (20)$$

we obtain that

$$\langle\tau(\vec{r})\rangle=-i\int\rho(\vec{r})\left.\frac{dB}{dn}\right|_{n=0}d\vec{r}_1=\int\rho(\vec{r})b\tau_{\mathrm{ind}}(\vec{r}-\vec{r}_1)d\vec{r}_1, \quad (21)$$

which is the self-consistent field created by the dislocation system at the point $\vec{r}$. As it is shown in Ref. 27 for edge dislocations it fulfills the field equation

$$\Delta^2\langle\tau(\vec{r})\rangle=-\frac{\mu b}{1-\nu}\frac{\partial^3}{\partial x\partial y^2}\rho(\vec{r}). \quad (22)$$

The second moment of $P(\tau)$ can be determined from the relation

$$\langle\tau^2(\vec{r})\rangle=-\frac{1}{A(\vec{r},0)}\left.\frac{d^2A(\vec{r},n)}{dn^2}\right|_{n=0}. \quad (23)$$

However, from Eqs. (17), (18) one gets that

$$\begin{aligned}\left.\frac{d^2A}{dn^2}\right|_{n=0}&=-\int\rho(\vec{r})b^2\tau_{\mathrm{ind}}^2(\vec{r}-\vec{r}_1)d\vec{r}_1+\cdots\\&=-\int\rho(\vec{r}-\vec{r}_1)b^2\tau_{\mathrm{ind}}^2(\vec{r}_1)d\vec{r}_1+\cdots, \quad (24)\end{aligned}$$

in which, due to the $1/r$ type decay of the stress field of a straight dislocation, the integrand has a $1/r_1$ singularity, and consequently the second moment of $P(\tau)$ is infinite. Therefore to determine further characteristic properties of the distribution function $P(\tau)$ its asymptotic behavior has to be investigated. First the behavior of $A_N(n)$ has to be analyzed in the regime of small n values. Let us consider the first term in expression (18)

$$f_0(\vec{r},n)=\int\rho(\vec{r}-\vec{r}_1)B(\vec{r}_1,n)d\vec{r}_1. \quad (25)$$

For the same reason as in expression (24) its second derivative at $n=0$

$$\left.\frac{d^2f_0}{dn^2}\right|_{n=0}=\int\rho(\vec{r}-\vec{r}_1)b^2\tau_{\mathrm{ind}}^2(\vec{r}_1)d\vec{r}_1 \quad (26)$$

is singular. However, if $\rho(\vec{r})$ was zero at the point $\vec{r}$ the integral would be finite. (If the dislocation density has a finite value at infinity the integral is divergent for $r_1\to\infty$, too. For avoiding this problem it has to be assumed that the dislocation density goes to zero at infinity. However, this restriction will be lifted later.) So, if instead of $f_0(\vec{r},n)$ the expression

$$f_1(\vec{r},n)=\int[\rho(\vec{r}-\vec{r}_1)-\rho(\vec{r}-2\vec{r}_1)]B(\vec{r}_1,n)d\vec{r}_1 \quad (27)$$

is considered the above singularity in the second derivative of $f_1(\vec{r},n)$ does not appear because $\rho(\vec{r}-\vec{r}_1)-\rho(\vec{r}-2\vec{r}_1)=0$ for $\vec{r}_1=0$. The newly defined f_0 and f_1 are not independent from each other:

$$f_1(\vec{r},n)=f_0(\vec{r},n)-\int \rho(\vec{r}-2\vec{r}_1)B(\vec{r}_1,n)d\vec{r}_1. \quad (28)$$

Since, $\tau_{\rm ind}(r)\sim x(x^2-y^2)/r^4$, if we take B at the point $1/2\vec{r}_1$, we find that

$$B\left(\frac{1}{2}\vec{r}_1,n\right)=B(\vec{r}_1,2n). \quad (29)$$

Using this relation with a $\vec{r}_1\rightarrow 2\vec{r}_1$ variable substitution in the second term of Eq. (27) we arrive at

$$f_1(\vec{r},n)=f_0(\vec{r},n)-\frac{1}{4}f_0(\vec{r},2n). \quad (30)$$

Because of the regular behavior of the second derivative of $f_1(\vec{r},n)$ it can be approximated with a parabolic expression

$$f_1(\vec{r},n)\approx a'(\vec{r})n+b(\vec{r})n^2. \quad (31)$$

Equations (30) and (31) determine a function equation for $f_0(\vec{r},n)$, the solution of which is

$$f_0(\vec{r},n)=a(\vec{r})n-\frac{b(\vec{r})}{\ln 2}n^2\ln\frac{n}{R}, \quad (32)$$

where $a(\vec{r})=i\langle\tau\rangle$ and R is a parameter which cannot be determined from the function equation. It corresponds to the αn^2 solution of the homogeneous equation

$$0=f_0(\vec{r},n)-\frac{1}{4}f_0(\vec{r},2n). \quad (33)$$

According to Eqs. (26) and (31) the actual value of $b(\vec{r})$ can be given by the expression

$$b(\vec{r})=\frac{1}{2}\frac{d^2f_1}{dn^2}\bigg|_{n=0}=\frac{1}{2}\int[\rho(\vec{r}-\vec{r}_1)-\rho(\vec{r}-2\vec{r}_1)]b^2\tau_{\rm ind}^2(\vec{r}_1)d\vec{r}_1. \quad (34)$$

The stress field created by a straight dislocation has the following form:

$$\tau_{\rm ind}(\vec{r})=\frac{K(\varphi)}{|\vec{r}|}, \quad (35)$$

where φ is the angle between the x axis and the position vector $\vec{r}$ and $K(\varphi)$ is a trigonometric polynomial of φ determined by the actual type of the dislocation under consideration. Introducing polar coordinates (r_1,φ) for the variable $\vec{r}_1$, Eq. (34) gets the form

$$b(\vec{r})=\lim_{\varepsilon\rightarrow 0}\frac{1}{2}\int_0^{2\pi}d\varphi\int_{\varepsilon}^{\infty}dr_1[\rho(\vec{r}-\vec{r}_1)-\rho(\vec{r}-2\vec{r}_1)]b^2\frac{K^2(\varphi)}{|\vec{r}_1|} \quad (36)$$

in which in order to avoid the singularity in the integrand around $r_1=0$ a circular area with radius ε is excluded from the integral. After splitting it into two integrals, with the $2\vec{r}_1\rightarrow\vec{r}_1$ variable substitution in the second one we find that

$$b(\vec{r})=\frac{1}{2}\int_0^{2\pi}d\varphi\int_{\varepsilon/2}^{\varepsilon}dr_1\rho(\vec{r}-\vec{r}_1)b^2\frac{K^2(\varphi)}{|\vec{r}_1|}. \quad (37)$$

Since the integral has to be carried out for an area close to the origin of the coordinate system, $\rho(\vec{r}-\vec{r}_1)$ can be approximated by its value at $\vec{r}_1=0$

$$b(\vec{r})=\frac{1}{2}\rho(\vec{r})\int_0^{2\pi}d\varphi\int_{\varepsilon/2}^{\varepsilon}dr_1b^2\frac{K^2(\varphi)}{|\vec{r}_1|} \quad (38)$$

from which

$$b(\vec{r})=\rho(\vec{r})\ln(2)C, \quad (39)$$

where

$$C=\frac{b^2}{2}\int_0^{2\pi}K^2(\varphi)d\varphi \quad (40)$$

is a constant determined by the type of dislocation under consideration, and by the elastic moduli. In an isotropic medium for edge dislocations

$$C=\frac{(\mu b)^2}{8\pi^2(1-\nu)^2}\int_0^{2\pi}\cos^2(\varphi)\cos^2(2\varphi)d\varphi=\frac{(\mu b)^2}{16\pi(1-\nu)^2}. \quad (41)$$

According to Eqs. (32) and (39) we conclude that up to second order terms $f_0(\vec{r},n)$ can be approximated with the expression

$$f_0(\vec{r},n)\approx i\langle\tau(\vec{r})\rangle n-C\rho(\vec{r})n^2\ln\frac{n}{R}. \quad (42)$$

As was mentioned earlier the actual values of parameter R cannot be determined by the method described above. It can be obtained from the analysis of expression (25) that it is proportional to the crystal size, consequently $f_0(\vec{r},n)$ diverges logarithmically with the crystal size. However, by taking into account the dislocation-dislocation correlation described by the function $D_2(\vec{r}_1,\vec{r}_2)$, the divergence can be canceled. Namely, for small n values the second term in expression (18) can be approximated by

$$\int D_2(\vec{r}_1,\vec{r}_2)B(\vec{r}-\vec{r}_1,n)B(\vec{r}-\vec{r}_2,n)d\vec{r}_1d\vec{r}_2\approx -G(\vec{r})n^2. \quad (43)$$

Assuming that $G(\vec{r})$ diverges also logarithmically with the crystal size, the sum of the two terms in Eq. (18) becomes crystal size independent. So up to second order terms the Fourier transform of the stress distribution has the form

$$A(\vec{r},n)=\exp\left\{i\langle\tau(\vec{r})\rangle n+C\rho(\vec{r})n^2\ln\frac{n}{R_{\rm eff}}+\cdots\right\}, \quad (44)$$

where $R_{\rm eff}$ can be regarded as effective outer cutoff radius. It is important to emphasize that in order to avoid crystal size dependence in $P(\tau)$ the dislocation-dislocation correlation has to be taken into account.

For obtaining the connection between the asymptotic behavior of $P(\tau)$ and $A(\vec{r},n)$ let us consider the variance of the stress distribution function

$$v(\tau)=\int_{-\tau}^{\tau}\tau'^2P(\tau')d\tau'. \tag{45}$$

As was mentioned earlier the second order moment of $P(\tau)$ is infinite, so $\lim_{\tau\to\infty}v(\tau)=\infty$. However, introducing the function

$$A_1(\vec{r},n)=A(\vec{r},n)-\frac{1}{4}A(\vec{r},2n) \tag{46}$$

and its Fourier transform

$$P_1(\vec{r},\tau)=\mathcal{F}[A_1(\vec{r},n)], \tag{47}$$

from Eq. (44) we obtain that

$$\lim_{\tau\to\infty}\int_{-\tau}^{\tau}\tau'^2P_1(\vec{r},\tau')d\tau'=-\left.\frac{d^2A_1}{dn^2}\right|_{n=0}=\ln 2C\rho(\vec{r}). \tag{48}$$

This means that for large stress values the variance of $P_1(\vec{r},\tau')$ can be approximated by

$$\int_{-\tau}^{\tau}\tau'^2P_1(\vec{r},\tau')d\tau'\approx\ln 2C\rho(\vec{r}), \tag{49}$$

i.e., its second moment is finite. On the other hand from Eqs. (46) and (47) one finds that

$$\int_{-\tau}^{\tau}\tau'^2P_1(\vec{r},\tau')d\tau'=\int_{-\tau}^{\tau}d\tau'\int_{-\infty}^{\infty}dn\,\tau'^2\left[A(n)-\frac{1}{4}A(2n)\right]\exp\{2\pi in\tau'\}. \tag{50}$$

After splitting the integral into two terms, and performing the $n\to 2n$ variable substitution in the second one we arrive at

$$\begin{aligned}\int_{-\tau}^{\tau}\tau'^2P_1(\vec{r},\tau')d\tau'&=\int_{-\tau}^{\tau}d\tau'\,\tau'^2\left[P(\tau')-\frac{1}{8}P(\tau'/2)\right]\\&=\int_{-\tau}^{\tau}d\tau'\,\tau'^2P(\tau')-\int_{-\tau/2}^{\tau/2}d\tau'\,\tau'^2P(\tau')\\&=v(\tau)-v(\tau/2).\end{aligned} \tag{51}$$

From Eqs. (49) and (51) the following function equation can be concluded for the variance $v(\tau)$:

$$v(\tau)-v(\tau/2)=2\ \ln 2C\rho(\vec{r}), \tag{52}$$

the solution of which is

$$v(\tau)=2C\rho(\vec{r})\ln\frac{\tau}{\tau'}, \tag{53}$$

where τ' is a parameter which cannot be determined from Eq. (52). It follows that the asymptotic behavior of the probability distribution has the form

$$P(\tau)\approx C\rho(\vec{r})\frac{1}{\tau^3}. \tag{54}$$

The results obtained above can be generalized for the case in which dislocations with opposite sign Burgers vectors are allowed. Without going into detail we mention that in the first moment of the distribution function $P(\tau)$ given by the expression (21), and in the asymptotic form (54) the dislocation density $\rho(\vec{r})$ has to be replaced by $\rho_+(\vec{r})-\rho_-(\vec{r})$ and $\rho_+(\vec{r})+\rho_-(\vec{r})$, respectively, where $\rho_+(\vec{r})$ and $\rho_-(\vec{r})$ denote the density of dislocations with positive and negative sign Burgers vectors.

CONCLUSIONS

The collective behavior of a system of parallel edge dislocations was investigated. Results of numerical simulations show that the stress field created by the dislocations can be approximated as the sum of a slowly varying and a stochastic component. According to our numerical observations the stochastic component can be well described as white noise. For determining the probability distribution of the stochastic stress component Markoff's method was applied. Since for avoiding crystal size dependence of the distribution function the dislocation-dislocation correlation function defined by expression (19) cannot be neglected Markoff's original formula[30] applied for several other systems and was generalized. It was found that the first order moment of the distribution function is equal to the self-consistent field of the dislocation system. The same stress field was obtained from the BBGKY hierarchy of different order dislocation distribution functions by neglecting dislocation correlations.[27] Furthermore, it was obtained that the probability distribution asymptotically decays with the inverse third power of the stress. For the homogeneous dislocation distribution (apart from a constant) this behavior can be easily obtained from dimensional analysis. Namely, the only expression which has the required inverse stress dimension and is proportional to the dislocation density is $cb^2\mu^2\rho/\tau^3$, where c is a constant. It is important to note, however, that the obtained asymptotic behavior is valid for an inhomogeneous dislocation distribution too, and depends only on the local dislocation density, i.e., it is independent from the nonlocal properties of the dislocation configuration and from the dislocation-dislocation correlation. The actual form of the correlation function $D_2(\vec{r}_1,\vec{r}_2)$ determines the half width of the probability distribution function through the correlation parameter $R_{\rm eff}$ (which can be approximated by the dipole width). A further important consequence of the $\sim 1/\tau^3$ asymptotic decay is that the second and higher order moments of the distribution function are infinite.

The results obtained make it possible to set up the framework of an $O(N)$ dislocation dynamics simulation method based on the stochastic approximation. The numerical simulations above show that each dislocation experiences a stress field with random character (see Fig. 1). According to expression (44) this random stress is described by the distribution function $P(\tau)$ which depends on the smoothed out dislocation densities $\rho_+(\vec{r})$, $\rho_-(\vec{r})$, and the correlation parameter $R_{\text{eff}}(\vec{r})$. [Since expression (44) determines only the Fourier transform of $P(\tau)$ for small Fourier parameters, $P(\tau)$ needs to be approximated by a function the Fourier transform which follows the form (44).] So, for the numerical investigation of the dynamic properties of an assembly of N dislocations the following stochastic algorithm is proposed.

(1) With an appropriate coarse-grain size the simulation area is divided into cells.

(2) In each cell the values of the smoothed out parameters $\rho(\vec{r})$, $\langle\tau(\vec{r})\rangle$, and $R_{\text{eff}}(\vec{r})$ are determined.

(3) Each dislocation is displaced by a random value generated according to the local stress distribution function $P(\tau)$.

(4) Go to 2.

The advantage of the method compared to the direct numerical integration of the equations of motion of dislocations demanding $O(N^2)$ calculation is that it requires only a $O(N)$ calculation. In addition the algorithm can be very efficiently implemented on parallel computers. Preliminary results show that the algorithm is able to reproduce similar dislocation configurations as the direct integration.

The method outlined above leads to a stochastic dislocation dynamics, but it needs to be stressed that it differs strongly from the one proposed by Hähner.[12,13] In that model the dislocation system is described by a single variable, the dislocation density time evolution of which is governed by a Langevin type equation. To determine the connection between the two approaches requires further investigations. Finally we mention that since in the derivation of the formula the $1/r$ nature of the dislocation interaction was used, rather than the special properties, the obtained expression can be generalized for other similarly interacting objects such as, for example, vortices in liquids.

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