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Statistical properties of dislocation mutual interactions

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Abstract. We compute the probability distribution density of mutual forces between edge and screw dislocation assemblies. The distribution is directly related to the internal stress distribution and can be revealed experimentally from x-ray profiles. Using numerical simulations, we compare the tail of the probability distribution for homogeneous and fractal dislocation arrangements.

Keywords: defects (theory), plasticity (theory)

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Contents

1. Introduction

The collective behaviour of interacting dislocations represents an interesting theoretical problem with direct applications to crystal plasticity. Dislocations are linear lattice defects interacting via long range anisotropic forces directly related to internal stresses in the material [1]–[5]. For this reason, dislocation dynamics displays complex features, such as avalanche motion [6]–[10], slow creep relaxation [11] and pattern formation [12]. Fractal dislocation structures have been observed directly by transmission electron micrography on plastically deformed metals [12] and indirectly by localizing acoustic emission sources during the viscoplastic deformation of ice crystals. Acoustic emission measurements represent as well a valuable tool to investigate the dislocation dynamics, which shows an intermittent widely fluctuating signal, distributed as a power law [9].

Numerical simulations represent an important method to investigate the mechanisms underlying plastic deformation [13]–[17], [9, 18]. The problem can be formulated at an atomistic scale, but due to numerical limitations it is difficult to understand in this way large scale collective effects. In this respect, a valid alternative is represented by mesoscopic simulations, considering the dynamics of interacting dislocations [13]–[17], [9, 18]. Dislocation dynamics simulations have been used mostly to study pattern formation [13]–[17], but also avalanches [9] and creep relaxation [18]. While a complete analytic treatment of these collective effects appears to be extremely complex, progress has recently been made by use of statistical methods [19].

Since dislocation arrangements are typically disordered, the internal stress in the material will also fluctuate from site to site. Linking the internal stress distribution to the dislocation arrangement is a well defined statistical problem, that has been recently studied for some particular cases [20]. This problem has direct analogies with the calculation of the gravitational force distribution to a random arrangement of stars [21] or the velocity distribution induced by vortexes in a turbulent fluid [22]. The internal stress distribution is an experimentally accessible quantity since it is directly related to the shape of the x-ray scattering peak [23]–[25]. Analytical results have been derived from some simple random dislocation arrangements: the amplitude of the distribution tail is proportional to the dislocation density ρ and it decays as $P(\sigma) \sim \sigma^{-3}$ [20]. Apart from its direct experimental implication, the internal stress distribution can be useful for numerical

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modelling. The contribution to the force acting on a dislocation due to near dislocation can be replaced by a random value, drawn from the appropriate distribution [26].

In this paper we complement previous results on internal stress distributions, deriving the force distribution for an uncorrelated random arrangement of edge and screw straight dislocation lines. The results are in agreement with previous estimates. Next we analyse the case of a fractal dislocation arrangement, computing numerically the internal stress distribution. We find that the tail of the distribution can be affected by the fractal structure. The presence of a small scale cut-off to the fractal behaviour has a strong effect on the distribution, screening the effect of large scale fractality. This fact has implications in the analysis of x-ray profiles from fractal dislocation arrangements.

2. Probability distribution of the interaction force for a dislocation system

We investigate the stress field probability density function (PDF) in a system of infinite dislocations. Under the assumption of straight parallel interacting dislocations, the stress field that the system exerts on a dislocation is proportional to the force that the dislocation undergoes and the system can be treated as a two-dimensional system of long range interacting points. We calculate therefore the force PDF, that, for an infinite system of uniform distributed self-gravitating particles, has already been calculated by Holzmark [27]. The force between two dislocations is given by the following expression, the Peach and Koehler formula [2]:

$$\vec{F}_{ij} = \hat{l}_i \times (\hat{\sigma}_j \cdot \vec{b}_i), \tag{1}$$

where $\vec{F}_{ij}$ is the force that a dislocation j exerts through the stress field $\hat{\sigma}_j$ on a dislocation i with Burgers vector $\vec{b}_i$ and a line versor $\hat{l}_i$. With the assumptions made above, the interacting force (1) between screw and edge parallel dislocations is zero. For two interacting screw dislocations according to (1) the force has only a radial component

$$\vec{F}_{ij} = \vec{F}_r = \frac{\mu b_i b_j}{2\pi r_{ij}} \hat{r}_{ij}, \tag{2}$$

where r_{ij} is distance between the dislocations i and j, b is the modulus of the Burgers vector and μ is the shear modulus of the metal. In the case of edge dislocations instead, the interaction force has a radial and a tangential component (in this case the Burgers vector is perpendicular to the dislocation line)

$$\vec{F}_r = \frac{\mu b_i b_j}{2(1-\nu)\pi r_{ij}} \hat{r}_{ij}; \qquad \vec{F}_{ij\perp} = \frac{\mu b_i b_j \sin 2\theta}{2(1-\nu)\pi r_{ij}} \hat{r}_{ij\perp}, \tag{3}$$

where $r_{ij\perp}$ is a versor perpendicular to the radial one $\hat{r}_{ij}$, θ is the angle between the Burgers vector and $\hat{r}_{ij}$ and ν is the Poisson ratio. From the expressions above it is clear that the interactions between dislocations have a long range character.

We consider the case of N uniformly distributed screw or edge dislocations, all with Burgers vector of modulus b. The distribution function we are looking for has the following form:

$$W(\vec{F}) = \frac{1}{(2\pi)^2} \int_{-\infty}^{+\infty} \left[\tilde{p}(\vec{k})\right]^N \exp(-\mathrm{i}\vec{k} \cdot \vec{F})\, \mathrm{d}^2\vec{k}, \tag{4}$$

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where $[\tilde{p}(\vec{k})]^N$ is its generating function. The condition of random spatial distribution for the dislocations allows its factorization. The function $\tilde{p}$ depends therefore on the spatial dislocations distribution $p(\vec{r})$ in the following way:

$$\tilde{p}(\vec{k}) = \int \exp\left(\mathrm{i}\vec{k}\cdot\vec{F}(\vec{r})\right) p(\vec{r})\,\mathrm{d}^2 r,$$

where for $p(\vec{r})$ the relation

$$p(\vec{r})\,\mathrm{d}^2 r = \frac{1}{\pi L^2}\,\mathrm{d}^2 r = W(\vec{F})\,\mathrm{d}^2 F$$

holds. Rewriting (4) we get

$$W(\vec{F}) = \frac{1}{(2\pi)^2}\int_{-\infty}^{+\infty}\left[\int_{r=0}^{L}\frac{1}{\pi L^2}\exp\{\mathrm{i}\vec{F}(\vec{r})\cdot\vec{k}\}\,\mathrm{d}^2 r\right]^N \exp\left(-\mathrm{i}\vec{k}\cdot\vec{F}\right)\mathrm{d}^2\vec{k}. \quad (5)$$

Letting $n = N/\pi L^2$ be the spatial distribution function, the generating function then has the simpler form

$$\lim_{L^2\to+\infty}\left[\tilde{p}(\vec{k})\right]^N = \exp\left[-n\int_0^L (1-\mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{F}(\vec{r})})\,\mathrm{d}^2\vec{r}\right] = \mathrm{e}^{-nC(\vec{k},L)}. \quad (6)$$

In the expression (6) we do not consider the integration extrema tending to infinity. As we will show later on, these extrema generate convergence problems for the probability function.

Screw dislocations. We express $C(\vec{k},L)$ as a function of the force. The Jacobian for the change of variable from r to F is in this case

$$|J| = \frac{\mu^2 b^4}{4\pi^2|F|^4}.$$

The function (6) is then

$$C(\vec{k},L) = \int_{|\vec{F}|=\epsilon}^{+\infty} a^2(1-\mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{F}})|F|^{-4}\,\mathrm{d}^2\vec{F}, \quad (7)$$

where, for sake of simplicity, we introduce the constant $a = \mu b^2/2\pi$ and $\epsilon = \mu b^2/2\pi L$. From the integration of the angular variable a Bessel function appears. Using the substitution $u = kF$ we get

$$C(\vec{k},L) = 2\pi a^2\int_{|\vec{F}|=\epsilon}^{+\infty}|F|^{-3}(1-J_0(kF))\,\mathrm{d}F$$
$$\cong \frac{\pi a^2 k^2}{2}\log\left(\frac{L}{ak}\right). \quad (8)$$

In the limit of $\vec{k}$ going to infinity, it holds that

$$C(\vec{k},L) \underset{k\to\infty}{\simeq} \frac{\pi a^2 k^2}{2}\log\left(\frac{L}{a}\right). \quad (9)$$

This approximation permits us to evaluate the PDF in the case of small forces. Under this approximation we get a Gaussian generating function. For this class of density functions the calculation of the variance is straightforward; we have

$$\langle F^2\rangle = \pi a^2 n\log L. \quad (10)$$

The variance diverges logarithmically with the extension of the dislocation assembly, but actually it is not possible for a Gaussian density function to have infinite moments. Such a pathology comes from the hypothesis that the dislocations can lie infinitely near to each other.

For small k, the behaviour of $C(\vec{k}, L)$ changes completely; we get

$$C(\vec{k}, L) \underset{k\to 0}{\simeq} -\frac{\pi a^2 k^2}{2}\log(k). \tag{11}$$

Substituting (11) and (6) in the relation (4) we obtain the PDF in the case of strong interactions, i.e.

$$W(\vec{F}) = \frac{1}{2\pi^2}\int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}\vec{F}\cdot\vec{k}} \mathrm{e}^{(\pi a^2/2)nk^2 \log k}\, \mathrm{d}^2 k. \tag{12}$$

Letting $\cos\theta = -t$ and $z = kF$, we find then

$$W(\vec{F}) = \frac{1}{2\pi^2}\,\mathrm{Re}\int_{-1}^{+1} \frac{\mathrm{d}t}{(1-t^2)^{1/2}} F^{-2}\int_{0}^{+\infty} \mathrm{e}^{\mathrm{i}zt}\mathrm{e}^{-nC(z/F)}\,\mathrm{d}z. \tag{13}$$

Written in this way the function $W(\vec{F})$ can be further simplified, first considering a Taylor expansion of the function $C(z/F)$ (we are considering now only the effect coming from strong forces), and secondly exploiting properties of the integral $\int_{-1}^{+1}\mathrm{d}t/(1-t^2)^{1/2}$. We get for the probability density of the modulus of the force the following expression:

$$W(F) \simeq \frac{n\mu^2 b^4}{12\pi F^3}\Gamma(4) = \frac{n\mu^2 b^4}{2\pi F^3}. \tag{14}$$

This result describes the behaviour of the tail of the force PDF for a homogeneous distributed parallel screw dislocation assembly: $W(F)$ is inversely proportional to the cube of the force intensity and proportional to the dislocation density n. Moreover, we get a logarithmically divergent second moment for the PDF. Such behaviour is not really astonishing; it is in fact already known that the elastic force for a homogeneous dislocation distribution has the same divergence problems.

Edge dislocations. We turn now our attention to edge dislocations. The calculation for this case proceeds in an analogous way as the calculations done above for the screw ones. Again, we calculate the Jacobian matrix for the change of variable $\vec{r} \to (\vec{F}_r, \vec{F}_\perp)$. In this case we get

$$|J| = \frac{\mu^2 b^4}{8(1-\nu)^2\pi^2} F_r^{-4}\left[1 - \left(\frac{F_\perp^2}{F_r^2}\right)\right]^{-1/2}.$$

Even here, let us consider $a = \mu b^2/2(1-\nu)\pi$. The function C, the exponent of the generating function, has the form

$$C(\vec{k}, L) = \frac{a^2}{2}\int_{F_r=\epsilon}^{+\infty}\int_{F_\perp=-\infty}^{+\infty} F_r^{-4}\left[1 - \left(\frac{F_\perp^2}{F_r^2}\right)\right]^{-1/2}(1-\mathrm{e}^{\mathrm{i}\vec{F}\cdot\vec{k}})\,\mathrm{d}F_r\,\mathrm{d}F_\perp, \tag{15}$$

where we take into account the dependence of the integral from the size of the system through the parameter $\epsilon = \mu b^2/2\pi(1-\nu)L$. Later on we will take the limit for $L \to +\infty$.

After trivial calculations we arrive at the following expression:

$$C(\vec{k},L) = \frac{\pi a^2 k^2}{\sqrt{2}} \int_{k\epsilon}^{+\infty} \frac{\cos(\bar{f}u)}{\bar{g}u}\,\mathrm{d}u$$
$$= \frac{a^2 k^2}{\bar{g}\sqrt{2}} \log\left(\frac{L}{a\bar{f}k}\right) \tag{16}$$

where $\bar{f} = 0.86$ and $\bar{g} = 1.50$ are numerical evaluated mean values over the interval $[0, \pi/2]$ of the functions $f(x) = (1+\sin^2 x)^{1/2}$ and $g(x) = 1 + \sin^2 x$. Even here the generating function C has a logarithmic dependence.

Again we evaluate C in the two limiting behaviours, one in the case of small values of k, i.e. strong forces, and one for big values of k, i.e. small force values. In the first case we get a Gaussian PDF; C is in fact

$$C(\vec{k},L) \simeq \frac{a^2 k^2}{\bar{g}\sqrt{2}} \log\left(\frac{L}{a\bar{f}}\right), \tag{17}$$

and the variance of the distribution diverges logarithmically with the system size

$$\langle F^2 \rangle = \frac{n\sqrt{2}}{\bar{g}} a^2 \log\left(\frac{L}{\bar{f}}\right). \tag{18}$$

In the limit for $k \to +\infty$ instead we get

$$C(\vec{k},L) \simeq -\frac{a^2 k^2}{\bar{g}\sqrt{2}} \log(a\bar{f}k). \tag{19}$$

The results found above differ from the case of screw dislocations just for a multiplicative factor. For strong forces we get the same power dependence of the probability density on the force intensity

$$W(F) \simeq \frac{na^2 8\sqrt{2}}{\bar{g}F^3}. \tag{20}$$

These results show how the distribution tail does not depend on the dislocation geometry, but just on the dislocation interaction type and on the dislocation distribution. These are in fact the only elements exploited for the derivation of the expressions (14) and (20).

3. The nearest neighbour distribution function

The behaviour of the force PDF for strong forces can be obtained considering the contributions to these forces due to the nearest neighbour dislocations. The nearest neighbour distribution (NND) gives the probability density of finding the first neighbour at a distance r and it is solution of the integral equation

$$p_{\mathrm{nn}}(r) = n(r)\left(1 - \int_0^r p_{\mathrm{nn}}(s)\,\mathrm{d}s\right), \tag{21}$$

$n(r)$ being the spatial distribution of dislocations. We assume that the force distribution for the nearest neighbour is given by

$$W_{\mathrm{nn}}(F) = \lim_{F\to+\infty} W(F) = \frac{\mu^2 b^4}{2\pi} nF^{-3}, \tag{22}$$

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as obtained in equations (14) and (20). We use the rule of change of variable for a density function, $p_{\mathrm{nn}}(r)\,\mathrm{d}r = W_{\mathrm{nn}}(F)\,\mathrm{d}F$; we can thus rewrite equation (21) getting an integral expression for $W_{\mathrm{nn}}(F)$.

We consider a fractal dislocation distribution with a lower cut-off below which the distribution is purely random. We then substitute the constant n in equation (22) with the following expression for the spatial distribution:

$$n(r) = \begin{cases} \rho_1 \left(\dfrac{r}{\lambda}\right)^{D-2} & \text{if } r > \lambda \\ \rho_1 & \text{otherwise} \end{cases} \tag{23}$$

where D is the fractal dimension of the distribution, λ is the lower cut-off and ρ_1 is the local density. In this case the solution of equation (21) is

$$W_{\mathrm{nn}}(F) = 2\pi\rho_1\lambda^{2-D}\left(\frac{\mu b^2}{2\pi}\right)^{D} F^{-(D+1)}. \tag{24}$$

Equation (24) shows that the amplitude of the PDF tail is proportional to the local distribution density and suggests that the power law decay of the internal stress PDF depends on the fractal dimension.

4. Numerical simulations

For a random dislocation arrangement, the PDF of mutual interactions should display at large forces a power law tail decaying as F^{-3}. When the arrangement is fractal, a simple argument shows that the tail of the distribution should change. In order to check this point, we generate a fractal arrangement of screw dislocations and compute the force PDF. A fractal arrangement with a given fractal dimension is obtained by a random Cantor set [28]. The random beta model is constructed considering a square system and dividing it equally in four squares. Each square is occupied with a given probability p. Occupied squares are subsequently divided into four parts, which are again occupied with probability p. The process is iterated a certain number of times (ideally *ad infinitum*), and finally dislocations are placed in the occupied squares. In this way, dislocations lie in a fractal with fractal dimension $D = 1 + \log(1+p)/\log 2$.

In figure 1 we report the force PDF for different values of the fractal dimension D. We notice that for low D the prediction of the simple argument described above is fulfilled: the PDF has a power law tail with exponent roughly equal to $D + 1$. However, as the fractal dimension is raised the power law tail disappears. This result is counterintuitive since one would naively expect that as D tends to 2 one should recover a power law tail with exponent -3. The argument fails and the tails are not observable because in a fractal the average quadratic force diverges unless the fractal dimension is small [28].

A more remarkable case is that of a fractal arrangement with a low scale cut-off. We consider a random Cantor set, but we randomly place dislocations with a density ρ_1 in the occupied squares. As shown in figure 2, the resulting force PDF tail is not affected by the large scale fractality of the arrangement: the tail decays as F^{-3} instead of $F^{-2.2}$. We compare this PDF with another class of correlated arrangement, the restricted random distribution introduced by Wilkens [29]. In this model, the lattice is divided into squares of linear size l, where we randomly place M dislocations. This creates a correlated

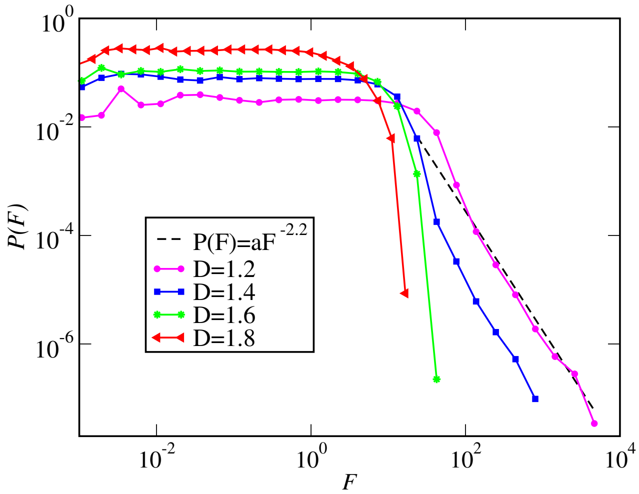

Figure 1. Comparison of the tail of the force PDF for fractal distributions with different fractal dimensions.

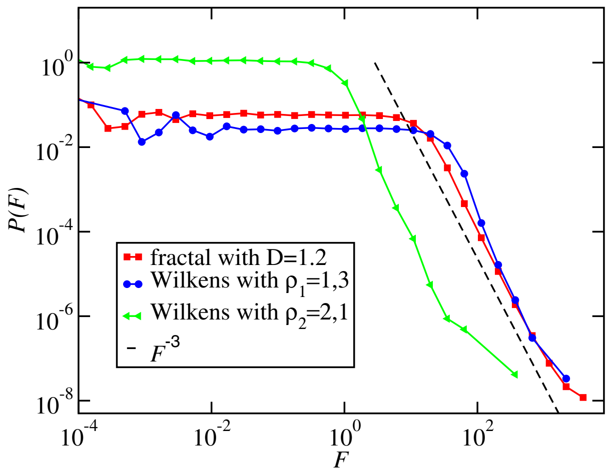

Figure 2. Comparison of the tail of the force PDF for fractal distribution with $D = 1.2$ and a lower cut-off. The PDF is compared with those obtained with a Wilkens model with local and global densities ρ_1 and ρ_2.

arrangement, and the force distribution scales as ρ/F^3, with $\rho = M/l^2$. For a fractal with a lower cut-off we can define two densities, the local density ρ_1 and a global density ρ_2, obtained dividing the total dislocation number by the size of the sample. Our simulations show that the PDF for the fractal is very close to an equivalent Wilkens model with a density ρ_1. This implies that in x-ray experiments the width of the profile may reflect the short scale dislocation density rather than the global dislocation density. The reason behind this observation is due to the fact that the tail of the distribution is dominated by the nearest neighbour distribution. This creates no problem for homogenous arrangements where the local and the global density are the same, but has drastic effects in the case of fractal arrangements.

5. Conclusions

In this paper we have analysed the statistical properties of the mutual interactions of random assemblies of dislocations. Using analogies with related calculations for a self-gravitating gas, we have computed the force PDF for a random distribution of edge and screw dislocations. The main features of the force PDF are in good agreement with results on the internal stress distribution computed in [30] with a similar approach. Next we have analysed the effect of large scale dislocation correlations on the internal stress distribution, using numerical simulations. In particular, we have considered fractal dislocation arrangements, which are relevant for several experimental situations [12]. An important result is that the short scale cut-off plays a key role in determining the distribution shape.

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