Complexity in dislocation dynamics: model

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We propose a numerical model to study the viscoplastic deformation of ice single crystals. We consider long-range elastic interactions among dislocations, the possibility of mutual annihilation, and a multiplication mechanism representing the activation of Frank-Read sources due to dislocation pinning. The overdamped equations of motion for a collection of dislocations are integrated numerically using different externally applied stresses. Using this approach we analyze the avalanche-like rearrangements of dislocations during the dynamic evolution. We observe a power law distribution of avalanche sizes which we compare with acoustic emission experiments in ice single crystals under creep deformation. We emphasize the connections of our model with non-equilibrium phase transitions and critical phenomena.

I. INTRODUCTION

The viscoplastic deformation of crystalline materials, such as ice single crystals, involves the motion of a large number of dislocations. Dislocations may be incorporated into a crystal in its growth process, or under deformation conditions. They can penetrate into the material from the sample surfaces, or be generated by various mechanisms, as for example, in what is usually called a Frank-Read source, activated by the pinning of a dislocation loop. The elastic force between a pair of dislocation lines decreases algebraically with the interline distance; it can be attractive or repulsive, depending on the orientation of their respective Burgers vectors; and eventually a pair of dislocations may annihilate at relatively short distances. As a consequence of all of these features, the collective behavior of a large number of these defects appears to be an amazingly rich problem, suitable to be studied from very different points of view.

A new insight into the classical issue of viscoplasticity was recently opened by Weiss and Grasso after their experimental study of the acoustic activity of ice crystals under creep. The complex character of the collective dislocation dynamics reveals itself in experiments of acoustic emission (AE), as reported in our companion paper in this volume. As a matter of fact, when a material is deformed under constant load (creep experiment) and dislocation motion is the dominant mechanism for viscoplastic deformation, a constant strain-rate regime usually follows after the initial transient stage. Orowan’s relation \( \dot{\gamma} = \rho_mbv \) is known to prevail under such conditions, where \( \gamma \) is the strain of the sample, \( \rho_m \) is the density of mobile dislocations, \( b \) is the Burgers’ vector, and \( v \) is the mean velocity of the dislocations. Obviously, this is a mean-field relation which neglects temporal and spatial fluctuations of both the density and the velocity fields. As a result of their interactions, however, dislocations tend to move cooperatively giving rise to a rather complex and heterogeneous slip process. Dislocations move in groups to form slip bands. Moving dislocations can pile-up against stable dislocation configurations such as walls or boundaries, which may eventually break apart.

Given the amplitude threshold and the frequency range accessible to the experimental apparatus, the AE signals detected seem to correspond to the synchronous motion of several dislocations, likely to occur during the breakaway of a pile of these defects, or the activation of a multiplication source. Various measurements of the acoustic activity recorded during a stress-constant step show that the AE signal takes place in the form of bursts distributed according to a power law. This behavior is certainly a consequence of the collective motion of dislocations which spontaneously gives rise to an avalanche-like dynamics, typical of slowly driven dissipative systems. The power law distribution provides evidence of scale-free cooperative behavior whose origin could be ascribed to nonequilibrium continuous phase transitions or self-organized criticality.

The AE experiments, however, have only access to information resulting from the interplay of various magnitudes. Thus, the physical interpretation of the generated AE waves remains a major difficulty, and constitutes the main motivation of this work.

II. DESCRIPTION OF THE MODEL

Our goal is to characterize the viscoplastic deformation of ice or a similar crystalline material from the perspective of nonequilibrium statistical mechanics. To do so, we propose a simplified model to study the dynamics of a collection of dislocations.
Ice crystals deform essentially by slip on the basal plane (0001) (xy plane), i.e. the motion of dislocation lines or loops takes place by gliding on the xy planes. The simplest Burgers vectors $b$ of a dislocation in a crystal of hexagonal ice are the primitive cell vectors of the conventional hexagonal lattice. We start studying a two-dimensional (2d) model representing a cross section of the crystal which is perpendicular to the basal planes and parallel to one of these lattice vectors, that is, for example, the xz plane. In this way, the dislocations constrained to move in this plane have all Burgers vectors parallel to the chosen lattice vector $b = (b,0,0)$ and move along fixed lines parallel to the x axis. We also consider that all $N$ dislocations are of edge type, and that, on average over many realizations, the number of dislocations with positive and negative Burgers vectors is the same.

Several 2d-models containing similar basic ingredients have been proposed in the literature in the last few years. A basic feature common to most models, is that dislocations interact with each other through the long-range elastic stress field they produce in the host material. An edge dislocation with Burgers vector $b$ located at the origin gives rise to a shear stress $\sigma^s$ at a point $(x, z)$ of the form

$$\sigma^s = bD\frac{x(x^2 - z^2)}{(x^2 + z^2)^2},$$

where $D = \mu/2\pi(1 - \sigma)$ is a coefficient involving the shear modulus $\mu$ and the Poisson’s ratio $\sigma$ for the material. In our model, we further assume that Peierls stress is zero and that the dislocation velocities are linearly proportional to the local stress. Experimental evidence supports such a relationship for low stress conditions, which is indeed the case in our model. Accordingly, the velocity of the $n$th dislocation, if an external shear stress $\sigma^e$ is also applied, is given by

$$v_n = b_n\left(\sigma^s_{nm} - \sigma^e\right).$$

As the number of dislocations in any real crystal exceeds by far the number of defects we can handle in a computer, one usually introduces periodic boundary conditions (PBC) to effectively extend the size of our system. To avoid the discontinuities arising from truncating long-range elastic interactions (see Eq. 1), we resort to the Ewald summation method. In this way, we have exactly accounted for the interaction of a dislocation with all the infinite periodic replicas of another dislocation in a finite cell of dimensions $L \times L$. Contrary to what is stated in Ref. 10, we do not find any spurious results coming from the implementation of PBC in this fashion.

When the distance between two dislocations is of the order of a few Burgers vectors, the high stress and strain conditions close to the dislocation core invalidate the results obtained from a linear elasticity theory (i.e. Eq. 1). In these instances, phenomenological nonlinear reactions describe more accurately the real behavior of dislocations in a crystal. In particular in our model, we account for the annihilation of dislocations with opposite Burgers vectors when the distance between them is shorter than $2b$. Thus the core of one dislocation in our model has a radius of size $b$.

Another important feature of any computer model is the implementation of a mechanism for the multiplication of dislocations in the sample. It is widely believed that the Frank-Read mechanism is the most relevant for a gliding process of dislocations under creep deformation. Indeed Frank-Read sources (FRS) have been observed in ice. In a FRS multiplication occurs by pinning of a dislocation segment on the basal planes due, for example, to a defect in the crystal, or to the very presence of dislocation dipoles, piles, and walls. If the local stress concentration is less than a critical value, the pinned segment bows out by glide. Beyond this critical value, the dislocation segment wraps around itself, creating a new dislocation loop and restoring the original configuration. Thus a sequence of loops forms continuously from the source until the local shear stress drops below the activation value. In order to simulate this mechanism, we split our system of size $L$ into smaller cells where, at each time step, we keep track of both the local fraction of pinned dislocations and the stress. Pairs of dislocations of opposite Burgers vectors are generated in a given cell if (i) there are pinned particles and (ii) if the local stress is large compared to a threshold value (the pair creation probability is proportional to the local stress). Each pair of dislocations reduces the local value of the stress, and we keep on generating pairs until the local stress drops below the threshold value. In such a way, we simulate the procession of dislocations often seen experimentally when a FRS is activated in a material.

To follow the time evolution of $N$ dislocations, we integrate numerically the $N$ coupled equations $dx_n/dt = b_n(\sum_{m\neq n}\sigma^s_{nm} - \sigma^e)$, where $\sigma^s_{nm}$ is given by Eq. 1, using an adaptive step size fifth-order Runge-Kutta algorithm. Simulations start from a configuration of $N$ point-dislocations randomly placed on a square cell of size $L$. So far, we have considered two different box sizes $L = 200b$, and $L = 300b$, with an initial number of dislocations $N_0 = 800$, and $N_0 = 1500$, respectively. We let the system relax in the absence of external stress, until it reaches a metastable arrangement. Annihilation and multiplication processes imply that the number of dislocations $N$ in our system is not fixed in the course of time. After the system has reached a metastable arrangement, the volume fraction of dislocations $\phi = N\pi b^2/(Lb)^2$ ranges between $1 - 5\%$. 


Once in these conditions, we apply a small external shear stress and keep track of the various quantities describing the dynamics of the dislocations. Averages are made over at least 50 realizations starting with different random initial conditions.

### III. CREEP DYNAMICS

In the evolution of our model, dislocations build up complex and highly fluctuating patterns containing, for example, dislocation dipoles and walls, similar to those experimentally observed [13,14].

If the external stress applied is not high enough to activate a FRS [15], our system simply relaxes very slowly. After a short initial transient, the root-mean-square velocity $(\sum_i v_i^2)^{1/2}$ and the mean strain rate $d\gamma/dt \sim \sum b_iv_i$ enter into a regime of power-law relaxation. In Fig. 1, we show in a double logarithmic scale the relaxation of $d\gamma/dt$. The power-law exponent is around $-0.65$. This scale-free behavior seems to correspond to what in the literature is known as Andrade’s power law creep, where the strain rate decays as $t^{-2/3}$, and, consequently, the strain grows like $t^{1/3}$. The inset of Fig. 1 shows the strain curve. Our best fit is obtained with an exponent of 0.28.

The features of this signal resemble those observed in apparently very different systems, such as fracturing of wood and concrete [10], Barkhausen effect [17], and flux lines in high-$T_c$ superconductors [18], and induces us to think in terms of avalanches. To define what an avalanche is in our system, we introduce an offset value of the signal to eliminate what we call the background noise. The latter can be thought of as the lower experimental resolution, but at the same time corresponds to the incoherent motion of $N_m$ independent dislocations. Thus, when the signal exceeds this offset, we will have an avalanche. The avalanche duration $T$ and magnitude $s = \sum T V$ increase until the signal drops down below the offset value. The cumulative distribution $P_c(s)$ of the avalanches obtained after averaging over several realizations is depicted in Figure 3 for the two system sizes studied $L = 200, 300$. We recover a clear power law distribution ($P_c(s) \sim s^{-\tau}$) extending over close to two decades. The exponent $\tau \simeq 0.6$ is in reasonable agreement with experimental data [3]. The universal properties of the distribution do not depend on the particular choice of the offset value. The distribution cut-off for large values of $s$ is due to the finite size of the sample. (As one would expect, the cut-off is scaling accordingly to the system size.) This

![FIG. 1. Mean strain rate as a function of time in our model of collective dislocation dynamics. The curve shown in the inset represents the global strain.](image1)

![FIG. 2. Number of dislocations $N$ and mean velocity $V$ as a function of time in a given run of our model with generation of dislocation pairs in FRS’s.](image2)
clearly points out the presence of a very large (or infinite) characteristic size for the acoustic events. It is worth remarking that larger stresses [15] introduce a characteristic scale in the process. A more detailed study as a function of the applied stress is in progress [12].

\[ P_c(s) \sim s^{-0.6} \]

**FIG. 3.** The cumulative avalanche size distribution \( P_c \) for two system sizes \( L = 200, 300 \) represented in a double logarithmic scale. The curves in the inset represent the raw distributions \( P(s) \).

**IV. CONCLUSIONS AND DISCUSSION**

The numerical investigation of the present model provides striking evidence for the collective critical behavior of dislocation motion under external stress. We have found two different regimes depending on the externally applied stress: i) For low stresses, the mean dislocation velocity and the mean strain-rate relax according to Andrade’s power law creep. ii) For higher stress values, the system activates FRS’s to which it responds exhibiting singular behavior in the guise of avalanches distributed over many length scales. The avalanche distribution is a power law which signals the absence of any characteristic size in the process. Avalanche dynamics is the rule rather the exception in slowly driven disordered systems [16–18]. Under the external drive (the stress in the present case), the system jumps between metastable or pinned configurations in which the dynamics is virtually frozen. In the limit of a very slow driving the disordered energy landscape is explored quasistatically and the response function exhibits critical properties [19]. Typically, a basic ingredient for this behavior is the presence of quenched disorder acting as the source of pinning in the system. Noticeably, the system under study does not contain any external source of disorder. Pinned states are due to the various structures such as dipoles, piles, and dislocation walls, that play the role of self-generated pinning centers that create the pinning force landscape. The new scenario poses many new and interesting questions for a definitive identification and understanding of the critical nature of dislocation dynamics.

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