Dislocation Glasses: Ageing during Relaxation and Coarsening

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The dynamics of dislocations is reported to exhibit a range of glassy properties. We study numerically various versions of 2d edge dislocation systems, in the absence of externally applied stress. Two types of glassy behavior are identified: (i) dislocations gliding along randomly placed, but fixed, axes exhibit relaxation to their spatially disordered stable state; (ii) if both climb and annihilation is allowed, irregular cellular structures can form on a growing length scale before all dislocations annihilate. In all cases both the correlation function and the diffusion coefficient are found to exhibit ageing. Relaxation in case (i) is a slow power law, furthermore, in the transient process (ii) the dynamical exponent \( z \approx 6 \), i.e., the cellular structure coarsens relatively slowly.

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Since dislocations are ubiquitous in crystals and they can have a dramatic effect on physical properties of materials, understanding the morphology and dynamics of dislocations is of fundamental importance. They are the carriers of plastic deformation in solids [1] and are unwelcome impurities in single-crystal growth [2]. In 2d they play a crucial role in melting [2], appear in Wigner crystals [2], and dislocations in vortex lattices [3] determine properties of superconducting films [3]. Further examples where dislocations arise include magnetic bubble structures [7], charge density waves [8], colloidal lattices [9], and dusty plasma [10].

The morphology of dislocations is one of the most studied and least understood aspects of crystal defects. While there is a multitude of dislocation patterns, one can discern a few generic types. Such are fractals and ladders in the presence of external shear [11], as well as cellular and diffuse configurations in unsheared crystals. The latter ones were discussed in the remarkable recent experimental papers by Rudolph et al. [2, 12] with the conclusion that climb mobility of dislocations has an important effect on morphology. Specifically, when there is climb then cells of some characteristic length scale can form, or, if climb is suppressed, dislocations freeze into a diffuse-looking random distribution. A recent work by the present authors corroborated this finding on the basis of mesoscale simulations [13].

Just a glance at disordered dislocation configurations from experiments [2] and simulations [13, 14] suffices to raise the question, to what extent dislocations exhibit glassy properties. Indications of slow equilibration came recently from numerical studies of relaxing 2d dislocation systems [15]. A physical argument for the glass analogy is that the long-range interaction between dislocations can change sign as function of relative angles, thus making frustration possible. Frustrated interactions are known to give rise to spin glasses in the presence of quenched disorder [16]. Furthermore, there is an external element of randomness in dislocation systems that arises from initial conditions. This reinforces the analogy, because random initial conditions due to quenching from the high-\( T \) state are an essential ingredient in structural-glass-formers, like in Lennard-Jones systems [17], and lead to slow growth of irregular domains even in systems as simple as the Ising model [18].

There is a growing body of knowledge about the dynamics of glasses (see [18] and refs. therein). A central feature of glassy dynamics is the dramatic slowing down when the temperature is lowered [19]. Not only does the dynamics slow down, but it also exhibits ageing, widely considered as a hallmark of glassy dynamics [20]. There are several qualitatively different types of systems exhibiting ageing, such as (i) spin glasses with quenched disordered interactions, (ii) systems approaching a non-glassy equilibrium state, while random initial condition, possibly augmented with kinetic constraints, slow down relaxation, and (iii) structural glasses wherein long-time disorder originates in initial condition.

In this Letter we study the dynamics of edge dislocations in 2d by mesoscale simulations [13], wherein dislocations are the particles interacting by their stress fields and obeying overdamped dynamics. While this is a strong simplification of real 3d dislocation networks, for FCC crystals under certain conditions it is a reasonable approximation, and it is of course relevant for defects in 2d lattices. Two main situations are considered, in the first one dislocations only glide along the axis of their Burgers vector, in the second one they can also climb perpendicular to it, and here we also allow annihilation. Climb has a dramatic effect, without it dislocations relax to a (meta)stable state, while climb with annihilation results in an increasingly dilute system and eventually all dislocations vanish, corresponding to the dipolized state predicted long time ago [3]. In both situations we study the cases of a single and three glide axes. The effect of temperature on ageing is tested by the addition of a
Our main observations are as follows. (1) Dislocation configurations after a fast initial transient depend on whether climb is possible and on the number of glide axes. With climb, walls form for both the 1- and 3-slip systems, in the latter leading to a cellular structure with a pronounced length scale, whereas without climb typical configurations appear more disordered. (2) All systems exhibit ageing, that is, both the correlation function and the effective diffusion coefficient of dislocations depend on the waiting time. (3) In the absence of climb the correlation functions decay by a power law while a stable state is approached. (4) Sufficiently high temperature restores non-ageing dynamics. (5) With climb, the time exponent $z$ is identified, characterizing the growth of the mean domain diameter.

First we discuss the details of the simulation. Three different possible Burgers vectors defined by the directions $\pm (\cos(m\uppi/3), \sin(m\uppi/3))$, $m = 0, 1, 2$ in a square area of size $L \times L$ was considered with periodic boundary conditions. This geometry emulates a hexagonal underlying lattice. In order to calculate the stress field of a dislocation with Burgers vector $(b_x, b_y)$, we use the formalism developed by Kroner [1]. The stress function $\chi(r)$ for this problem fulfills the biharmonic equation

$$\nabla^4 \chi = C(b_x \partial_y - b_y \partial_x) \delta(x) \delta(y),$$

(1)

with $C = 2\mu/(1 - \nu)$ in 3d and $C = 2\mu(1 + \nu)$ in 2d, where $\mu$ is the shear modulus and $\nu$ Poisson’s ratio. From $\chi(r)$ the stress components are $\sigma_{xx} = -\partial_y \partial_x \chi$, $\sigma_{yy} = -\partial_x \partial_y \chi$, $\sigma_{xy} = \partial_x \partial_y \chi$. The force $F$ per unit length acting on a dislocation with Burgers vector $b$ is given by the Peach-Koehler formula $F = (\tilde{\sigma} b) \times l$ in which $l = (0, 0, 1)$ and the stress $\tilde{\sigma}$ is due to all other dislocations. Equation (1), discretized to $M^2$ points, with periodic boundary conditions, can be solved for $\chi$ by using the Fourier transform (FT) of the partial difference operator, $D_m = \frac{2\uppi}{\sqrt{2\uppi}L} \sin \left( \frac{\uppi m}{L} \right)$, where $m = 0, \ldots, M - 1$. Then one obtains the FT of the stress function as

$$\hat{\chi}_{lm} = C(b_x D_m - b_y D_l) / [D^2_x + D^2_m];$$

(2)

yielding the FT of the stress components $\tilde{\sigma}_{xx} = -D_l D_l \hat{\chi}_{lm}$, $\tilde{\sigma}_{yy} = -D_m D_m \hat{\chi}_{lm}$, $\tilde{\sigma}_{xy} = D_l D_m \hat{\chi}_{lm}$. Inverse FT gives the stress components at the grid points for a single dislocation. For the effect of all dislocations, in $\hat{\chi}_{lm}$ we replace $b$ by the FT of the discretized Burgers vector field. While we keep track of the dislocation positions to high precision, the stress field is discretized to $M = 256$. Note that this recipe suppresses interactions between dislocations in the same box, but in our case such concurrence is rare. By applying fast FT, for up to 10000 dislocations the above algorithm is about 10 times faster than the direct calculation of the pair interactions, for more details see [13]. Assuming overdamped dislocation dynamics, the $\mathbf{v}^g_i$ glide and $\mathbf{v}^c_i$ climb velocity components of the $i$th dislocation are

$$\mathbf{v}^g_{g,c} = \Gamma_{g,c} (\mathbf{F}^i a^i_{g,c}) + \sqrt{2\uppi T_{g,c} \xi^g_{g,c}} a^i_{g,c},$$

(3)

where $\mathbf{F}^i$ is the Peach-Koehler force given above, $\Gamma_g$ and $\Gamma_c$ are the glide and the climb mobilities, respectively, $a^i_{g,c} = b_i/|b_i|$, and $a^i_{g,c}$ is a unit vector perpendicular to $a^i_{g,c}$. Thermal fluctuations at temperature $T$ are included as white noise $\xi_{g,c}(\mathbf{r}, t) = \delta(t - t')$. (So as to eliminate material parameters the dimensionless variables $r \Rightarrow r/L$, $t \Rightarrow T \xi_{g,c} C^2/4\pi L^2$, and $T \Rightarrow 4\pi T/C^2$ are used henceforth.)

In order to study the morphology of dislocations, we considered dynamics without and with climb, and in either case we took 1 as well as 3 glide axes. Simulation started out from random initial conditions of 10000 dislocations, specifically, axes were placed independently, with a uniform distribution, and the sign of the Burgers vector was also randomly chosen such that for each axis direction they compensated each other. No shear is imposed through external traction, as we intend to study dislocations originating from some internal inhomogeneities. If climb is present, dislocations can get arbitrarily close to each other, so we annihilated dislocations of opposite Burgers vectors in the same box. Figures 1h–d show typical configurations, without climb (a,b) and with climb and annihilation (c,d), in each case for 1 and 3 slip axes, respectively. Configurations (a,b) are near equilibrium, they show diffuse distributions, but in the single slip case the formation of walls is apparent, in accordance with recent analytic results [21]. On (c,d) transient states are snapshot, where the predominance of walls is apparent. Dislocations eventually annihilate, in agreement with the classic prediction [3] of dipolized equilibrium well below the melting point. As we have reported in [12], walls form cells in the 3-slip case as seen in Fig. 1i. The picture shows a close resemblance to some dislocation patterns in 2d dusty plasmas [10], highlighting the experimental relevance of our simulation. Furthermore, our results are in qualitative concordance with recent experimental studies [12], where, in off stoichiometric GaAs, cell formation was attributed to increased climb mobility. So we can conclude that first and foremost the presence of climb, but also the number of slip axes, strongly affect the morphology of dislocations. It is common for all cases presented here, that random initial conditions result in disordered configurations, calling for studies into glassy properties of dislocation systems.

Aiming at quantifying the glassy character of dislocation dynamics we focus on ageing (see [18]). In particular, we study the dependence on the waiting time of the correlation, or overlap, function

$$C(t, t_0) = \frac{1}{N} \sum_{i=1}^{N} \exp \left[ -|\mathbf{r}_i(t + t_0) - \mathbf{r}_i(t_0)|/\xi_0 \right].$$

(4)
indicates power law with
This is shown on the right inset, where the straight line
due to limitations in computational power) for a se-
function on Fig. 2. The asymptotic value
−
\( C(t_w, t) \approx \frac{1}{N_d} \sum_{i=1}^{N_d} |\mathbf{r}_i(t + t_w) - \mathbf{r}_i(t_w)|^2 \), \[ (5) \]
where somewhat arbitrarily \( r_0 = 5/\sqrt{N_d} \), and the effective diffusion coefficient
\( D(t_w, t) = \frac{1}{N_d} \sum_{i=1}^{N_d} |\mathbf{r}_i(t + t_w) - \mathbf{r}_i(t_w)|^2 \),
where \( N_d \) is the number of dislocations remaining at the final observation time. Here \( C \) and \( D \) should be conceived as time \( t \) dependent quantities, recorded after a waiting time \( t_w \).
FIG. 1: Snapshots of relaxed dislocation configurations without climb (\( \Gamma_c = 0 \)): (a) single slip (b) 3-slip, and typical wall structures with climb (\( \Gamma_c/\Gamma_b = 0.1 \)): (c) single slip, (d) 3-slip.
First we consider the situation without climb, with 3 slip axes, at zero temperature, and plot the correlation function on Fig. 2. The asymptotic value \( C_\infty(t_w) = C(t_w, \infty) \) markedly depends on \( t_w \) (left inset). Generically, beyond the inflexion point correlations decay exponentially, followed by a power form \( t^{-\beta} \). Thus it is natural to consider the curves \( 1 - (1 - C)/(1 - C_\infty) \) decaying in time \( t \) from 1 to 0, which are found to collapse approximately to a master curve as function of \( t/t_w^{2/3} \). This is shown on the right inset, where the straight line indicates power law with \( \beta \approx 0.54 \). Note that the fact that \( t_w \) and \( t \) have different exponents contradicts standard scaling formulas in ageing (see [15]), an anomaly for which we do not have an explanation and requires further studies. It is worth recalling here that power decay of the elastic energy was found before in [15]. So we can conclude here that there is a strong analogy with spin glasses inasmuch that there is a quenched randomness in the placement of the slip axes, which confine dislocations along the entire dynamics, and the relaxation towards a disordered ground state exhibits ageing. Next we study the dynamics of the 3 slip system without climb in the presence of a small Langevin noise, \( T = 0.025 \). Then the system never fully relaxes, but before some stationary state is reached it also exhibits ageing, as demonstrated in Fig. 3. Plot (a) shows the correlation function decaying expectedly to zero (we did not reach the asymptote due to limitations in computational power) for a sequence of waiting times. On (b) the diffusion coefficient is shown, where lower lying curves correspond to increasing \( t_w \). Asymptotically we found \( D(t_w, t) \approx D_0 + D_1(t_w)t^{-\gamma} \) with \( D_0 \approx 2.2 \times 10^{-7}, \gamma \approx 0.8 \), see upper right log-log inset. The power decay to \( D_0 \) can be considered as a manifestation of slowed-down dynamics, which may appear for intermediate \( t \)-s as effectively subdiffusive. To test whether the remanent diffusion constant \( D_0 \) is physically relevant or only due to finite size effects, we halved the effective linear system size by running a simulation with \( N_d = 2500 \). The lower left inset shows that the asymptotic \( D_0 \) does not change significantly for varying system size, so ordinary diffusion indeed prevails.
Finally, we considered dislocations with climb and annihilation for 3 slip axes. Here the number of dislocations \( N_d \) is a decreasing function of time, and after an initial transient the dislocations order into cellular structures, whose characteristic length scale grows while dislocations annihilate. Figure 4 shows the ageing effect in the over-
FIG. 2: Correlation function \( C(t_w, t) \) for 3-slip, without climb at \( T = 0 \) as function of \( t \) for different \( t_w = 1, 2, ..., 2048 \). Increasing \( t_w \) leads to slower decay. Left and right inset show the asymptote and the scaling form, resp.
be associated with the logarithmic growth in the random field model can.

Ising model with Glauber and Kawasaki dynamics, and the exponent here is in the order of approximately like in Fig. 3. Inset in (a) is the plot of the correlation function at a sufficiently high temperature showing that the dependence on the waiting time $t_w$ is practically lost.

FIG. 4: Correlation function (a) and diffusion coefficient (b) for 3-slip, without climb, $T = 0.025$, as function of $t$ for various $t_w$-s. Upper inset in (b) shows the decay to the asymptotic $D_0 = 2.2 \times 10^{-7}$ and lower inset gives $D(0,t)$ for two system sizes.

their transients do show ageing and, on short time scales, further glassy characteristics were detected recently. A common property of those systems is the asymptotic scaling of the characteristic domain size $\ell$ with time as $\ell \propto t^{1/z}$. For instance, $z = 2, 3$ corresponds to the 3d Ising model with Glauber and Kawasaki dynamics, and the logarithmic growth in the random field model can be associated with $z = \infty$, see [13]. Earlier we found numerically that the number of dislocations decreased approximately like $N_d \propto t^{-\delta}$ with $\delta$ approximately 1/3 [13]. Hence, based on the scaling of all lengths by the dislocation number we can conclude that the dynamical exponent here is in the order of $z \approx 6(1)$, where the error estimate is subjective. This relatively large exponent means that the glassy transient lasts for comparatively long times and may explain why the cellular structure can persist under experimental conditions.

We can summarize the physical picture of disordered dislocation systems as follows. In the absence of climb, where the external disorder is in the random but fixed placement of glide axes, there is an analogy with spin glasses in that the dislocation system has a multitude of near ground states, to one of which it relaxes. No increasing length scale was discerned at this stage of simulation. On the other hand, with climb, the ever growing cellular structure resembles the domain growth in, say, the Ising model launched after a quench from a paramagnetic state and showing glass-like dynamics. In each case there is a pronounced ageing effect in both the correlation function and the diffusion coefficient at zero and small temperatures. Interestingly, we did not encounter dislocation states analogous to structural glasses, probably because dislocations moving without constraints can annihilate. Our results are, however, strongly suggestive that we can speak about dislocation glasses, where the types of glasses are distinguished by different morphologies.

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