Jamming, Pattern Formation, and Dynamic Phases for Driven Dislocation Assemblies

Caizhi Zhou, CNLS/T-3;
Irene J. Beyerlein, T-3;
Charles Reichhardt, T-4;
Cynthia Olson-Reichhardt, T-1

Dislocation structures within individual crystals organize into patterns ranging from tangles to cells to planar walls, becoming more refined as stress or strain increases. Under a drive, pileups and intermittent dynamics arise near the depinning transition, but correlations between patterning and the intensity of applied stress or strain have not been established. We demonstrate that driven dislocation assemblies exhibit the same non-equilibrium phases as those observed for collectively interacting particle systems, such as vortices in superconductors or sliding charge-density waves. The analogous phases are a jammed state below yielding, a strongly fluctuating intermediate state above yielding, and a quasi-ordered phase at higher drives, detectable via dislocation structure, mobility, velocity distribution, and velocity noise. This implies that many established results obtained for driven vortices can be applied to dislocation dynamics.

The dynamics and pattern formation of dislocations are of tremendous importance for understanding materials properties. Driven dislocations are also an outstanding example of a non-equilibrium many-body system where a number of competing interactions come into play. Of particular interest is how the dislocations can organize themselves into patterns under different applied loads, how these patterns can be characterized, and whether there are distinct dynamic phases as a function of load. It is known that organized dislocation structures within individual crystals, such as tangles, cells, or planar walls, can become more refined and better defined as stress or strain increases.

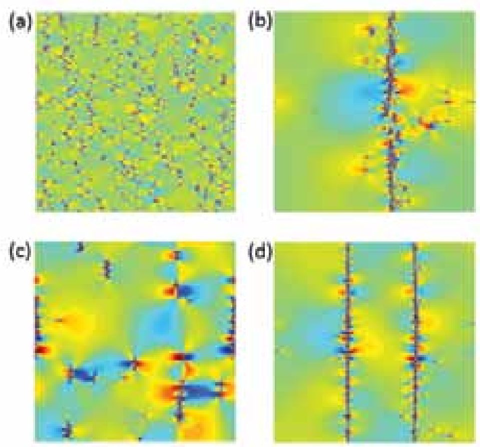

Fig . 1. Stress maps of the sample range from large negative (blue) to large positive (red) stress. (a) The initial dislocation positions at zero load. (b) Just before yielding, the dislocations are predominantly located at pile-ups to form a single bipolar wall. (c) Above yielding at F_d = 3.6, the wall breaks apart and the structure exhibits intermittent dynamics. (d) At F_d = 8.0 there is a dynamical ordering into polarized walls, each composed of dislocations with the same Burgers vector orientation.

2D and 3D dislocation dynamics simulations based on linear elasticity theory predict self-organization of dislocation assemblies into varying configurations, such as pileups near the yielding or depinning transition [1] and 2D mobile walls [2] or 3D slip bands [3,4] under an external drive. Below a critical stress where dislocations show no net motion, the system is considered jammed [5], while intermittent or strongly fluctuating behavior with highly jerky or avalanche-like motion occurs above the critical stress [1,4]. Avalanche behavior with power-law velocity distributions is proposed to be a signature of critical dynamics [1,4-6]. No correlations between the transitions in patterning and the intensity of applied stress or strain have been established before now. Another important problem is whether the patterning could determine how the yielding changes as a function of dislocation density.

We utilize a discrete dislocation dynamics model with periodic boundary conditions for a 2D cross-section of a sample containing straight-edge dislocations that glide along parallel slip planes. The dislocations interact via a long-range anisotropic stress field that is attractive between two oppositely signed dislocations and repulsive for liked-signed pairs. Under an external applied stress τ_{ext}, dislocation i moves along x in its assigned plane according to an over-damped equation of motion given by

$$\eta \frac{dx_i}{dt} = b_i \sum_{j\neq i}^{N} \tau_{\text{int}}\left(r_j - r_i\right) - \tau_{ext} \qquad (1)$$

where x_i is the x coordinate of ith dislocation at point $r_i = (x_i, y_i)$ with Burgers vector b_i, η is the effective friction and $\tau_{\text{int}}(r_j - r_i)$ is the long-range shear stress on dislocation i generated by dislocation j. For $r = (x, y) = (x_j, y_j) - (x_i, y_i)$, $\tau_{\text{int}}(r_j - r_i)$ for an edge dislocation with Burgers vector b is

$$\tau_{\text{int}}\left(\boldsymbol{r}\right) = b\mu \frac{x(x^2 - y^2)}{2\pi(1-\nu)\left(x^2 + y^2\right)^2} \qquad (2)$$

where μ is the shear modulus and ν is the Poisson's ratio.

After randomly placing the dislocations in the simulation volume, the system is allowed to relax without external load, so that the dislocations can achieve an equilibrium configuration to minimize the system energy (Fig. 1(a)). With external load F_d increasing, the dislocation structure changes(Fig. 1(a)-(d)) and produces signatures in $\langle|v|\rangle$ versus F_d as shown in Fig. 2.

Below yielding, the dislocation pattern slowly changes and gradually forms a dipolar wall (Fig. 1(b)) after each load increment but $\langle|v|\rangle$goes to zero in the long-time limit, indicating that the system is in the jammed phase below the critical yield. Just above yielding, the dipolar wall structure breaks down as shown in Fig. 1(c) and the system enters a state characterized by strong fluctuations in the dislocation positions.

For more information contact Irene J. Beyerlein at irene@lanl.gov.

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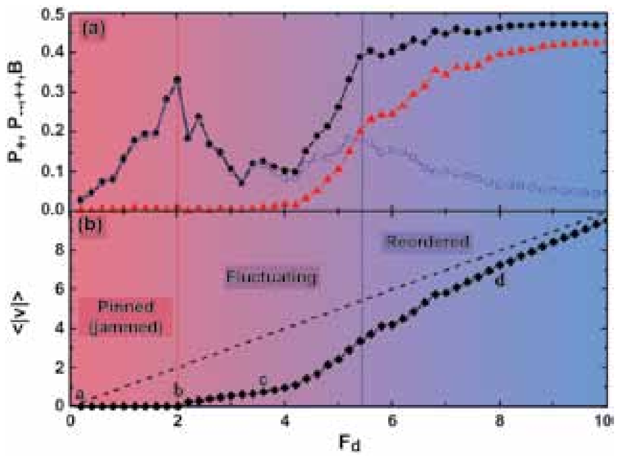

Fig. 2. (a) P_{+-} (blue squares), the fraction of dipolar walls, versus F_d has a peak just below yielding. $P_{--,++}$ (black circles), the fraction of uni-polar walls, passes through a plateau when the polarized wall state forms. B (red triangles) is a measure of the net Burgers vector in the walls. (b) The average absolute value of the dislocation velocity <|v|> (solid lower curve) versus F_d. The upper dashed curve shows <|v|> for non-interacting dislocations. Visible in the lower curve is a yielding point, a nonlinear region corresponding to the disordered or fluctuating regime, and a linear region at high drives when the system is dynamically ordered. Points a, b, c, and d indicate the F_d values illustrated in Fig. 1.

Under high drive, the dislocations form unipolar walls composed of only one type of dislocation, either negative or positive as shown in Fig. 1(d).

By conducting a series of simulations for varied dislocation densities, ρ, and analyzing the ordering dynamics, we construct the dynamic phase diagram shown in Fig. 3. The lower curve indicates the yielding transition from the low drive jammed or pinned phase of dipolar walls to the fluctuating disordered phase. The onset of the dynamically ordered phase is defined as the force at which the unipolar wall structures start to form, and is plotted in the upper curve. As ρ increases, the yielding point rises to higher F_d since the dislocations have a more difficult time breaking through the dipolar walls that form. The increase in yield threshold with increasing ρ remains robust when we perform simulations with different initial dislocation configurations. In addition, the onset of the high-drive dynamically ordered phase also increases in a similar fashion with increasing ρ. This phase diagram exhibits the same features observed for vortex systems as a function of pinning strength versus external drive, where both the critical depinning force and the onset of the ordering rise to higher drives with increasing pinning strength [7].

To summarize, we have shown that driven dislocation assemblies exhibit several distinct non-equilibrium phases as a function of drive that are associated with the formation of distinct dislocation patterns. The jammed to yielding transition is correlated with the formation of 1D dislocation pile ups, and above yielding the system transitions into a fluctuating intermittent phase where the dislocation structures break apart and reform. This is followed at higher loads by a more ordered state of moving polarized dislocation walls. All of the states are associated with transport signatures such as changes in the transport noise fluctuations as well as features in the dislocation velocity versus applied shear, in analogy with velocity-force curves. We also find that the transition from the jammed state to the polarized moving wall state moves linearly to higher load with the dislocation density. Finally, we note that many of the features described here are remarkably similar to the dynamic phases observed in driven many-body systems with quenched disorder, such as vortices in type-II superconductors.

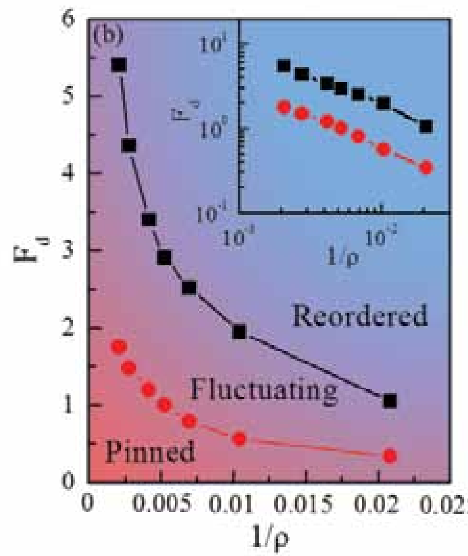

Fig. 3. The dynamical phase diagram F_d versus $1/\rho$, where ρ is the dislocation density. The lower curve (red circles) indicates the onset of yielding and the upper curve (black squares) is the onset of the dynamically induced ordered phase; the fluctuating phase falls between the two curves. Both the critical yielding and the dynamical ordering shift to higher drives as the ρ increases. Inset: The same curves plotted on a log-log scale.

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