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Nonequilibrium states of driven disordered polymorphic solids

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Abstract

Condensed matter systems, when driven far from equilibrium, often exhibit a far more varied set of phases than their equilibrium counterparts. The existence of non-equilibrium analogs of 'solids' and 'liquids' has been demonstrated earlier in the context of models for driven disordered vortex lattices in superconductors. Here we study the effects of a structural (polymorphic) transition in a driven two-dimensional crystal placed in a quenched random background. Such a polymorphic crystal is shown to exhibit a complex sequence of unusual dynamical phases as the external drive is varied, including some which have no analog in the undriven pure system. We propose that such states should be accessible in experiments.

Keywords: Driven systems; Nonequilibrium phase transitions; Structural transitions; Vortex matter; Hexatic glass

1. Introduction

Many condensed matter systems are capable of existing in more than one crystalline form (polymorphs). Even non-material lattices, such as Abrikosov flux-line lattices in the mixed state of type-II superconductors [1] or Skyrmion lattices in quantum Hall systems [2] can transit between different (triangular and rectangular) crystalline symmetries [3] as parameters such as the magnetic field are varied. Colloidal PMMA spheres coated with a low-molecular weight polymer undergo a remarkable variety of solid–solid transformations in an external field [4]. What is the effect of quenched disorder on the static and dynamical properties of such systems? While the depinning and flow of periodic media over a quenched randomly pinned (disordered) background has been extensively studied [1], the implications of an underlying structural transition remains unexplored. Here we report recent results on the complex non-equilibrium phase behaviour exhibited by a two-dimensional crystal driven across a disordered background, when the ground state of the crystal is tuned through a square–triangular transition.

Our model solid is a two-dimensional system of particles interacting via two and three-body interactions [6]. In addition, particles also interact with a one-body substrate potential which acts as a quenched random

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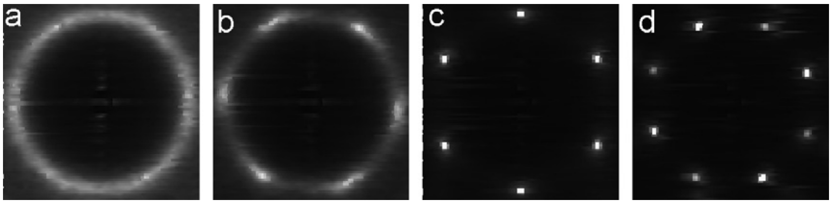

Fig. 1. Structure factor $S(\mathbf{q})$ for the plastic flow state (a), driven hexatic glass (b), moving triangle (c) and moving square solid phases (d) at $v_3 = 6.0$ and $F_x = 10, 20, 60$ and 140, respectively. To obtain $S(\mathbf{q})$, 50 independent configurations were used. The structure in (d) reflects the presence of two mutually misoriented square crystallites.

background. The interaction Hamiltonian is:

$$H_{int} = 1/2\sum_{i\neq j} V_2(r_{ij}) + 1/6\sum_{i\neq j\neq k} V_3(r_i, r_j, r_k) + \sum_i V_d(r_i),$$

where $\mathbf{r}_i$ is the position vector of particle i, $r_{ij} \equiv |\mathbf{r}_{ij}| \equiv |\mathbf{r}_j - \mathbf{r}_i|$, $V_2(r_{ij}) = v_2(\sigma_0/r_{ij})^{12}$ and $V_3(r_i, r_j, r_k) = v_3[f_{ij}\sin^2(4\theta_{ijk})f_{jk} + \text{permutations}]$ [6]. The function $f_{ij} \equiv f(r_{ij}) = (r_{ij} - r_0)^2$ for $r_{ij} < 1.8\sigma_0$ and 0 otherwise and θ_{ijk} is the angle between $\mathbf{r}_{ji}$ and $\mathbf{r}_{jk}$. The two-body (three-body) interaction favours a triangular (square) ground state. Energy and length scales are set using $v_2 = 1$ and $\sigma_0 = 1$. The three-body interaction, parametrized through a single parameter v_3, tunes the system across a square–triangular phase transition. The quenched random background is modeled as a Gaussian random potential [7] $\mathrm{V}_d(\mathbf{r})$ with zero mean and exponentially decaying (short-range) correlations. The disorder variance is set to $v_d^2 = 1$ and its spatial correlation length is $\xi = 0.12$.

Our system consists of 1600 particles in a square box with periodic boundary conditions, and at number density $\rho = 1.1$. In what follows, we chose a typical value $v_3 = 6$ that supports a square-symmetry in the ground state. The system is subject to a constant force $\mathbf{F} = \{F_x, 0\}$ at a fixed temperature T and evolves through standard Langevin dynamics; $\dot{\mathbf{r}}_i = \mathbf{v}_i$ and $\dot{\mathbf{v}}_i = \mathbf{f}_i^{\text{int}} - \alpha\mathbf{v}_i + \mathbf{F} + \eta_i(t)$. Here $\mathbf{v}_i$ is the velocity, $\mathbf{f}_i^{\text{int}}$ the total interaction force, and $\eta_i(t)$ the random force acting on particle i. The zero-mean thermal noise $\eta_i(t)$ is specified by $\langle\eta_i(t)\eta_j(t')\rangle = 2T\delta_{ij}\delta(t - t')$ with $T = 0.1$, well below the equilibrium melting temperature of the system. The unit of time $\tau = \alpha\sigma_0^2/v_2$, with $\alpha = 1$ the viscosity.

Configurations obtained through a simulated annealing procedure are the initial inputs to our Langevin simulations. We evolve the system using a time step of $10^{-4}\tau$. The external force F_x is ramped up from a starting value of 0, with the system maintained at up to 10^8 steps at each F_x. Below a critical force F_c, the system remains pinned to the substrate and above F_c it depins and starts to move. In the moving non-equilibrium steady state we obtain a variety of phases: a moving liquid/glass phase, a moving anisotropic hexatic glass phase, flowing triangular and square states ordered over the size of our simulation cell and a dynamic coexistence regime between these ordered phases. Fig. 1 displays the static structure factors, $S(\mathbf{q}) = \sum_{ij}\exp(-i\mathbf{q}\cdot\mathbf{r}_{ij})$, for the liquid, hexatic, and the drive-stabilized periodic phases. For a lower v_3 that supports a triangular ground state structure, the final non-equilibrium state is the moving triangular structure.

2. The depinning transition

For small F_x the solid is pinned. At $F_x = F_c$, the critical depinning force, the system undergoes a *discontinuous* depinning transition which exhibits a prominent hysteresis behaviour (Fig. 2(middle)). This is the *plastic* depinning transition, and the system above F_c changes to a liquid-like structure (Fig. 1(a)) and flows plastically. The centre of mass velocity v_{CM} of the system relaxes from zero to the steady-state value which increases with further increase of the drive. The time relaxation of v_{CM} at various driving forces is shown in Fig. 2(left). The velocity distribution among the particles broadens and its width in this non-equilibrium isotropic phase no longer reproduces the temperature of the stuck-phase (Fig. 2(right)). While the velocity component along the drive direction averages to the steady-state v_{CM} after depinning; the transverse component distribution is centred around zero. The widths of the velocity distributions along the drive and transverse direction are nearly similar in the liquid phase just at the depinning; but begin to deviate considerably with increasing F_x. In the *co-moving* frame, random disorder can be thought of as providing an