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Nonlinear response and dynamical transitions in a phase-field crystal model for adsorbed overlayers

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Abstract. The nonlinear response and sliding friction behavior of a phase-field crystal model for driven adsorbed atomic layers is determined numerically. The model describes the layer as a continuous density field coupled to the pinning potential of the substrate and under an external driving force. Dynamical equations which take into account both thermal fluctuations and inertial effects are used for numerical simulations of commensurate and incommensurate layers. At low temperatures, the velocity response of an initially commensurate layer shows hysteresis with dynamical melting and freezing transitions at different critical forces. The main features of the sliding friction behavior are similar to the results obtained previously from molecular dynamics simulations of particle models. However, the dynamical transitions correspond to nucleations of stripes rather than closed domains.

1. Introduction
The nonlinear response of an adsorbed atomic monolayer under an external force is a central problem for understanding friction phenomena \cite{1,2} in experiments on sliding friction between two surfaces with a lubricant \cite{3} or between adsorbed overlayers on an oscillating substrate \cite{4,5}. A fundamental issue in modeling such systems is the origin of the hysteresis and the dynamical melting and freezing transitions associated with the different static and kinetic frictional forces when increasing the driving force from zero and decreasing from a large value, respectively. Various elastic and simplified particle models have been used to study the driven dynamical transitions and the sliding friction behavior \cite{1,2,6,7}. However, it is still not fully understood which features are universal and what are the most relevant parameters in such models.

In this work, we present results for the nonlinear response and sliding friction behavior of an adsorbed layer using a phase-field crystal (PFC) model with pinning \cite{9} in presence of thermal fluctuations and inertial effects \cite{10}. The model describes the layer in terms of a continuous density field coupled to a periodic pinning potential and external driving force. At low
temperatures, the velocity response of commensurate and incommensurate layers are qualitative different. For an initially commensurate layer, the nonlinear response shows hysteresis with dynamical melting and freezing transitions at different critical values of the force. The main features of the velocity response are similar to the results obtained previously with molecular dynamics simulations of particles. However, the dynamical melting and freezing mechanisms are significantly different, corresponding to nucleation of stripes rather than closed domains.

2. Model and simulation
In the PFC model with pinning [9, 11, 12], the potential energy contribution due to the interacting particles forming the layer and the pinning potential can be written in a dimensionless form as

\[ H_{\text{pfc}} = F_0 \int d\vec{x} \left\{ \frac{1}{2} \psi[r + (1 + \nabla^2)^2] \psi + \frac{\psi^4}{4} + V(\psi) \right\}, \quad (1) \]

where \( \psi(\vec{x}) \) is a continuous field and \( V(\vec{x}) \) is the external pinning potential. The phase field \( \psi(\vec{x}) \) is a measure of deviations of the particle density \( \rho(\vec{x}) \) from a uniform reference value \( \rho_0 \), such that \( \psi(\vec{x}) = (\rho(\vec{x}) - \rho_0)/\rho_0 \). The overall constant \( F_0 \) sets the energy scale and \( r \) is a parameter. In Eq. (1), \( \psi(\vec{x}) \) is a conserved field and the energy minima depend on the average value \( \bar{\psi} \) of \( \psi(\vec{x}) \). When \( V(\vec{x}) = 0 \), the minimum energy configuration consists of an hexagonal pattern of peaks in \( \psi(\vec{x}) \) with wave vector \( k_h \approx 1 \). This phase-field crystal of an hexagonal array of peaks [13] is taken here as a simple model of an atomic layer with the pinning potential representing the effects of a rigid substrate.

To take into account inertial effects, we also include the momentum density \( \vec{g}(\vec{x}) = \rho(\vec{x}) \vec{v}(x) \) as an additional dynamical variable. As obtained recently [10], the resulting coupled dynamical equations of motion can be written as

\[ \frac{\partial \psi}{\partial t} = -\nabla \cdot \vec{g}; \quad (2) \]

\[ \frac{\partial g_i}{\partial t} = -\nabla_i \frac{\delta H_{\text{pfc}}}{\delta \psi} + \psi f_i - \eta g_i + \nu_i(\vec{x}, t); \]

\[ \langle \nu_i(\vec{x}, t) \nu_j(\vec{x}', t') \rangle = 2k_B T \delta(t - t') \delta(t - t') \delta_{i,j}, \]

where \( \vec{f} \) is the spatially uniform external force and the thermal noise \( \nu_i(\vec{x}, t) \) satisfies the fluctuation-dissipation relation corresponding to a temperature \( T \) and damping parameter \( \eta \).

We have considered a pinning potential \( V(\vec{x}) \) representing a substrate with square symmetry

\[ V(\vec{x}) = -V_0 [\cos(k_0 x) + \cos(k_0 y)]. \quad (3) \]

The parameters of the PFC model were fixed to \( r = -0.25 \), \( \bar{\psi} = -0.25 \), with a lattice mismatch between the layer and the pinning potential \( \delta_m = (k_h - k_0)/k_h = -0.5 \).

For numerical calculations, the phase field \( \psi(\vec{x}) \) and momentum density field \( \vec{g}(\vec{x}) \) are defined on a space square grid with \( dx = dy = \pi/4 \) in systems with linear sizes \( L = 64 \) to \( 128 \) and periodic boundary conditions. The Laplacians and gradients were evaluated using finite differences. The coupled equations (2) are solved numerically using time steps \( dt = 0.001 - 0.005 \).

3. Numerical results and discussion
The velocity response was studied for commensurate and incommensurate layers. Different pinning amplitudes \( V_0 \) with the external force set to zero, were chosen to obtain the equilibrium states [9, 11]. For a small pinning amplitude \( V_0 = 0.05 \), the ground state and low temperature configurations consist of an incommensurate hexagonal phase (inset of Fig. 1a) while for a larger pinning amplitude \( V_0 = 0.15 \), the configuration is a commensurate \( c(2 \times 2) \) structure.
Figure 1. (a) Velocity as a function of applied force for an incommensurate layer. Inset: snapshot of the density field configuration at $f = 0$. (b) Scaled structure-factor peak $S(Q)/N_p$ as a function of applied force. Here $\vec{Q}$ stands for the primary reciprocal lattice vector of the hexagonal structure ($\vec{k}_h$). Filled and open symbols correspond to increasing and decreasing forces, respectively.

(inset of Fig. 2a), where every second site of the lattice of the pinning potential corresponds to a peak in the phase field $\psi(\vec{x})$. The solid commensurate configuration is stable against thermal fluctuations [11] below a melting transition temperature $T_c \approx 0.055$ and the incommensurate one below $T_h \approx 0.035$. We focus on equilibrium states which correspond to well ordered $c(2 \times 2)$ or incommensurate phases, at a temperature ($T = 0.01$) well below both transition temperatures ($T_h, T_c$) and a fixed damping parameter $\eta = 0.4$.

To obtain the driven response, a force along the $x$ direction is increased from zero to a maximum value and then decreased back to zero. For each value of the force, $10^6$ time steps were used to reach a steady state and an additional equal number were used to obtain time-averaged quantities. The velocity is measured by tracking the position of the peaks in the phase-field pattern as $\psi(\vec{x})$ during the simulation [11, 12] and then the steady-state drift velocity $\vec{v}$ is obtained as a time average over all the peaks.

The main features of the velocity response to the driving force are shown in Fig. 1 for the incommensurate phase and in Fig. 2 for the commensurate phase. While for the incommensurate phase the response is nonzero even for small driving forces and shows no hysteresis behavior (Fig. 1a), for the commensurate phase the nonlinear response shows clear hysteresis behavior with two different critical force thresholds $f_a \approx 0.075$ for increasing forces and $f_b \approx 0.045$ for decreasing forces (Fig. 2a). At $f_a$, the velocity jumps abruptly from zero to a finite value whereas at $f_b$ the velocity of the sliding layer drops abruptly to zero and the layer become pinned by the external potential to form an immobile commensurate state. These two threshold values correspond to the static frictional force and kinetic frictional force, respectively.

To characterize the dynamical transitions at $f_a$ and $f_b$ in more detail, we examine the behavior of the steady state structure factor $S(\vec{k})$ which is a measure of the translational order of the layer. It can be calculated from the the positions $\vec{R}_j$ of the peaks in the phase-field pattern as $S(\vec{k}) = \langle \sum_{j,j'=1}^{N_p} \exp(-i\vec{k} \cdot (\vec{R}_j - \vec{R}_{j'}))/N_p \rangle$, where, $\langle ... \rangle$ denotes a time average and $N_p$ is the number of peaks. The structure factor evaluated at the dominant lattice wave vector $Q$ of the layer is shown in Fig. 1b and 2b. Here $Q = \vec{k}_c$ corresponds to the primary reciprocal lattice vector for a $c(2 \times 2)$ structure and $Q = \vec{k}_h$ to the reciprocal lattice vector of a hexagonal structure. For the incommensurate case where there is no critical force, $S(k_c)$ remains almost unchanged with the applied force indicating that the sliding layer remains ordered as an hexagonal structure. However, for the commensurate case, on increasing the force beyond $f_a$, $S(k_c)$ drops abruptly to
Figure 2. (a) Velocity as a function of applied force for a commensurate layer. The letters indicate the dynamical transitions at $f_a$, $f_b$ and $f_c$. Inset: snapshot of the density field configuration at $f = 0$. (b) Scaled structure-factor peak $S(Q)/N_p$ as a function of applied force. Here $Q$ stands for the primary reciprocal lattice vector for either the c(2×2) structure ($k_c$) or the hexagonal structure ($k_h$). Filled and open symbols correspond to increasing and decreasing forces, respectively.

zero consistent with the velocity response behavior in Fig. 2a. This is the onset of a force induced dynamical melting transition of the initial c(2×2) commensurate state. In fact, the behavior of $S(k_c)$ is analogous to the temperature induced melting transition in absence of a driving force [11]. On decreasing the force, the value of $S(k_c)$ stays vanishingly small until the force drops below the threshold $f_b$ of a dynamical freezing transition, at which point $S(k_c)$ rapidly increases to a value corresponding to the commensurate pinned state. Further understanding of these dynamical transitions can be obtained from an analysis of the neighbors coordination numbers of the peaks in $\psi(x)$ using a Voronoi diagram construction [9, 10]. The qualitative behavior of the structure factor and the coordination number strongly suggest that the transitions at $f_a$ and $f_b$ can be regarded as a force induced dynamical melting and freezing transition respectively.

Finally, we examine snapshots of the phase field $\psi(x)$ obtained in the steady state. For driving forces above the dynamical melting threshold $f_a$ (Fig. 3a) and the dynamical freezing threshold $f_b$ (Fig. 3b), the configuration consists of stripes of commensurate c(2×2) phase separated by disordered domain walls. These domain walls are mobile liquid like regions as confirmed by a count of the fraction of various coordination numbers. The commensurate stripes have only 4-fold coordination numbers, while in the liquid like domain walls, there is a mixture of 5-fold, 6-fold and 7-fold coordination numbers. Starting from the steady state above $f_b$ which still has a non-zero average sliding velocity, an examination of the time sequence of the freezing shows that the domain wall regions gradually shrink and eventually disappear. Above $f_c$ the sliding layer shows an hexagonal structure with defects (Fig. 3c), indicating that at the crossover critical value $f_c$ (Fig. 2a), there is another dynamic transition from a disordered phase into an incommensurate hexagonal phase corresponding to the increase of the structure factor $S(k_h)$ in Fig. 2b. This dynamical phase emerges as the average effect of the external pinning potential becomes less and less important at high sliding velocities and the steady state then corresponds effectively to the case of a weak pinning potential.

4. Conclusions
We have investigated the nonlinear response and sliding friction behavior of an adsorbed layer using a PFC model with pinning, where the adsorbed structure is described as a continuous density field allowing for elastic and plastic deformations. The main features of the velocity
Figure 3. Snapshots of the density field at different values of the applied force in Fig. 2a: (a) $f_x = 0.0975$ (near $f_a$); (b) $f_x = 0.0525$ (near $f_b$) and (c) $f_x = 0.1425$ ($f_x > f_c$).

response, in particular the hysteresis loop separating the static friction and sliding friction thresholds for the commensurate layer, are similar to the results obtained previously with particle models with interacting Lennard-Jones potentials [1, 2, 7]. The similarity of results from these very different models demonstrates the universality of the hysteresis loop for models with inertial effects and the macroscopic consequence of stick and slip motion. However, the details of the dynamical melting and freezing mechanisms are significantly different. In the PFC model, they correspond to nucleation of stripes rather than closed domains found in particle models. The origin of this intriguing difference requires further investigation of both atomistic and PFC models.

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