Shear Friction and Elastic Breakdown of Strained Layers

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Stability of a strained monolayer on a substrate as a function of lattice mismatch and disorder is considered. Disorder arises from microscopic roughness of the substrate surface resulting in local critical shear forces which are random. A simplified two-dimensional atomic model with Lennard-Jones interactions and a diluted pining potential is used to model the system. The stability of lattice registry is determined via molecular dynamics calculations. An initially strained overlayer is found to always become unstable, with vanishing static shear friction, for increasing dilution via an elastic breakdown due to disorder.

I. Introduction

A great deal of work has been devoted to the study of coherently strained layered structures, which are particularly important for device applications[1]. However, the applicability of these systems is often limited by a lattice mismatch between the layers which leads to an instability with generation of interfacial defects in the form of misfit dislocations[2]. It is important then to understand the limitations of the stability of these structures in order to develop applications with well-controlled parameters. Most of the analytical and numerical work[3-6] for these systems consider a perfect substrate. For small lattice mismatch, the overlayer remains in registry with the substrate but for larger mismatch the system is unstable to the formation of misfit dislocations at a critical value of the misfit parameter δ_c. In practice however, overlayers are often grown on substrates which are likely to have some degree of disorder. While much work has been devoted to the thickness dependence[5,6] of δ_c, the effect of substrate disorder on the stability of the system is a problem much less understood.

In this work, we consider the stability of a single monolayer on a substrate as a function of lattice mismatch and disorder[7]. We consider a type of disorder that could result from microscopic roughness of the substrate surface[8]. If the surface is relative rough on the microscopic scale it is likely that different surface areas of the interface between substrate and overlayer experience different surface stresses or pinning potentials. A simplified two- limensional atomic model with Lennard-Jones interactions and a diluted pinning potential is used to model this system. The dilution is taken to represent a finite concentration of vanishing pinning centers. The stability of lattice registry is determined using molecular dynamics calculations. We find that this kind of disorder have a strong effect on the stability of the system. An strained overlayer which is in registry on a perfect substrate is found to become unstable, with vanishing static shear friction, for increasing dilution.

The model system consists of a two-dimensional monolayer of particles interacting with a pair potential

$$v(r) = \epsilon[(r_0/r)^{12} - 2(r_0/r)^6] \tag{1}$$

were ϵ is the potential well depth and r_0 is related to the particle separation, b, at the minima of the potential by $b = 2^{1/6} r_0$. In addition, each particle also interact with pinning centers, representing the substrate, with a separable gaussian potential of the form

$$u(r) = \sum_j A_j[\exp(-(x-x_j)^2/2\sigma^2)+\exp(-y-y_j)^2)/2\sigma^2] \tag{2}$$

where A_j is the strength of the pinning potential at site j of a square lattice of lattice spacing a and σ is the effective range of the pinning center. Microscopic roughness of the substrate on the length scale defined by a leads to different local shear stresses of a pinned overlayer which are proportional to A_i. So, to take into account this kind of disorder in the simplest possible form, we assume that A_i has only two values, U or zero, given by the probability distribution

$$P(A_i) = x\delta(_i) + (1-x)\delta(A_i - U) \tag{3}$$

where x is the concentration of diluted pinning centers.

We determine the response of the overlayer to an applied external shear force using molecular dynamics techniques[9]. The equation of motion for the particles with coordinates $\vec{r}_i(t)$ is given by

$$m\ddot{\vec{r}}_i + m\eta\dot{\vec{r}}_i = -\frac{\partial u}{\partial r_i} - \frac{\partial v}{\partial r_i} + \vec{\xi}_i + \vec{F} \tag{4}$$

where F is the external shear force, u and v are the interacting potentials, η is a microscopic friction constant and ξ_i is a stochastically fluctuating force satisfying the fluctuation-dissipation theorem

$$< \vec{\xi}_{i,\mu}(t)\vec{\xi}_{j,\nu}(0) >= 2\eta mkT\delta_{ij}\delta_{\mu,\nu}\delta(t) \tag{5}$$

where m is the mass of the particles, T is the temperature and ν, μ represent the components of ξ. We use dimensionless variables r/a, t/τ, kT/U where $\tau = (ma/U)^{1/2}$ and a dimensionless force Fa/U. In the simulations, the time variable was discretized in time steps of $dt = 0.001\tau$ and typically 2×10^5 time steps were used to obtain averages. We used $\sigma/a = 0.005$ and $\epsilon/U = 1$. The temperature, $kT/U = 0.2$, was chosen small compared to the pinning strength so that collective diffusion of the overlayer is not a dominant effect.

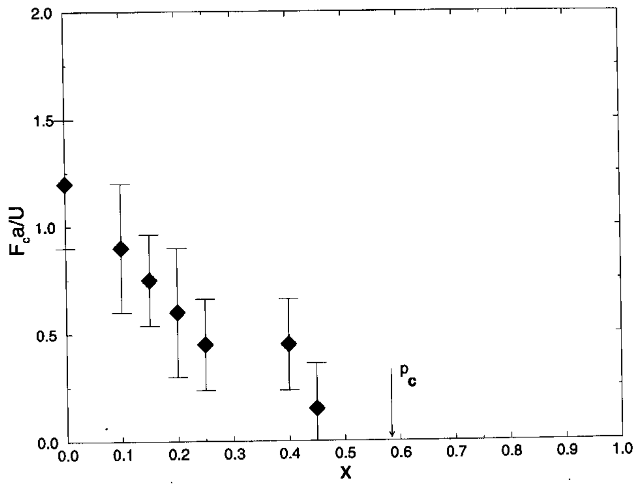

Figure 1. Static shear friction F_c as a function of dilution x. The vertical arrow indicates the percolation threshold, p_c for site dilution on a square lattice.

When $F = 0$ the overlayer is either pinned or unpinned with zero drift velocity, depending on the misfit parameter δ. The misfit parameter is defined by $\delta = (b-a)/a$ so that for $\delta = 0$ and without disorder the particles are in registry with the substrate, forming a square lattice, and a critical shear force $F_c(\delta)$, the static friction, is required to depin the overlayer inducing an average drift velocity $\dot{\vec{r}} = \vec{F}/m\eta$. The critical misfit, δ_c, for stability of the overlayer can be associated with the lowest value of δ at which F_c vanishes. We extend this criterion to study the disordered case. In Fig. 1, we show the results of the calculation of F_c as a function of dilution x for small misfit $\delta = 0.05$ averaged over different realizations of disorder. For $x = 0$, the overlayer is in perfect registry with the substrate leading to a finite F_c but, as x increases, F_c decreases significantly even for small x and appears to vanishes at a value x_c close to p_c. The quantity $p_c = 0.5927$ is the known value of the site percolation threshold[10] for the formation of an infinite cluster of diluted sites. Our data is not precise enough do determine if F_c vanishes before or at p_c. However, in simple models of percolation in elastic networks[10] the onset of nonzero elastic constant coincides with the percolation threshold which suggests that similar behavior could result for F_c as a function of x. Since F_c is a measure of the stability of the pinned overlayer, the decrease of F_c can be associated with a decrease in the critical misfit δ_c as a function of disorder. This implies that an overlayer which has a misfit $\delta < \delta_c$ on a perfect substrate could be out of registry on a substrate with surface disorder. The static friction F_c and the decrease of δ_c as a function of dilution can be regarded as an elastic breakdown problem induced by the presence of defects (unpinned particles) on an otherwise pinned overlayer. In fact, current work on breakdown in random media[11] suggests that the dominant factor limiting the elastic strength of these systems are defects. In our model, since the local static, shear friction at a diluted pinning center vanishes, it follows that the particles close to this center will have an initial sliding proportional to the external force which will in turn increase the external force on neighbouring particles even further leading to depinning. At F_c, breakdown occurs producing an overall sliding of the overlayer, as more and more particles are unpinned. It should be interesting to study this phenomenon in detail and its effect on adhesion of strained layers on disordered substrates.

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