Local Melting and Drag for a Particle Driven Through a Colloidal Crystal

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We numerically investigate a colloidal particle driven through a colloidal crystal as a function of temperature. When the charge of the driven particle is larger or comparable to that of the colloids comprising the crystal, a local melting can occur, characterized by defect generation in the lattice surrounding the driven particle. The generation of the defects is accompanied by an increase in the drag force on the driven particle, as well as large noise fluctuations. We discuss the similarities of these results to the peak effect phenomena observed for vortices in superconductors.

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Colloidal crystals are an ideal system for studying a variety of issues that arise in two-dimensional (2D) systems such as melting [1], defect dynamics [2], and ordering on 2D [3] and 1D [4] periodic substrates. A particular advantage of this system is that, due to the particle size, the individual colloidal positions and motions can be directly observed, unlike other systems in which this information is generally inaccessible.

Recently there has been growing interest in controlling colloids individually or in small groups by means of optical techniques such as holographic optical trap arrays [5]. With such methods, individual colloids can be captured and moved, or collections of colloids can be driven through single traps or periodic arrays of traps [6–8]. Alternative methods for driving individual colloids include moving single magnetic particles through assemblies of non-magnetic colloids [9]. These methods of manipulating and driving individual colloids offer a wealth of new ways to explore the dynamical properties of colloidal crystals and glasses, and can also be used to manipulate particles in other systems such as dusty plasmas [10].

A relatively simple example of manipulating single colloids to probe collective properties of a surrounding colloidal crystal is to drive a single colloid through a crystalline array of other colloids. One question that arises in this system is how the size of the driven particle affects both its motion and the response of the surrounding colloids. A very small driven particle is unlikely to generate enough stress in the surrounding lattice to create defects, and therefore the driven particle motion and the response of the system will be elastic. As the particle size or the temperature is increased, defect generation may become possible and a transition to plastic flow can occur. The defects may remain localized near the driven particle and strongly affect the frictional drag. The drag should also depend on the orientation of the driving direction with respect to the colloidal lattice. For example, in a triangular lattice, easy flow directions should occur along 60° angles. Work on systems of particles flowing over different orientations of rigid substrates has shown that a series of magic angles can arise where the flow locks into particular orientations [7].

By studying colloids moving through a periodic substrate created by other colloids, it may be possible to gain insight into related phenomena such as the role played by dislocations in friction and depinning. For example, in the case of atomic friction [11] where one lattice is driven over another, dislocations may nucleate in either of the lattices and can strongly affect the friction coefficient. In the case of driven vortices in superconductors, the onset of dislocations or plasticity at or near melting can give rise to a phenomena known as the peak effect, where the vortices slow considerably or become pinned as a function of external magnetic field or temperature [12–15].

In order to investigate the dynamics of a single driven colloidal particle moving through a triangular colloidal lattice we conduct a series of Langevin simulations of the type employed in Refs. [16,17]. We consider a 2D system of $N$ colloidal particles interacting with a repulsive Yukawa potential in the absence of a substrate. We impose periodic boundary conditions in the $x$ and $y$ directions. The initial configuration of the colloids is a triangular lattice. For a fixed density $n$ there is a well defined melting temperature $T_m$, measured either by diffusion or by the density of non-sixfold coordinated particles as determined by a Voronoi tessellation. An additional colloid is placed in the system, and a constant driving force $f_d$ is applied only to that particle.

The equation of motion for a colloid $i$ is

$$\frac{d\mathbf{r}_i}{dt} = f_{ij} + f_d + f_T$$  \hspace{1cm} (1)

Here $f_{ij} = -\sum_{j \neq i}^N \nabla_i V(r_{ij})$ is the interaction force from the other colloids. The colloid-colloid interaction is a Yukawa or screened Coulomb potential given by $V(r_{ij}) = q_i q_j / r_{ij} \exp(-\kappa r_{ij})$, where $q_{i(j)}$ is the particle charge, $1/\kappa$ is the screening length, and $r_{ij}$ is the position of particle $j$. All the particles have the same charge $q$ except for the driven particle which has charge $q_d$ that may differ from $q$. The applied driving force $f_d$ is finite if colloid $i$ is the driven colloid and zero otherwise. The system size is measured in units of the lattice constant $a_0$ and we use a screening length of $\kappa = 3/a_0$. The thermal force $f_T$ is a randomly fluctuating force from random kicks. For most of the results in this work we fix the colloid density (thus fixing the melting temperature...
FIG. 1. (a,c,e): Colloid configurations (black dots) and trajectory lines at different temperatures for a driven particle with charge $q_d/q = 3$. (b,d,f): Corresponding Voronoi construction colored according to the number of neighbors: five (black), six (white), and seven (gray). (a,b) $T/T_m = 0.1$; (c,d) $T/T_m = 0.57$; (e,f) $T/T_m = 1.07$.

We first consider the case where a particle with $q_d/q = 3$ is driven along the zero degree angle with respect to the lattice. Three distinct phases occur for increasing $T/T_m$. In Fig. 1(a,c,e) we show the colloids and particle trajectories for different $T/T_m$. In Fig. 1(b,d,f) we show the corresponding Voronoi construction or Wigner-Seitz cells, in which a single colloid is located at the center of each polygon. The cells are colored according to the number of nearest neighbors: white for six neighbors, black for five neighbors, and gray for seven neighbors. In Fig. 1(a,b) at $T/T_m = 0.1$, the flow is elastic and the particle moves along a 1D path while causing small distortions in the surrounding lattice. Fig. 1(b) shows that although a group of defects surrounds the driven particle, which is an extra or interstitial particle in the triangular lattice, there are no other dislocations induced elsewhere in the lattice. At $T/T_m = 0.3$, we find a transition to plastic flow where the particle no longer moves strictly in a straight line, and defects form in the surrounding lattice. Additionally, some colloids from the surrounding lattice are pushed in front of the driven particle over distances larger than a lattice constant $a_0$. Fig. 1(c,d) illustrates this behavior for $T/T_m = 0.57$. A localized molten region surrounds the moving particle, and ejects 5-7 defects into the lattice over time. Fig. 1(e,f) shows the system above melting at $T/T_m = 1.07$, where defects are generated in the sample even in the absence of the driven particle. In this globally molten phase, the driven particle is still able to push other particles in front of it.

We next show the effect of the defect generation on the colloidal velocity in the different phases. In Fig. 2(a) we plot the percentage of sixfold coordinated particles, $P_6$, for a system with $q_d/q = 1$, fixed $f_d$, and increasing temperature. We find a transition from elastic to plastic flow at a temperature close to $T/T_m = 0.57$. A localized molten region surrounds the moving particle, and ejects 5-7 defects into the lattice over time. Fig. 2(b) shows the system above melting at $T/T_m = 1.07$, where defects are generated in the sample even in the absence of the driven particle. In this globally molten phase, the driven particle is still able to push other particles in front of it.
loidal lattice slow the driven particle. As $T$ is further increased, $V_x$ eventually increases to $V_0$ for $T/T_m > 10$.

We next consider the effect of varying $q_d$. In Fig. 2(c) we plot $P_0$ for a system with $q_d/q = 0.25$, and in Fig. 2(d) the corresponding $V_x$. Here $V_x$ is only slightly lower than $V_0$. A small decrease in $V_x$ occurs close to melting; however, unlike the case of $q_d/q = 1$, there is little change in $V_x$ across $T_m$. In Fig. 2(e) we show $P_0$ for $q_d/q = 6$, and in Fig. 2(f) the corresponding $V_x$. $P_0$ is more rounded than for $q_d/q = 0.25$. This is due to the dislocations created by the driven particle, which become more numerous as the melting transition is approached. $V_x$ drops dramatically well below the melting temperature, at a much lower $T$ than observed for smaller $q_d$. The decrease in $V_x$ coincides with the creation of dislocations in the lattice near the driven particle. Far from the driven particle, the colloidal lattice remains ordered.

We observe that at the onset of the local dislocation or defect creation, the driven particle often drags an additional colloid in front of it. Once the dragged colloid falls away to one side, another colloid is captured and dragged. The presence of an extra dragged particle produces extra resistance to the motion of the driven particle. In Fig. 2(b), at high temperatures $T > T_m$, the drag effect is reduced and the particle velocity increases when the thermal fluctuations become so strong that the driven particle can no longer capture other particles. Small driven particles do not have a strong enough colloidal-colloid interaction to push any additional particles, so no additional drag effect occurs. The small driven particle of Fig. 2(c) creates little distortion in the surrounding colloidal lattice, so the formation of dislocations occurs only due to $T$. In Fig. 2(e) the driven particle is large enough to create a significant amount of distortion in the surrounding lattice, and thus produce dislocations at low $T$ well below melting. Thus, the combination of lattice distortions from the driven particle and the temperature produces the onset of dislocations. Dislocations appear at a lower temperature in the presence of a large driven particle than they do for a small or for no particle, when no lattice distortions are introduced. We therefore expect that as $q_d$ increases, the local melting transition will shift to lower $T$. We have also considered the effect of varying $f_d$, and observe the same results whenever the particle velocity is slower than the propagation of disturbances in the surrounding media.

In Fig. 3 we plot the curve separating the crystal phase $C$, the local melting phase $LM$, and the global melting phase $M$. The line separating $C$ and $LM$ is obtained from the decrease of $V_x$. Within $LM$, the moving particle creates dislocations but only locally as seen in Fig. 1(d).

We note that these results have many similarities with a phenomena called the peak effect for vortices in superconductors [12–15]. An immediate difference between the two systems is that the vortices interact with a background of quenched disorder which is not present in our system. The peak effect is generally believed to occur due to a transition from an elastic, dislocation free vortex lattice to a disordered glassy state containing many dislocations. The relatively stiff elastic lattice cannot adjust to the disorder and is thus weakly pinned, whereas the soft disordered state can adjust well to the disorder and is strongly pinned. The peak effect is observed by monitoring the vortex velocity in the form of a voltage as a function of temperature. At the peak effect transition the voltage drops abruptly, indicating that the vortices are slowing or being pinned. The peak effect can also be observed by constructing IV curves. There is still controversy over whether the true nature of the peak effect is a thermal melting or a disorder induced transition [13,14]. Distinguishing between these two scenarios is made difficult by the fact that the entire vortex lattice becomes disordered at the peak effect transition.

In our system there is a transition from an elastic (defect free) flow to a plastic (defected) flow which coincides with a drop in the velocity of the moving particle. The velocity drop occurs even when the defects do not occur in the whole sample but only surround the driven particle. Additionally we find strong $1/f$ type velocity noise fluctuations in the disordered flow. In our system, the velocity transition is not caused by thermal fluctuations, but is instead due to the distortions of the surrounding lattice by the driven particle. In the case of the vortices, lattice distortions could arise from the relative motion of vortices trapped at pinning sites. If the distortions in the surrounding lattice are large enough, dislocations nucleate and the overall vortex velocity drops.

To further explore similarities between the peak effect and our system, we slowly increase $f_d$ and measure the velocity at fixed $T$, in analogy with IV measurements. A
particular characteristic of the peak effect is crossing IV curves [15]. Due to thermal activation, the more disordered system has a lower threshold for motion than the ordered system. In contrast, at higher drives when thermal creep is negligible, the overall velocity is lower in the disordered system than in the ordered system. This implies that the velocity-force curves for the two cases must cross at intermediate drives.

In Fig. 4 we plot the velocity vs force curves for \( qd/q = 3 \) at fixed \( T/T_m = 0.5 \) in the ordered regime (solid line) and at \( T/T_m = 1.1 \) just into the liquid regime (dotted line). For the disordered (melted) system there is no true depinning threshold and we observe a finite velocity almost to zero applied drive. The velocity in the ordered regime for \( f_d < 0.2 \) is less than that of the disordered regime and is almost zero, with a clear depinning threshold. By contrast, at higher drives the velocity in the ordered regime is higher than the melted regime. Thus we observe a crossing of the velocity force curves similar the crossing of the IV curves [15] for the peak effect. We have also examined the velocity in the local melting case and again find a finite depinning threshold; however, here the velocity is always lower than the ordered case, even at high drives. Our results lend support to the idea that the peak effect phenomena in superconductors is not a thermal melting phenomena, but is instead a disorder induced transition.

We have also explored the effect of driving the particle at various angles with respect to the undriven lattice. For certain angles such as 60° the results are unchanged. For incommensurate angles, the plastic flow transition shifts to a lower \( T/T_m \) since the moving particle generates larger distortions in the surrounding lattice and defect creation is easier.

In conclusion, we have studied a single colloid driven through an ordered colloidal crystal. We find that as a function of temperature and charge of the driven colloid, there is a transition from elastic flow, where no defects are generated in the surrounding lattice, to plastic flow, where defects proliferate. This transition coincides with an increased drag on the driven particle, due to the driven particle trapping and pushing surrounding colloids in front of it. As the charge of the driven particle increases, the elastic-plastic transition shifts to lower temperatures. This system has several similarities to the peak effect phenomena found in vortex matter in superconductors: The onset of defect formation slows the particle, and there is a crossing in the velocity force curves. Our results suggest that the peak effect is due to a disorder induced transition rather than a thermal melting transition. These results should be accessible experimentally by driving single colloids with optical tweezers or dragging a magnetic bead though an ordered colloidal crystal. Another variation on this would be to drive a colloidal crystal past obstacles of varied size. Other systems in which these effects could be observed include driving particles through dusty plasma crystals or ordered foams.

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