Krypton clusters adsorbed on graphite: A low-temperature commensurate-incommensurate transition

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Clusters of Lennard-Jones atoms adsorbed on a graphite surface are studied using Monte Carlo simulation. We investigate the stability of registered and nonregistered structures at low temperatures. The model is two dimensional with adatom-adatom interactions specific to krypton, while the amplitude of the hexagonal substrate corrugation potential V_1 is taken as a variable. In order to allow the density to change continuously, free boundaries have been employed. We locate a thermally induced as well as a field induced phase transition in the plane of temperature and corrugation amplitude. The transition is from a modulated (incommensurate) structure at low corrugation amplitude and low temperature to a registered (commensurate) lattice at stronger corrugation and/or higher temperature. We find that free surfaces enhance the stability of the $\sqrt{3}\times\sqrt{3}R30°$ structure. Our results support the existence of an incommensurate-commensurate transition driven by thermal expansion as proposed by Gordon and Villain [J. Phys. C **18**, 3919 (1985)].

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I. INTRODUCTION

Rare gases physisorbed on the basal plane of graphite provide an experimental realization of an effectively two-dimensional system [1–4]. Experiments performed for krypton adsorbed on graphite have indicated a complex phase diagram, including registered or commensurate (C) structures, incommensurate (IC) phases, and a number of multicritical points [5,6]. The assumption of a planar solid for not too high coverages is justified by a total adsorption energy of about 1400 K [7,8] more than an order of magnitude larger than the lateral modulation of the krypton-graphite potential. The interactions responsible for physisorption processes are sufficiently well known to allow for realistic microscopic models that can be analyzed using approximate analytic techniques and phenomenological theories, or computer simulation techniques. The graphite substrate modulates the interaction among the krypton atoms, but is otherwise assumed to be perfectly rigid in the temperature range of interest here. The modulation has the hexagonal symmetry of the first graphite layer and forms a triangular array of adsorption sites with lattice spacing 2.46 Å. The lattice constant of a two-dimensional krypton solid is about [1,9] 4 Å and the 1×1 structure is therefore highly unfavorable. Instead, adsorption can take place by occupation of next-nearest graphite hexagons and formation of a $\sqrt{3}\times\sqrt{3}R30°$ commensurate lattice with lattice constant $a_C=4.26$ Å. In this case, the adsorbed layer has to expand relative to an isolated two-dimensional Kr solid. Alternatively, the competition between the Kr-Kr interactions and the Kr-graphite interactions, each favoring a particular length scale, can result in an incommensurate phase with an average lattice constant closer to that of the Kr solid itself.

Computer simulation studies of krypton adsorbed on graphite have been performed using both Monte Carlo techniques [10,11] and the method of molecular dynamics [10,12–14]. Much effort has been devoted to the question of two-dimensional melting and properties of the incommensurate phase. An important result is the observation of an IC phase with hexagonal symmetry [10,13] supporting the domain wall description of the IC phase. There is, however, considerable uncertainty concerning the magnitude of the modulation of the Kr-graphite potential. Zero-temperature calculations [15,16] have shown that the commonly accepted value for the corrugation amplitude [7] is too small to ensure a registered phase at zero temperature. The experimental measurements indicate [5] that a low-temperature, low pressure monolayer is commensurate. Moreover, it has been suggested [4] that thermal expansion of the Kr solid can stabilize a registered phase, even if the potential is insufficiently corrugated at zero temperature. We address these questions by performing numerical simulations as a function of substrate corrugation and temperature.

Previous molecular dynamics calculations [14] have shown that boundary conditions play an important role in numerical studies of the commensurate-incommensurate transition. In order to allow for a con-

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tinuously changing density and to allow an adsorbed island of atoms to contract and rotate freely [17], we have done Monte Carlo simulations on an isolated two-dimensional cluster of atoms with free bonds along the surface. At zero temperature, we calculate the minimum-energy configuration depending on the ratio of adatom-adatom energy to adatom-substrate energy. At finite temperatures, we calculate thermodynamic functions along two paths in the plane of temperature and corrugation strength. The critical value of the substrate field at constant temperature $T=30$ K is found to be lower than the value determined at zero temperature. This is in agreement with theoretical arguments predicting that the commensurate phase will be stabilized at finite temperatures due to thermal expansion of the adlayer. The same procedure is used to locate a phase transition as a function of temperature when the substrate potential is kept constant. For a corrugation amplitude four times weaker than the value estimated at zero temperature, we observe a registered-modulated transition at $T\sim 48$ K based on finite-size extrapolation. In both cases, hysteresis effects can be observed, indicating a first order transition.

We note that simulations of this type are subject to several drawbacks. First, since there is no restoring force for particles leaving the cluster, it will, in principle, be thermodynamically unstable whenever the vapor pressure of the cluster is greater than zero. At low temperatures, we may assume that this particle flux is negligible on the time scale of a simulation. This assumption is supported by direct inspection of particle configurations generated in the simulations. Secondly, the boundaries of the cluster must be expected to be unstable against long wavelength (roughening) fluctuations at finite temperatures [18]. These excitations contribute to greatly enhanced fluctuations in the Monte Carlo data.

The paper is organized as follows. The model is defined in Sec. II. In Sec. III we describe zero-temperature energy minimization calculations as a function of corrugation amplitude. In Sec. IV we present finite temperature Monte Carlo simulations, and, finally, Sec. V contains our conclusions.

II. MODEL SYSTEM

We assume that the adlayer is confined to a two-dimensional plane $z=z_{\rm eq}$, where $z_{\rm eq}$ is an average equilibrium distance above an ideal graphite surface. The adatom-adatom interactions are taken to be Lennard-Jones pair interactions

$$v_{\rm LJ}(r)=4\epsilon\{(\sigma/r)^{12}-(\sigma/r)^{6}\}\ , \tag{2.1}$$

where $r=|\mathbf{r}_i-\mathbf{r}_j|$ is the distance between two atoms and ϵ and σ are the Lennard-Jones parameters for krypton. The substrate potential has the form

$$V(\mathbf{r}_i)=V_0(z_{\rm eq})+2V_1(z_{\rm eq})\{\cos(\mathbf{b}_1\cdot\mathbf{r}_i)+\cos(\mathbf{b}_2\cdot\mathbf{r}_i)+\cos[(\mathbf{b}_1+\mathbf{b}_2)\cdot\mathbf{r}_i]\}\ , \tag{2.2}$$

where $\mathbf{b}_1$ and $\mathbf{b}_2$ are the reciprocal lattice vectors of the graphite basal plane, $V_0(z_{\rm eq})$ is the laterally averaged adsorption energy, and $V_1(z_{\rm eq})$ is the amplitude of the corrugation. The configurational energy of N adsorbed particles is then

$$H=\sum_i V(\mathbf{r}_i)+\tfrac{1}{2}\sum_{i\neq j} v_{\rm LJ}(r_{ij})\ . \tag{2.3}$$

Thus we model a two-dimensional (2D) finite-cluster Lennard-Jones solid subject to an external field with hexagonal symmetry. There has been quite some controversy regarding the precise value of the corrugation amplitude V_1 [19,20]. Data used in the literature range from $-V_1\sim 5$ K [1,4] based on the method of Steele [7] to $-V_1\sim 14$ K [19] obtained from calculations that take into account the anisotropy of the graphite polarizability. The corrugation amplitude depends rather sensitively on the input parameters [20,21], in particular, small variations in $z_{\rm eq}$ will strongly affect the value of V_1. We calculate numerically the separate parts of the total energy $E_{\rm tot}=E_{\rm Kr/g}+E_{\rm Kr}$, where

$$E_{\rm Kr/g}=\frac{1}{N}\left\langle\sum_i V(\mathbf{r}_i)\right\rangle\ , \tag{2.4a}$$

and

$$E_{\rm Kr}=\frac{1}{2N}\left\langle\sum_{i\neq j} v_{\rm LJ}(r_{ij})\right\rangle\ . \tag{2.4b}$$

The Lennard-Jones potential is set equal to zero at a distance of either 2.5σ or 3.6σ. We define an order parameter for the registered phase proportional to the Kr-substrate energy

$$\Phi=\frac{1}{3N}\left\langle\sum_i\{\cos(\mathbf{b}_1\cdot\mathbf{r}_i)+\cos(\mathbf{b}_2\cdot\mathbf{r}_i)+\cos[(\mathbf{b}_1+\mathbf{b}_2)\cdot\mathbf{r}_i]\}\right\rangle\ . \tag{2.5}$$

This function is normalized so that $\Phi=1$ for a phase with all atoms in registry, while a state where atoms are randomly distributed over the surface will result in $\Phi=0$. A monolayer that is free to translate over the surface (floats) will also produce a zero thermal average for the order parameter. To further characterize modulated structures, a structure factor can be defined as

$$S(\mathbf{k})=\frac{1}{N^2}\left\langle\left|\sum_i\exp(i\mathbf{k}\cdot\mathbf{r}_i)\right|^2\right\rangle\ . \tag{2.6}$$

This quantity is proportional to the scattered intensity from the overlayer. We have calculated (2.6) at zero temperature for wave vectors along the (10) and (11) directions.

III. ZERO-TEMPERATURE CALCULATIONS

A commensurate (registered) structure will be stable if the corrugation amplitude of the substrate potential exceeds a minimum value, otherwise the adlayer will contract into a denser nonregistered phase. This field induced commensurate-modulated transition has been studied at zero temperature by a number of authors, using various energy minimization schemes [15,16]. An estimate for the minimum corrugation amplitude needed to

produce a registered structure can be obtained from a simple energy balance argument. In the absence of substrate modulation, the minimum-energy configuration of a 2D Lennard-Jones solid without external fields is a close packed triangular lattice with cohesive energy [4,9]

$$E(a)=2\epsilon[C_{12}(\sigma/a)^{12}-C_6(\sigma/a)^6]\,, \tag{3.1}$$

where $C_{12}=6.0098$ and $C_6=6.3759$ are the triangular lattice sums. Minimum of $E(a)$ occurs for $a_{\rm LJ}=(2C_{12}/C_6)^{1/6}\sigma=1.111\sigma$ and $E(a_{\rm LJ})=-C_6^2/(2C_{12})\epsilon=-3.382\epsilon$. The cohesive energy of a registered triangular lattice with spacing $b=4.26$ Å is $E(b)=-3.050\epsilon$. Balancing the difference in cohesive energy against the adatom-substrate energy of the registered phase, $E(a_{\rm LJ})-E(b)=6V_1$, gives $V_1=-9.4$ K as an estimate of the corrugation amplitude needed to force the monolayer into the registered state. The argument does not account for the modulation energy of the nonregistered phase and surface effects arising from a finite cluster are not included. This estimate is, however, close to a numerical value of $-V_1\sim 11$ K found in a domain wall calculation [15] and in energy minimization calculations based on periodic boundary conditions [16].

We have calculated possible zero-temperature structures of N-particle clusters with free surfaces as a function of corrugation amplitude. Starting from registered islands of rectangular shape, we relax the total energy of the clusters by moving each atom at random, within a predefined area. The maximum step length is typically of the order $10^{-2}\sigma$. We have used one scheme in which the trail move is accepted if it lowers the total energy and is rejected otherwise. Particle clusters updated according to this algorithm eventually reach a state where the total energy does not change. Starting from a registered structure at strong corrugation we might expect, as the corrugation amplitude is varied, that different energy minima will connect smoothly. There is, of course, no guarantee that this procedure will lead to a global minimum. We have therefore checked the outcome of this calculation against a simulated annealing type algorithm, in which also moves that raise the total energy are allowed. In this scheme every tenth trial move will be accepted according to a Boltzmann distribution with temperature T. We find that this scheme leads to identical results independent of T for $T\leq 30$ K, but converges faster.

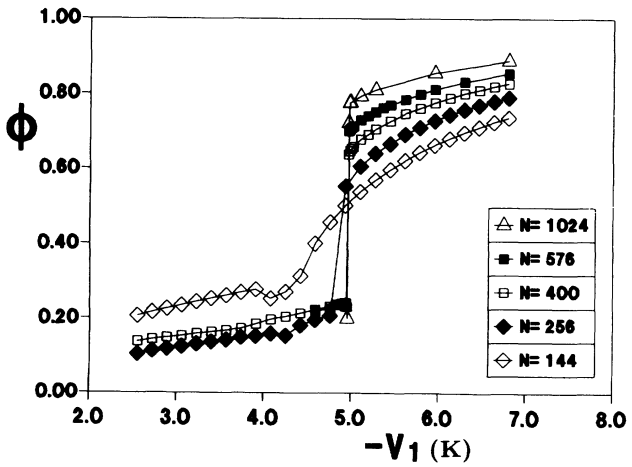

FIG. 1. Order parameter, as defined in Eq. (2.5), as a function of corrugation amplitude V_1 obtained from zero-temperature energy minimization calculations.

The zero-temperature results are shown in Figs. 1–3. A plot of order parameter as defined in Eq. (2.5) versus corrugation amplitude (Fig. 1) shows that the $\sqrt{3}\times\sqrt{3}R30°$ structure becomes unstable at an amplitude of $-V_1\sim 4.96$ K. At strong substrate corrugation, an $L\times L$ commensurate lattice remains in registry after the adatoms have relaxed from their initial positions. As the field is lowered, this structure transforms into a nonregistered, modulated phase with domains of hexagonal shape. The transition value for V_1 converges rapidly as a function of system size; the three largest lattices give almost the same result. Plots of the adatom-adatom energy [Eq. (2.4b)] as well as the total energy show a similar discontinuous behavior. Domain configurations illustrating the two different structures are shown in Figs. 2(a) and 2(b), respectively. Domains are distinguished by defining an order parameter for each of the three distinct sublattices. For a given atom a local order parameter

$$\phi=\cos(\mathbf{c}_1\cdot\mathbf{r}_i)+\cos(\mathbf{c}_2\cdot\mathbf{r}_i)+\cos[(\mathbf{c}_1+\mathbf{c}_2)\cdot\mathbf{r}_i]$$

is calculated for each of the three sublattices of the $\sqrt{3}\times\sqrt{3}R30°$ structure specified by reciprocal lattice vectors $\mathbf{c}_1$ and $\mathbf{c}_2$. If $\phi>0$, the atom belongs to a sublattice, otherwise it is taken as a member of a domain wall. The change in ordering is also apparent from plots of the structure factor calculated above and below the transition for a $N=20^2$ lattice. Along the (11) direction [Fig. 3(a)] (the horizontal axis in Fig. 2), as well as the (10) direction [Fig. 3(b)] (vertical axis in Fig. 2) the peak position of $S(\mathbf{k})$ increases from the commensurate values $|\mathbf{k}|=4\pi/(3a_C)$ and $|\mathbf{k}|=4\pi/(3\sqrt{3}a_C)$, respectively. This shows that the adlayer has a smaller average lattice constant for weak corrugation, but the cluster sizes studied are too small to obtain information about the possible modulation (domain structure) of the cluster. Snapshots of domain configurations also illustrate the mechanism driving the transition from a registered structure to a modulated structure. The contraction of the monolayer starts at the surface of the cluster, where atoms have more freedom to move and proceeds towards the center. The data in the high field registered phase scale asymptotically as $1/L$, where $L=\sqrt{N}$ is the linear size of the system. This is to be expected, since the leading finite-size correction is a surface term [22] proportional to $1/L$. The low field part of Fig. 1 is somewhat noisy and the size dependence is not monotonous with L. This behavior is probably due to the presence of a large number of close energy minima in the modulated phase. We have not been able to reproduce the hysteresis curve starting from a low field configuration with domains. As the corrugation strength is increased, each domain tends to become locked to its own sublattice, and we observe instead a curve that increases approximately linear with $-V_1$.

Our result $-V_1 \sim 4.96$ K for the minimum corrugation amplitude needed to stabilize a registered structure is a factor of 2 smaller than previous estimates [15,16]. Thus, we find that free surfaces enhance the stability of a registered rare gas cluster of atoms. This can be explained qualitatively by the "missing" interactions at the surface, which weakens the capability of a cluster to pull itself into registry.

IV. FINITE TEMPERATURE SIMULATIONS

We have located phase boundaries both as a function of temperature at a constant corrugation potential and as a function of corrugation amplitude at constant temperature. The simulations were performed for cluster sizes ranging from $N=144$ to 1296. Data are obtained for a minimum of 10^5 Monte Carlo steps per particle (MCS/P). In the transition region, up until 10^6 MCS/P data have been recorded. The influence of boundary conditions is illustrated in Fig. 4. The order parameter Φ defined in Eq. (2.5) is plotted as a function of $-V_1$ for a sample consisting of 256 Kr atoms. Both curves show the decrease of order that takes place as the amplitude of the substrate corrugation is relaxed at fixed temperature $T=30$ K. The starting configuration is again a lattice with perfect $\sqrt{3}\times\sqrt{3}R30°$ registry. The cluster has a rectangular shape corresponding to a 16×16 registered lattice. One simulation (solid diamonds) is done using a computational cell with periodic boundaries in both directions. In this case a smooth decrease of the order parameter is observed as the corrugation amplitude is decreased and the value of Φ is still high even at very weak corrugation. In the other simulation (diamonds), the adsorbed particles have free boundaries, and are thus treated as an isolated cluster on an infinite substrate. The data for this system coincide with the previous simulation at high substrate fields, but as $-V_1$ is lowered a jump in the order parameter is clearly seen, indicating a change of structure. A plot of total energy versus corrugation amplitude also shows a discontinuity for the simulation with free surfaces, in contrast to the smooth behavior seen when periodic boundaries are employed. The differences illustrated in Fig. 4 thus indicate that boundary effects are significant also at finite temperatures.

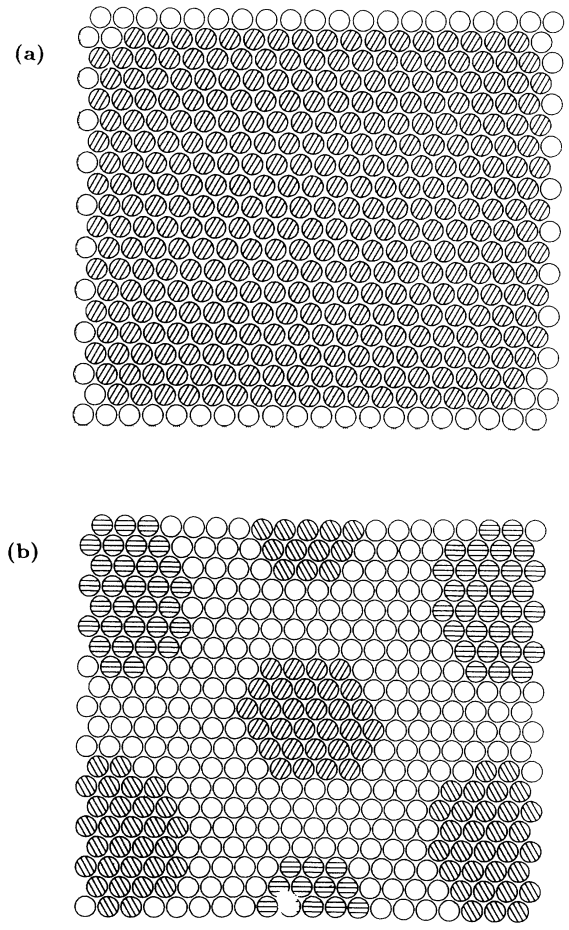

FIG. 2. Zero-temperature minimum-energy configurations resulting from energy relaxation ($N=400$): $V_1=-4.96$ K (a); $V_1=-2.3$ K (b). The hatched circles represent atoms belonging to one of the three different sublattices. Open circles indicate atoms belonging to domain walls. See text for a discussion of the criterion used for defining domains.

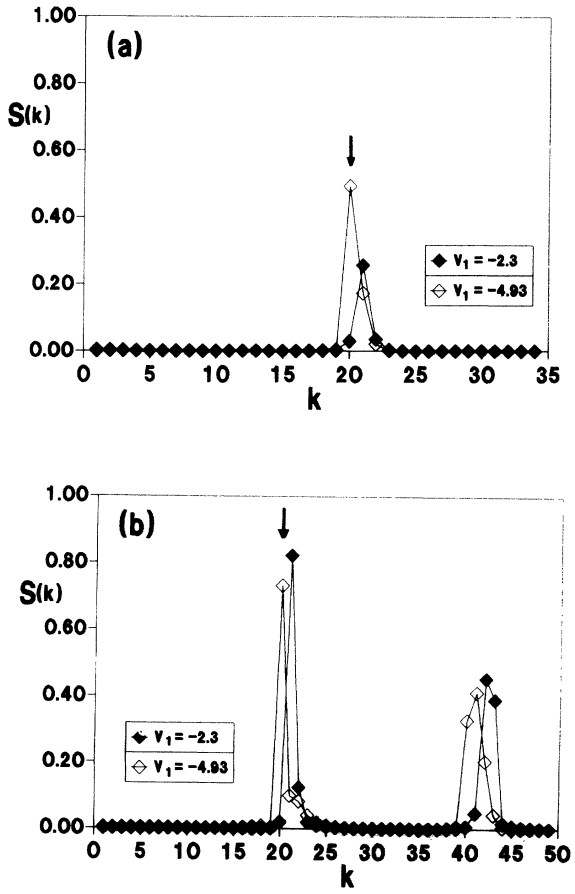

FIG. 3. Structure factor as defined in Eq. (2.6) calculated for the configurations shown in Fig. 2. (a) (11) direction, wave vector in units of $(4\pi/a_C)(k/20)$; (b) (10) direction, wave vector in units of $(4\pi/\sqrt{3}a_C)(k/20)$.

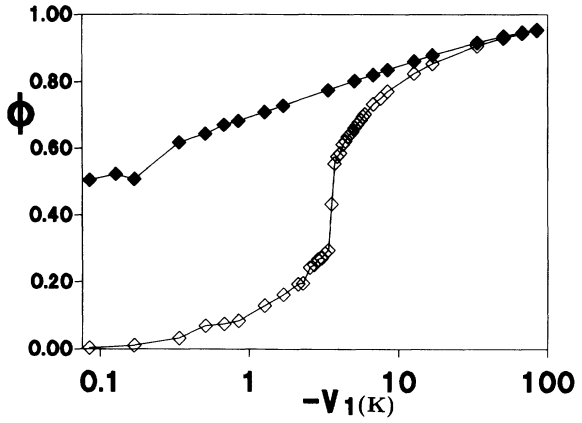

FIG. 4. Influence of boundary conditions in a Monte Carlo simulation of Kr atoms adsorbed on graphite. Shown is the order parameter [Eq. (2.5)] plotted as a function of corrugation amplitude V_1 at constant temperature $T=30$ K. The two curves represent a $N=256$ system with periodic boundaries (solid diamonds) and free surfaces (diamonds), respectively.

A. Constant amplitude

Our simulations at constant substrate corrugation are done at a fixed amplitude of $-V_1=2.3$ K. This is about half the value of the amplitude estimated by Steele [7]. Figure 5 illustrates the temperature variation of the order parameter $\Phi(T)$. The data have been obtained for lattice sizes $N=144,256,400,676$, and $N=1296$ with free surfaces. As the system size is increased, an apparent discontinuity is seen to develop in $\Phi(T)$ indicating that two different phases are present: a weakly registered structure ($\Phi<0.2$) at low temperatures and a partly registered phase ($\Phi>0.4$) at higher temperatures $T>50$ K. The temperature variation of the total energy and heat capacity shows a similar discontinuity. Inspection of snapshot configurations also supports a picture of thermal induced ordering in the clusters. At low temperatures (below the transition), the cluster occupies all three sublattices, while only a single domain is observed above the transition.

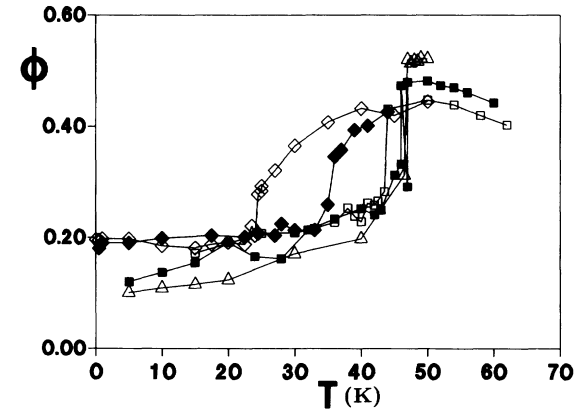

FIG. 5. Order parameter plotted against temperature at constant substrate corrugation $V_1=-2.3$ K. Lattice sizes are $N=144$ (diamonds); $N=256$ (solid diamonds); $N=400$ (squares); $N=676$ (solid squares); $N=1296$ (triangles). Solid lines are straight lines through the data points.

From Fig. 5, transition temperatures can be read off for each cluster size. In order to analyze these data in a systematic way, we invoke finite-size scaling expressions of the form $|T_c(L)-T_c(\infty)|\sim L^{-x}$, where $L=\sqrt{N}$ and x is a scaling exponent. For a first order transition x equals the dimensionality of the system, whereas $x=1/\nu$ for a continuous transition, where ν is the exponent describing the divergence of the correlation length. The scaling form given above is valid when L is sufficiently large so that bulk fluctuations are dominating. In our case, the clusters are small and the thermodynamic behavior is strongly influenced by surface fluctuations. These effects will lead to correction terms described by separate scaling exponents. A finite-size scaling plot of transition temperatures together with transition amplitudes obtained from fixed temperature simulations (Sec. IV B) is shown in Fig. 6. The straight line shown is obtained by adjusting $T_c(\infty)\sim 48$ K and $x\sim 3$. While a critical temperature of $T_c(\infty)=48\pm 1$ K can be consistently extrapolated from Fig. 6, our data set are too limited to extract a meaningful scaling exponent. If the transition is first order as indicated in Fig. 5, larger cluster sizes are clearly needed to enter a scaling regime described by $x=2$ (see also Fig. 7).

B. Constant temperature

The results of our simulations performed at constant temperature, $T=30$ K, are shown in Fig. 8. We have used lattice sizes $N=144,256,400$ and $N=1296$. Most of the runs are performed for decreasing substrate coupling using a commensurate lattice of rectangular shape as the initial configuration.

The order parameter depicted as a function of substrate corrugation amplitude exhibits a discontinuous variation reminiscent of that seen in simulations with fixed V_1. The limiting behavior is given either by the strong coupling limit $-V_1\rightarrow\infty$, where adatoms are forced into hexagon centers resulting in $\Phi=1$, or by an unperturbed Lennard-Jones cluster described by $\Phi\sim 0$ formed in the limit $V_1\rightarrow 0$. The discontinuity develops

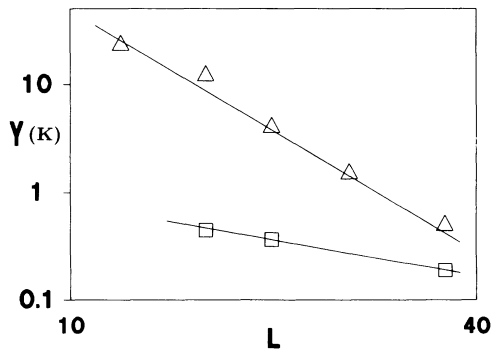

FIG. 6. Finite-size scaling plots of data from fixed amplitude simulations, $Y=|T_c(L)-T_c(\infty)|$, (triangles) and fixed temperature simulations, $Y=|V_{1c}(L)-V_{1c}(\infty)|$, (squares).

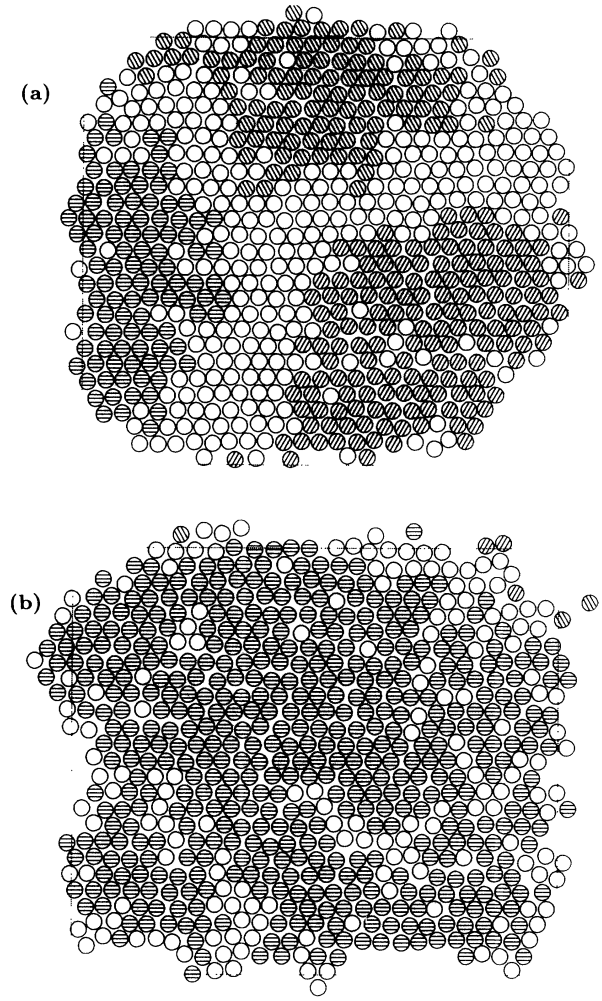

FIG. 7. Snapshot configurations ($N=676$) illustrating registered and modulated phases produced in simulations at constant corrugation strength $-V_1=2.3$ K. (a) $T=44.2$ K; (b): $T=54.4$ K. Domains are defined according to the same criterion as in Fig. 2.

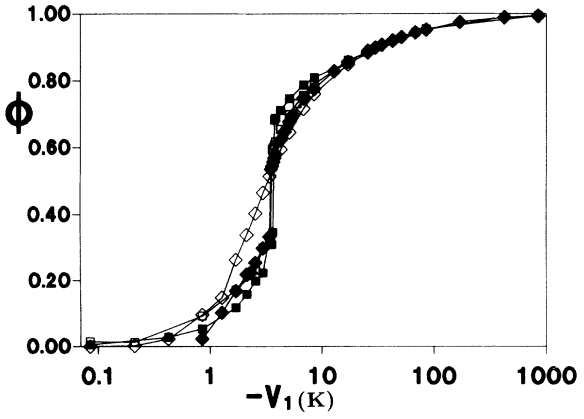

FIG. 8. Constant temperature simulations at $T=30$ K. Semilogarithmic plot of the order parameter versus corrugation amplitude V_1. Lattice sizes are $N=144$ (diamonds); $N=256$ (solid diamonds); $N=400$ (squares); $N=1296$ (solid squares). Solid lines are straight lines through the data points.

rapidly with system size, being clearly visible for $N \geq 256$. The transition cannot be resolved in the smallest cluster ($N=144$). A similar picture can be inferred from a plot of the total energy. From the position of the jump in Fig. 8, transition amplitudes are read off. A finite-size scaling plot of these data is also shown in Fig. 6. In this case, the data are described by a straight line with parameters $-V_{1c}(\infty) \sim 3.9$ K and $x \sim 1.1$. Again, the range of L is probably too small to measure a scaling exponent describing bulk fluctuations. Thus, the value found for the effective exponent x is not inconsistent with a first order transition.

V. CONCLUSION

From Monte Carlo simulations of relatively small particle clusters, we have identified a transition from a nonregistered state at low temperature and weak substrate corrugation to a registered state at high temperatures and/or large substrate corrugation. Our zero-temperature results show that free boundaries weaken the stability of the incommensurate krypton cluster relative to that of a registered island. We find a threshold amplitude of $-V_1 \sim 4.96$ K, below which the incommensurate structure has the lowest energy. This result is a factor of 2 lower than the outcome of calculations based on periodic boundaries [15,16]. At finite temperatures, we observe a further stabilization of the registered structure, relative to a modulated phase, in agreement with analytic predictions [4] and earlier molecular dynamics calculations [14]. Calculations were also performed at a finite temperature where the transition is fluctuation induced, and at a fixed corrugation where the transition is triggered by thermal expansion. For the cluster sizes studied, the surface fluctuations interfere rather strongly with properties of the bulk. Nevertheless, a transition point marking the stability of a registered cluster is clearly visible for clusters as small as $N \sim 200$ particles. Away from the transition point, the energy shows a $1/\sqrt{N}$ dependence arising from surface terms. The discontinuous behavior observed in our simulations in both parameter scans and in the molecular dynamics calculations of Koch and Abraham [14] indicates a first order transition. The effective scaling exponents obtained from a finite-size scaling plot deviate from the value $x=2$ expected for a first order transition. We expect that the cluster sizes studied are too small to be in the asymptotic scaling regime characteristic of bulk fluctuations. Our findings are in agreement with a C-IC transition driven by thermal expansion as suggested by Gordon and Villain [4]. Estimates of a transition from a locked commensurate adlayer to a floating monolayer have recently been obtained from self-consistent phonon calculations [23]. This work is restricted to large corrugation potentials producing a commensurate zero-temperature state.

In summary, we have observed a registered-nonregistered transition in Kr clusters adsorbed on graphite. The open boundary conditions applied allow us to study the stability of the registered structure for relatively small clusters in contrast to the large number of particles needed to simulate domain formation in fixed

density simulations [10]. The drawback is greatly enhanced fluctuations caused by a small bulk to surface ratio and the thermodynamic instability of the clusters due to lack of restoring forces. In spite of this, we believe the phenomena observed in our simulations are relevant for low-temperature experiments in the submonolayer regime [5]. Indeed, if the adlayer is composed of a mixture of islands of many different sizes with boundary conditions caused by impurities, heterogeneities, etc., the situation studied in this work might be appropriate. In particular, the detailed structure of the submonolayer will depend on surface effects in addition to the corrugation potential and the observation of a $\sqrt{3}\times\sqrt{3}R30°$ structure will not be a decisive indication for the size of the corrugation amplitude V_1.

ACKNOWLEDGMENTS

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