Self-organizing domain structure in a driven lattice gas

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Using Monte Carlo simulations, we have studied the self-organizing polydomain structure appearing at low temperatures in a square lattice-gas model with a repulsive nearest-neighbor interaction when the particle jumps are biased by a uniform electric field. These investigations confirm that the enhanced interfacial material transport is able to preserve the anisotropic self-organizing domain structure and to destroy the monodomain state via a nucleation mechanism. In the self-organizing state the size distribution of domains shows a power-law behavior. [S1063-651X(97)09205-2]

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I. INTRODUCTION

The introduction of driven lattice gases [1] was motivated by the demands to study nonequilibrium (open) systems that exhibit phase transitions and seem to be tractable with the improvement of dynamical methods using the concepts of equilibrium statistical physics. In these lattice-gas models the thermal jumps of interacting particles are biased by a uniform electric field E, resulting in a particle transport through the system when periodic boundary conditions are used. These systems exhibit many interesting phenomena (for a review see [2]). An attractive feature is that the equilibrium behavior should be reproduced in the limit $E \to 0$. From a practical point of view, these models are able to describe the effect of a driving field on the ordering processes in superionic conductors [3].

Now our consideration will be restricted to a half-filled driven lattice gas on a square lattice with repulsive nearest-neighbor interaction. The system has a twofold degenerate ground state in which the particles form a chessboardlike ordered structure. In equilibrium one of these structures will appear as a result of a sublattice ordering when cooling the system through the Néel temperature T_N. The early investigations apparently confirmed the naive expectation, namely, the universal behavior of the ordering process remains unchanged in the presence of a weak driving field. More precisely, dynamical mean-field analysis [4], field-theoretical investigation, and Monte Carlo (MC) simulations [5] have suggested that the Néel temperature decreases with E and the continuous transition becomes a first-order one above a threshold value.

In a previous paper [6] the MC simulations were reinvestigated using a system as large as 300×1500 for a fixed driving field. These simulations have demonstrated clearly that a self-organizing polydomain structure characterizes the stationary state at low temperatures. Here the ''self-organizing'' attribute refers to the motion of interfaces preserving the polydomain structure in the stationary state. Thus the low-temperature state remains translation invariant and the ordering process is not accompanied by the spontaneous symmetry breaking characteristic of the long-range order. The visualization of the particle configurations as a function of time has indicated that the self-organizing structure is preserved by the enhanced material transport along the interfaces separating the ordered phases. This phenomenon could be explained qualitatively by a simple phenomenological model describing the time evolution of interfaces. This phenomenological model predicts the appearance of some characteristic lengths leading to size effects that are responsible for some unexpected phenomena.

For sufficiently large fields these characteristic lengths become comparable with the lattice constant and we cannot observe a striking domain structure. In this case the revised dynamical mean-field analysis [7] confirms the absence of traditional phase transition.

Now we report on further MC simulations supporting the former picture for weak fields. It will be shown that the mentioned size effect resolves the discrepancy between the MC data obtained for small and large system sizes. We could distinguish three different types of stationary domain patterns when varying the temperature, field strength, and system sizes. Consequently, the self-organizing polydomain structure is considered as the real ''thermodynamic limit.'' In this phase we have found that the domain size distribution shows a power-law behavior. In agreement with this picture the homogeneous ordered phase is proved to be a metastable state that decays into the self-organizing polydomain structure via a nucleation mechanism. Several aspects of this nucleation process are also investigated.

II. MODEL

The driven lattice-gas model was introduced by Katz *et al.* [1] to study the effect of an external field on the ordering process. Using the traditional lattice-gas formalism, we will investigate the distribution of interacting particles on a square lattice. We assume repulsive interactions between the nearest-neighboring particles. In the half-filled system the time evolution is governed by particle jumps according to the Kawasaki dynamics. Taking the effect of external field into account, the jump rate depends on the ratio of the local potential energy difference (between the final and initial positions) and temperature T. Instead of the Metropolis rate we used the Kawasaki rate because it simplifies the analytical calculations [4,7]. Accepting the previous notations, the nearest-neighbor interaction is considered as an energy unit in which both the temperature ($k_B = 1$) and strength of a driving field are measured [1,2]. In the presence of a driving

field ($E \neq 0$) the jump rates are increased along the field and decreased in the opposite direction. The field direction is usually chosen to be parallel to one of the principal axes. Periodic boundary conditions are imposed to have a material transport through the system.

In the absence of a field the jump rate satisfies the condition of detailed balance and the stationary state can be investigated by the equilibrium techniques. It is well known that the corresponding equilibrium system undergoes a sublattice (antiferromagnetic) ordering when decreasing the temperature through the Néel temperature [$T_N = 0.5673(1)$]. The feature of this critical transition is well described in the literature [8].

In the presence of a driving field the ordering process is quite different. Instead of the homogeneous (monodomain) ordered phase a self-organizing polydomain structure was found at low temperatures. A typical particle configuration was shown in a previous paper [6]. During the simulations the visualization of the particle distribution makes clear that most of the jumps take place at the interfaces separating the ordered regions. Consequently, the particle transport is also localized along the interfaces in the presence of a driving field. For curved interfaces the induced current results in an accumulation of extra particles (holes) at the parts where the curvature is negative (positive). The interface is driven by the field with a velocity proportional to the accumulated charge density and perpendicular field component. These features are investigated by a simple phenomenological model in which the interface shape, the particle density, and the current along the interface are described by single-valued functions of time and the x coordinate [6]. The deterministic equations of motion take the effect of surface tension into consideration too.

The phenomenological model predicts that the neutral, tilted, standing, and planar interfaces are unstable against periodic perturbations in agreement with MC simulations [9], except for the interfaces parallel to the field. According to a linear stability analysis, the amplitude of the perturbation increases exponentially with time if the wavelength exceeds a threshold value. More precisely, the amplification rate has a maximum at a given wavelength (λ^*) proportional to $1/|E|$. Following the initial (exponential) increase of the periodic components there appears a finger formation controlled by nonlinear effects. In this case the typical finger width can be estimated as $d_\perp \approx \lambda^*/2$. Consequently, the growing domains are split into strips whose average length $d_\parallel$ depends on the thermal fluctuations decorating the deterministic evolution of interfaces. This picture explains why the system evolves into an anisotropic, self-organizing domain structure at sufficiently low temperatures. In this stationary state some parts of the moving interfaces can meet and annihilate each other, while the accumulated charges are neutralized (in part). This process unites two distinct domains and generates extra defects into the bulk phase. All these phenomena can be observed clearly when displaying the particle distribution during the MC simulations. The appearence of the two characteristic lengths ($d_\perp$ and $d_\parallel$) are responsible for size effects causing difficulties in the interpretation of MC data, as discussed in the subsequent section.

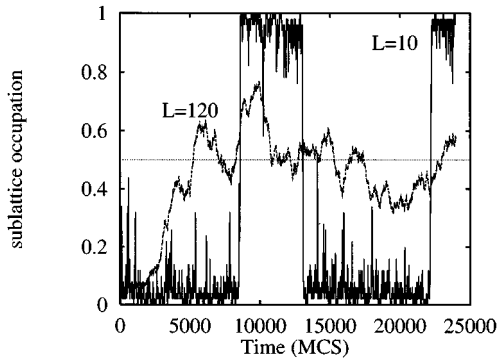

FIG. 1. Time dependence of the sublattice occupation in MC simulations at $E = 0.4$ and $T = 0.48$ for different L.

III. RESULTS OF MONTE CARLO SIMULATIONS

To justify the above statements we have performed a series of MC simulations using the standard technique [10]. Henceforth we will concentrate on the results because many details of simulations are described in our previous work [6].

First we discuss the size effects due to the appearance of different characteristic lengths mentioned above. The self-organizing domain structure is preserved by the interfacial phenomena when the system sizes are chosen to be much larger than these former values. However, if the MC simulation is performed on a small system then one can observe an ordered monodomain structure at low temperatures and a phase transition can be concluded. Thus the finite-size scaling of the order parameter can be performed for sizes $L \leqslant 40$ and one can deduce a ''critical temperature'' $T_N(E = 0.4) = 0.488(1)$. For larger system size (e.g., $L = 100$), however, the scaled data deviate significantly from the scaling function.

In a small system the ordered (chessboard) structure evolves into its counterpart (anti-chessboard) and vice versa via a nucleation mechanism as demonstrated in Fig. 1 (for $L = 10$), where the time is measured in Monte Carlo steps per particles (MCS). In this case the sublattice occupation indicates that the system is dominantly standing in one of the ordered (monodomain) states. With the increase of L the duration of the transition becomes longer and longer. For sufficiantly large sizes the monodomain structure cannot be observed in the system.

Figure 1 demontrates clearly that the evolution of sublattice occupation shows different behavior for $L = 120$ if the system is started from an ordered structure. Evidently, the fluctuation of the sublattice occupation (around 1/2) decreases when choosing even larger systems.

Beside the mono- and polydomain structures we can distinguish a third type of domain pattern when the system size equals approximately the longitudinal correlation length, which is generally larger than $d_\perp$. In a narrow range of system sizes closed strips are formed with interfaces parallel to the field. These interfaces are not affected by the interfacial instability mentioned above. Due to the thermal fluctuations the interfaces move randomly; the neighboring ones can meet and annihilate each other. The ''multistrip'' state can be considered as a stationary one because the nucleation mechanism recreates the annihilated domains.

The common feature of the above situations is the disap-

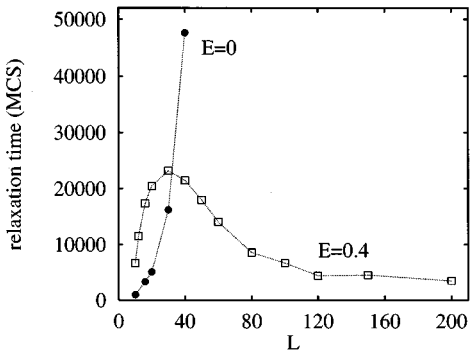

FIG. 2. Size dependence of the relaxation time in a driven system (open squares) for $E=0$ (closed circles) at $T=0.48$.

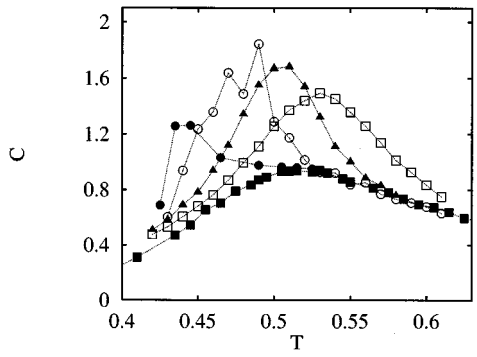

FIG. 3. Specific heat vs temperature at $E=0.4$ for different system sizes $L=16$ (open squares), 32 (closed triangles), 64 (open circles), 128 (closed circles), and 256 (closed squares).

pearance of the time average of the order parameter defined as a difference of the average sublattice occupations. The process can be characterized by a relaxation time if the system is started from one of the ordered monodomain state. To study this phenomenon a series of MC simulations was performed varying the system size for fixed field and temperature. The time variation of the order parameter has been determined by averaging over 150 MC runs. Following the method introduced by Binder and Müller-Krumbhaar [11], we have evaluated the relaxation time as a function of L for $T=0.48$ and $E=0.4$ (see Fig. 2). Notice that the temperature is chosen to be less than the critical temperature derived from the mentioned finite-size scaling for $L\leqslant 40$.

For small sizes the relaxation time increases with L. The curve has a maximum for $L\approx 36$ and tends to a constant value when $L\rightarrow\infty$. As a comparison with the equilibrium system we have repeated these calculations for $E=0$ and $L\leqslant 40$. As shown, the relaxation (ergodic) time increases monotonically with L in contrast to the driven system. The preliminary results suggest similar behavior for lower temperatures. Unfortunately, the systematic analysis requires more and more computational time when decreasing the temperature and/or field strength.

The interfacial energy contributes significantly to the total energy in the driven system. Consequently, the size effect can be observed when studying the specific heat. In the driven system the fluctuation-dissipation theorem is no longer valid; therefore the specific heat has been evaluated by the numerical derivation of the average energy as usual. Figure 3 indicates that the peak increases and moves to left when choosing $L=16$, 32, and 64 as typical in equilibrium systems. However, this tendency breaks down for larger systems when the appearance of interfaces (representing extra energy) decreases the peak height and the data converge toward the results obtained for $L=256$ in our previous work [6].

In order to study the temperature dependence of the specific heat in the real stationary state we have performed a series of MC simulatons varying the temperature for different field strengths. In these simulations the system sizes are chosen to be much (more than 10 times) larger than the corresponding characteristic lengths. Figure 4 illustrates that the position of the maximum moves to left, while the peak becomes lower and wider when the field strength is increased.

These data suggest that the critical behavior appears only in the limit $E\rightarrow 0$. Unfortunately, the MC simulations are not adequate to study rigorously the crossover from the smooth transition to the critical one when decreasing $|E|$ because of the extremely large sizes required to avoid the mentioned size effects. At the same time, the results of simulations agree quantitatively with the predictions of a generalized mean-field analysis performed previously at the level of the six-point approximation [7] for $|E|>1$.

During the above simulations the absence of long-range order has been justified in the low-temperature region for $|E|>0.2$. These simulations have confirmed qualitatively that the characteristic lengths become shorter for stronger fields, in agreement with the prediction of the phenomenological model.

The polydomain structure formed by the ordered chessboard and antichessboard phases is topologically equivalent to a pattern like ''droplets inside of droplets inside droplets . . .'' characteristic of the critical domain picture of the Ising model [12]. According to the deterministic interfacial evolution model, the appearance of characteristic lengths leads to a minimum size for droplets. In the real system the smaller droplets appear as a consequence of thermal fluctuations. The resultant domain structure is topologically similar to a quenched state roughened for a given time. To demonstrate it we have determined the domain size distribution functions in both cases. The number of sites in a given domain is determined by the cluster labeling technique widely used in percolation problems [13]. Closed circles in Fig. 5 show the average number of domains of size s in a rectan-

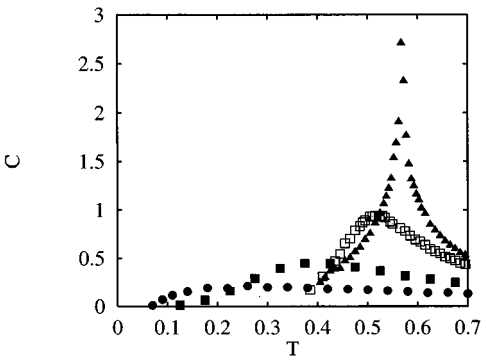

FIG. 4. Specific heat for different fields: $E=0$ (triangles), 0.4 (open squares), 1 (closed squares), and 1.5 (bullets).

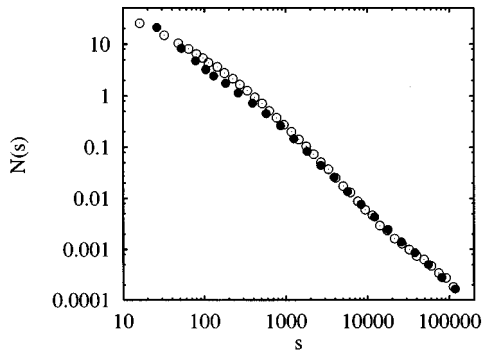

FIG. 5. Log-log plot of the average number of domains vs their sizes for a self-organizing domain structure (closed circle) and for a state (open circle) during the roughening process.

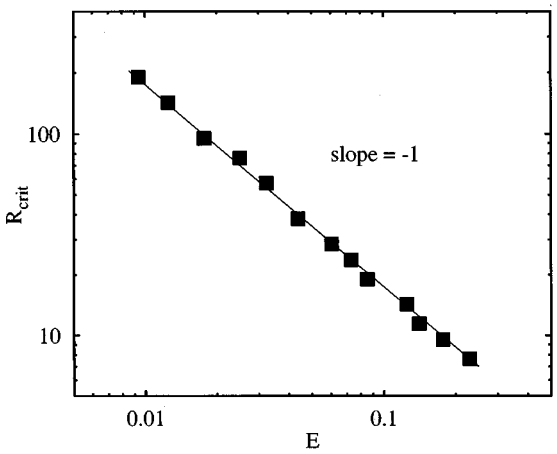

FIG. 6. Threshold value of the domain radius as a function of the driving field at fixed temperature $T=0.44$.

gular system with 500×1500 sites for $E=0.4$ and $T=0.4$. Here the open circles are obtained by averaging over 1000 patterns developed from a random distribution after a thermalization of 300 MCS in the absence of a driving field for a fixed temperature $T=0.4$. In this former case there also exists a characteristic domain size proportional to $t^{1/2}$.

The domain size distribution functions are generally sensitive to the choice of criteria defining domains and interfaces. In the above comparison we used the same criteria to demonstrate the similarity between the two types of states. Preliminary results suggest that this behavior is not affected by the anisotropy of the domain structure.

Beside the preservation of this self-organizing stationary state the enhanced interfacial particle transport breaks up the monodomain structure into a polydomain one via a nucleation mechanism as observed in MC simulations [6,14]. Due to thermal fluctuations ''islands'' of the counterphase are formed in the homogeneous initial state. These islands are polarized by the above mechanism and will elongate along the field if the driving force exceeds the shrinking effect of the surface tension. A detailed analysis of the mentioned phenomenological model predicts that the time derivatives of the interface shape and accumulated charges cannot vanish *simultaneously* for dropletlike (closed curve) solutions [15]. At the same time we are able to determine the variation of the domain area for any initial state. By this means we can distinguish domains whose area is growing or shrinking. First we have studied the time evolution of a circular domain. The initial charge distribution along its boundary is chosen to be the stationary solution for fixed radius. It is found that the area increases if the radius exceeds a threshold value R_t, which is proportional to $1/|E|$. It is emphasized that the interface motion is not isotropic and the initially circular island elongates along the field. This calculation can be repeated by assuming small elliptical distortion of the initial shape. It is found that the threshold value of the domain area as a function of ellipticity exhibits a local minimum. This fact indicates the enhanced role of the elongated islands during the nucleation process.

Unfortunately, a complete MC study of the nucleation process is not allowed by our computer facilities. We have studied only the variation of domain area when the ordered initial state contains a ''circular,'' polarized island of the counterphase. For this purpose the initial state in a square box was created as follows. In the completely ordered phase we generated a circular domain of the counterphase by shifting the inside particles along the field by one lattice constant. Thus the number of particles remains unchanged and we obtained a domain whose surface accumulates extra particles and holes (charges) with a distribution predicted by the phenomenological model for fixed radius. The appearance of such a domain is typical in the stationary state. Thermalizing the initial state for some time (10–40 MCS) we have determined the variation of the domain area. To suppress the thermal fluctuations this process was repeated several thousand times at a given field, radius R, and temperature ($T=0.44$). Due to the short run times we could vary the initial radius in a sufficiently wide range. The radius of the initial domain was chosen from 8 to 200 on an $L\times L$ lattice where L was increased simultaneously with R from 36 to 600.

From an average of data obtained for various radii we are able to determine the threshold value of the radius R_t separating the growing and shrinking domains. The results of MC simulations are illustrated in Fig. 6, where the size of the squares indicates the statistical error. These data confirm qualitatively the theoretically predicted $1/|E|$ behavior (see the solid line).

In these simulations we have chosen the radius to be significantly larger than the interface thickness, which is comparable with the lattice constant. For smaller radii the deviation of the actual interface from the circle becomes important and results in anomalous behavior. This phenomenon might have been the reason why the verification of the $1/|E|$ behavior was not successful in the early MC simulations [14].

Notice that R_t and $d_\perp$ increase with the inverse of $|E|$, while their temperature dependence seems to be negligible. At the same time the longitudinal correlation length or domain size increases when decreasing the temperature for a fixed driving field [6]. These facts make the reliable MC analysis difficult for low fields and temperatures because we should choose the system sizes to be much larger than the above characteristic lengths. Consequently, in these regions we need to search for other effective methods to check the predictions of the phenomenological model.

IV. CONCLUSION

The present MC simulations give further evidence that at low temperatures the driven lattice-gas model exhibits a self-

organizing polydomain structure that is topologically similar to those appearing during the roughening process. The interfacial effects not only preserve the self-organizing domain structure but they are able to destroy the monodomain structures via a nucleation mechanism. The related characteristic lengths are responsible for the significantly different features found between small and sufficiently large systems. For large fields these lengths become small and the results of simulations agree quantitatively with the predictions of generalized mean-field approximations at the level of six-point approximations.

In the present model the pattern formation is not surprising because similar phenomena are found in some other open systems. The best known example is the Rayleigh-Bénard instability [16]. The curiosity of the present driven lattice gas is related to the fact that here the pattern formation is preserved by an enhanced interfacial particle transport. This model represents that an interfacial phenomenon is able to prevent the formation of long-range order against the thermodynamic forces.

For weak fields the interfacial phenomena perturbed by noise affect dominantly the apparent domain structure while they allow nearly perfect order inside the domains. In this case the polydomain state can be considered as a noisy surface evolution problem. Such an approach raises many questions not yet investigated in the area of surface growth [17]. It is expected that this technique may give some predictions for the longitudinal domain (or correlation) length. Furthermore, it would be interesting to classify the interface evolution models that are able to preserve such a self-organizing domain structure.

ACKNOWLEDGMENT

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