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INTERFACE INSTABILITY IN DRIVEN LATTICE GASES

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Abstract

In driven lattice-gas models, the enhanced material transport along the interfaces results in an instability of the planar interfaces and leads to the formation of multistrip states. To study the interfacial instability, Monte Carlo simulations are performed on different square lattice-gas models. The amplification rate of a periodic perturbation depends on the wave number k; it has a positive maximum at a characteristic value of k on the analogy of the Mullins-Sekerka instability. Significant differences have been found in the dependence of amplification rate on k when comparing the systems with nearest neighbor repulsive and nearest and next-nearest neighbor attractive interactions. The results agree qualitatively with theories neglecting the fluctuations.

1. INTRODUCTION

The driven lattice-gas models were introduced to describe the effect of an electric field on the ordering process.[1] In these models, the particle hopping is biased by a uniform external field E. Monte Carlo (MC) simulations have demonstrated that the particles segregate into strips parallel to the applied field at low temperatures in the square lattice gas with attractive nearest neighbor interaction.[1,2] Analytical investigations have proved the stability of the parallel interfaces.[3,4] The tilted interface, however, is proved to be unstable.[5–7] On the analogy of the Mullins-Sekerka instability,[8,9] this morphological phenomenon may be considered as the initial stage of the formation of multistrip states in these driven systems.

Using the methods of field theory the above system is widely studied at the "coarse-grained" level (for a review see Ref. 10). Recently, the initial stage of the formation of

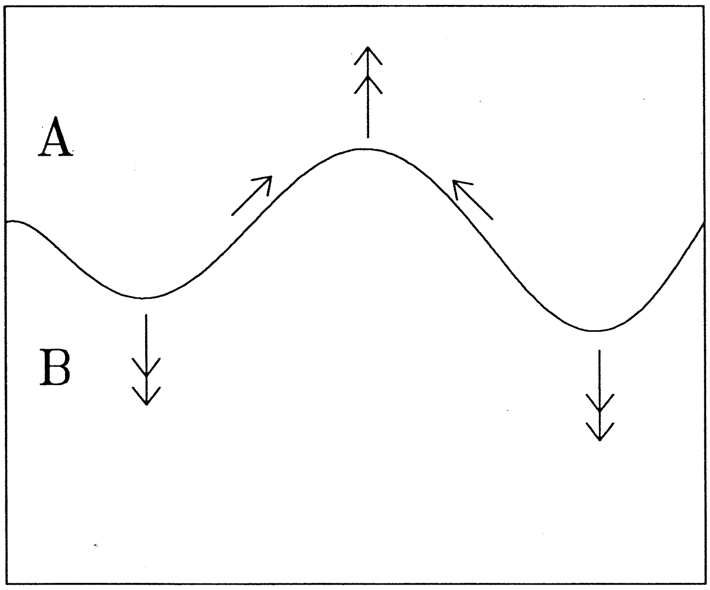

Fig. 1 The interface evolution is affected by the material transport (see arrows) induced by the vertical electric field along the interface (solid line) between the coexisting phases A and B. Double arrows indicate the motion of the interface.

the anisotropic domain structure is investigated by solving numerically the corresponding Cahn-Hilliard equation.[6,11] Yeung et al. has clarified that the interfacial instability is caused by the surface current induced by the driving field.[6,12] This mechanism has been confirmed by a very simple description of the interface evolution which neglects the interfacial thickness and bulk conductivity.[7]

The mechanism of the interfacial instability is sketched in Fig. 1. In this system, the particle transport is dominant at the interface separating the empty (A) and condensed (B) phases. The vertical field drives the particles along the interface as shown by the arrows. Figure 1 demonstrates such a situation where the particles are transported from the valley to the top, i.e., the amplitude of a periodic perturbation increases with time.

A different destabilizing mechanism is observed in the driven lattice gases if the nearest neighbor interaction is repulsive. In this case, the interface is positioned between two ordered phases (chessboard (A) and anti-chessboard (B)) in which the particle transport is negligible in comparison with interfacial current. Consequently, the particles are transported towards the top leaving holes in the valley. The interface regions with extra particles (holes) are driven upwards (downwards) as indicated by double arrows in Fig. 1. The final result is similar to those mentioned above; the planar interface is unstable against infinitesimal periodic perturbation if the wave number is less than a threshold value. A more detailed description of this mechanism including the stabilizing effects is given elsewhere.[13]

The interfacial instability and the following process can cut the large domains into strips in both systems discussed above. MC simulations have confirmed that the multistrip states are stable at low temperatures in two-dimensional driven lattice gases.[2,13] Displaying the time evolution of the particle distribution one can observe the formation of an anisotropic domain structure. The multistrip state may be considered as a result of the competition between traditional domain growth mechanism and interfacial instability.

The above theories of interfacial instability neglects the effect of fluctuations.[7,12,13] In the present paper, we concentrate on the role of fluctuations. For this purpose, MC simulations are performed in two different square lattice gases. Using the traditional technique,[1,2,13] the simulations are carried out on a rectangular box of $L \times M$ sites with periodic boundary conditions. The horizontal size is chosen to be $L = 512$. The simulations are started from an ordered configurations having two (or one) horizontal interface(s). After a thermalization, the vertical field is switched on and we have monitored the time evolution of the interface. During this process, we have determined the linear amplification rates for each Fourier component. These quantities are averaged over 200 runs.

In the first model, the attractive nearest and next nearest interaction is chosen to be unity. The next nearest neighbor interaction is introduced to reduce the evaporation of particles out of the interface. The same model is used by Manna et al.[14] for the investigation of the effect of gravitation on the shape of liquid drop sliding down on a wall. The simulations are carried out for a fixed temperature $T = 0.4$ and vertical size $M = 48$. In the initial state, the particles are condensed in a horizontal strip with planar interfaces and the upper interface is monitored followed a thermalization of 15000 Monte Carlo steps per particle (MCS). The Fourier components of the interface are determined step by step and we have evaluated their linear amplification rate λ as a function of wave number k. Using this method, the measurement of negative λ is excluded.

Figure 2 shows the data obtained for different electric fields. The results agree qualitatively with the theoretical prediction ($\lambda \propto (Ek^2 - Ak^4)$, where $A > 0$[7]) excepting the limit $k \to 0$, where λ tends toward a positive constant. This behavior may be related to the random motion of the interface due to escaping particles (holes).

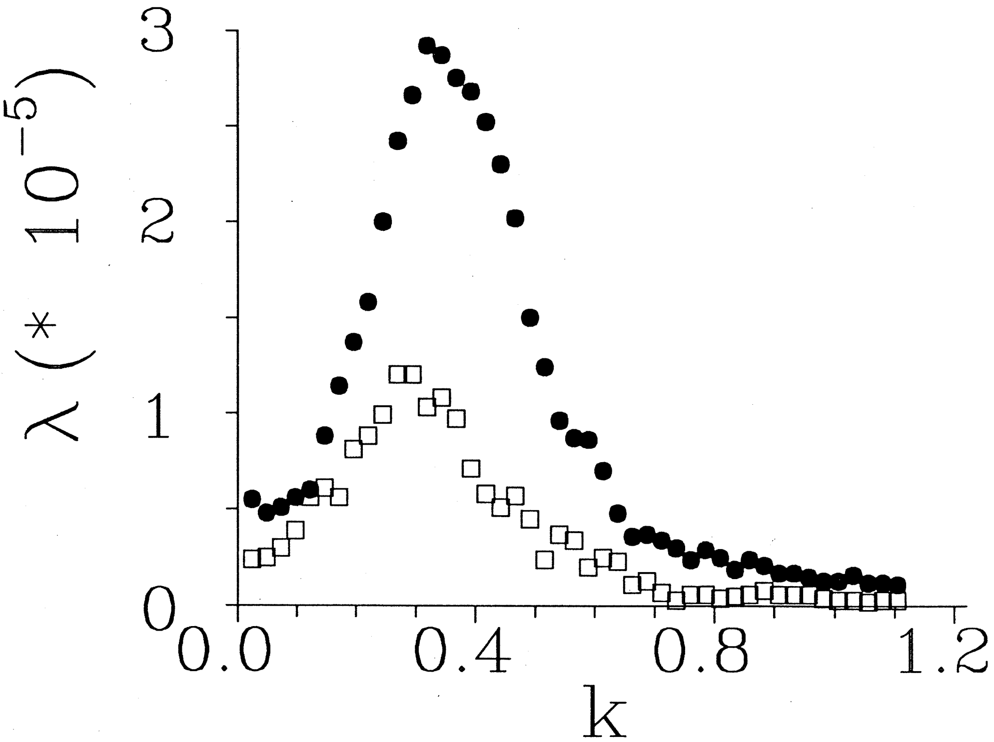

Fig. 2 Amplification rate of periodic perturbations as a function of wave number in a square lattice gas with attractive nearest and next-nearest neighbor interactions for $E = 0.4$ (boxes) and $E = 0.2$ (solid circles).

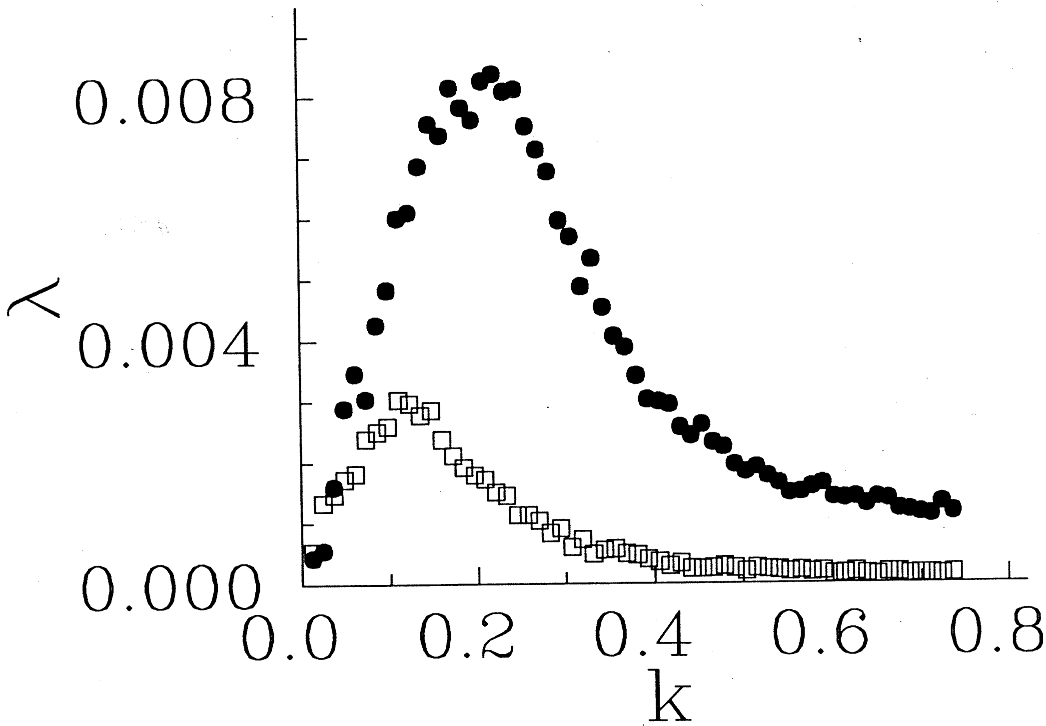

Fig. 3 Amplification rate of periodic perturbations vs. wave number in a square lattice gas with repulsive first-neighbor interactions for $E = 0.4$ (boxes) and 0.2 (closed circles).

In the second case, the square lattice-gas model is characterized by a repulsive nearest neighbor interaction. Our investigation is concentrated on a half-filled system which exhibits chessboard-like ordered phases (A and B) below a critical temperature $T_c = 0.567$. The simulation is started from such a state in which the ordered phases A and B are separated by a horizontal (planar) interface. The second interface is eliminated by choosing M to be odd ($M = 51$). In this case, we could choose a shorter thermalization (500 MCS) and period (250 MCS) to measure the amplification rate. The average amplification rate as the function of the wave number is illustrated in Fig. 3 for $E = 0.4$ and 0.2. These data confirm the theoretical predictions namely, $\lambda \propto |Ek|$ if $k \to 0$ and the position of maximum λ is proportional to the driving field.[13]

In summary, the present MC simulations have clearly demonstrated the interfacial instability and the subsequent processes cutting the large domains into strips in driven systems with both attractive and repulsive interactions. It is shown that the periodic perturbations increase with time in qualitative agreement with theoretical predictions. The effect of bulk diffusion and thermal fluctuations on the interfacial instability, however, requires further investigations.

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