Coarsening under Anisotropic Conditions in a Lattice Gas Model

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Abstract. Phase segregation under anisotropic non-equilibrium conditions is studied in the driven lattice gas. We show that, at early times, the degree of segregation of the nonequilibrium system is smaller than for the equilibrium counterpart, and that at late t there is a unique $t-$*dependent* length increasing $\ell(t) \sim t^{1/3}$ for a two-dimensional macroscopic system. We also identify the basic growth mechanisms, and demonstrate time self-similarity as well as other interesting features of both the structure factor and the scaling function. The chances are that our findings can be observed experimentally.

Many complex systems, e.g., binary alloys, polymers, and some hydrodynamical systems, undergo phase segregation after a quench below certain temperature. Many properties of the final state depend strongly on the kinetics of the segregation process. For instance, the alloy Al-Zn, which is homogeneous at high temperature, develops coarsening macroscopic grains after the quench. The details of the grains growth, and its competition with the progress of solidification from the melt determine the resistivity and hardness of the alloy, among other properties.

The underlying physics is now rather well understood, partially due to computer simulation of lattice gas models.[1, 2] There are some more general situations that have only been poorly studied, however. For instance, those that involve anisotropy and more, generally, non-equilibrium conditions, such as in the case of mixtures under shear flow. Alternatively, the driven lattice gas (DLG) evolving at low temperature provides a simple model situation for the kinetics of pattern formation in unstable mixtures under anisotropic non-equilibrium conditions. We studied the kinetics of the DLG by extensive Monte Carlo simulations, and concluded a coherent theoretical description.[3] In this paper we review some previous results and provide some additional interesting details.

The DLG consists of a d-dimensional lattice gas at temperature T in which nearest neighbors (NN) particle-hole exchanges are favored along one of the lattice principal directions, say $\vec{x}$. There is a variable, $n_i = 1$ (particle) or $n_i = 0$ (hole), defined at each node of the lattice, NN particle pairs interact via $H = -4\sum_{NN} n_i n_j$, and one assumes periodic boundary conditions and transition rates defined via a biased Metropolis rule, $\omega(\mathbf{n} \to \mathbf{n}^*) = min\{1, exp[-(\Delta H + E\delta)/T]\}$. Here $\mathbf{n}^*$ represents the configuration $\mathbf{n} = \{n_i\}$ after a particle-hole exchange, $\Delta H = H(\mathbf{n}^*) - H(\mathbf{n})$, $E\vec{x}$ may be interpreted as an (electric) field driving (charged) particles, and $\delta = (\mp 1, 0)$ for jumps along $\pm\vec{x}$ or jumps in any of the transverse directions, respectively. For $E = 0$ this model reduces

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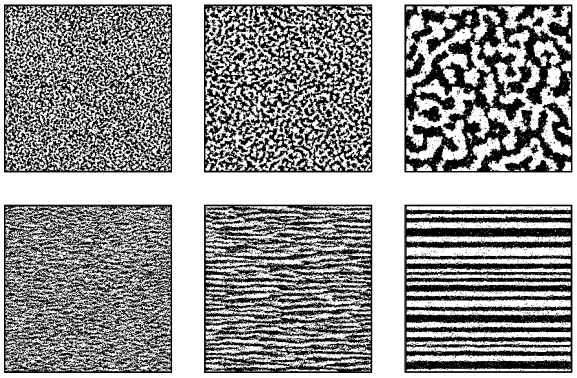

FIGURE 1. Snapshots of the coarsening process for LG (upper row) and DLG (lower row) defined on a 256×256 lattice for times (from left to right) $t = 10$, 100 and 10000 MC steps, respectively.

to the equilibrium lattice gas. However, the combination of the external field and periodic boundary conditions makes the system to constantly stay far from equilibrium. In particular, for any non-zero driving field, a particle current sets in. As E is increased, one eventually reaches saturation, i.e., particles cannot jump against the field. For $d = 2$, $\rho = \frac{1}{2}$ and $E = \infty$ (the only case we consider below) the system exhibits a critical point at $T = T_c^{\infty} \approx 1.41 T_c(E = 0)$. Steady states below this temperature consist of a single particle-rich stripe, which percolates along the field direction. The interfaces are then rather flat, showing only some microscopic roughness.[4]

In order to simulate a deep quench, we initialize our system in a completely random configuration, and let it to evolve under dynamics ω at temperature T (below the critical point) until one or a few stripes form. Our code involves a list $\lambda(t)$ of NN particle-hole pairs from where the next move is drawn. Time is increased by $\Delta t = \lambda(t)^{-1}$, so that the *MC step* involves a visit to all sites on the average. This corresponds to the standard Monte Carlo method only if the time increment Δt is drawn from a Poisson distribution. Taking constant $\Delta t = \lambda(t)^{-1}$ involves some approximation. However, if the number of particle-hole pairs in the system is sufficiently large (which is our case for $\rho = \frac{1}{2}$), the approximation is excellent. The lattice is rectangular, $L_{\|} \times L_{\perp}$, with sides ranging from 64 to 256. Averages correspond to one thousand independent runs.

The DLG exhibits different time regimes during phase segregation. Starting from complete disorder, there is a very short initial transient in which small grains form. A main novelty is that, as compared to the standard lattice gas (LG), typical grains are now stretched along the field direction (cf. Fig. 1). This initial anisotropy can be characterized quantitatively by measuring the number of broken bonds in the direction of the field, $n_{\|}(t)$, and perpendicular to it, $n_{\perp}(t)$, as a function of time. Fig. 2.a compares the difference $A(t) \equiv [n_{\perp}(t) - n_{\|}(t)]/2N$, which measures the degree of anisotropy ($2N$ is the total number of bonds in the system), as a function of time for the LG and the DLG. While $A(t)$ fluctuates around zero for the isotropic LG, it rapidly grows with time

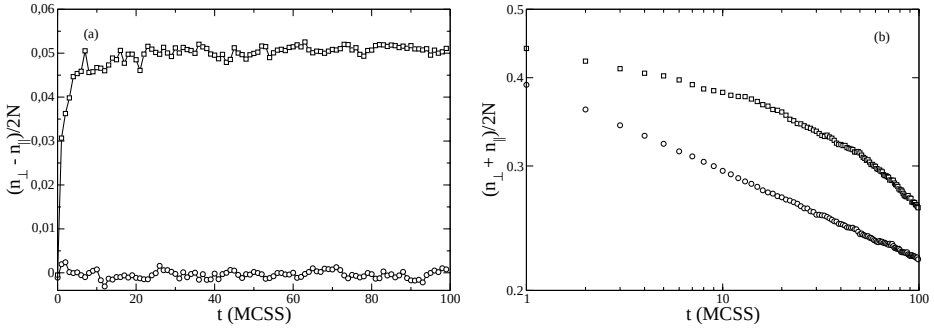

FIGURE 2. (a) The *anisotropy* function $A(t)$, as defined in the main text, as a function of time for both LG (circles) and DLG (squares); (b) Logarithmic plot of the *segregation* function $B(t)$ as a function of time for both LG (circles) and DLG (squares). See the main text for definitions. Both figures contain data from a single typical run.

for DLG, thus confirming anisotropy. On the other hand, close inspection of Figs. 1 suggests significant differences in the degree of segregation between LG and DLG at early stages of evolution. That is, for a fixed (early) time, LG seems more segregated than DLG. The observable $B(t) \equiv [n_\perp(t) + n_\parallel(t)]/2N$, which measures the density of broken bonds, illustrates the degree of segregation at time t. Fig. 2.b depicts $B(t)$ as a function of time for both LG and DLG as obtained from a single run. The smaller $B(t)$, the higher the degree of segregation is. We observe that $B(t) \sim t^{1/8}$ for LG, while $B(t)$ is compatible with a time dependence according to a stretched exponential with exponent $\alpha \approx 0.37$ for DLG. Although the stretched exponential relaxes faster than the power law, we observe $B_{LG}(t) < B_{DLG}(t)$ at early stages of evolution, confirming that LG is in fact more segregated than DLG at given early time. The reason for such different segregation relies on the effect that anisotropy induces on surface tension.[3]

The grains rapidly coarsen to form macroscopic strings, very similar to those observed in sheared fluids and other systems [5, 6]. The strings, as well as the anisotropic grains, can be characterized by two different typical length scales, namely $\ell_\parallel(t) \sim t^{\varphi_\parallel}$ and $\ell_\perp(t) \sim t^{\varphi_\perp}$, where $\varphi_\parallel \approx 1$ and $\varphi_\perp \approx 0.2$.[7] The multiplicity of length scales is a consequence of the underlying anisotropy. The DLG strings further segregate with time until well defined, relatively narrow stripes percolating in the field direction are formed. Strings give rise to stripes once $\ell_\parallel(t)$ equals $L_\parallel$. Hence the time τ_{st} the system needs to reach the striped state is $\tau_{st} \sim L_\parallel^{1/\varphi_\parallel}$.[7] Furthermore, the typical length in the direction perpendicular to the field at time τ_{st} is $\ell(\tau_{st}) \sim L_\parallel^{\phi}$, where $\phi = \varphi_\perp/\varphi_\parallel$, so that the number of stripes formed is $n_{st} \sim L_\perp L_\parallel^{-\phi}$.[7] Consequently, for rectangular lattices such that $L_\perp \leq L_\parallel^{\phi}$, the resulting state exhibits a single stripe, and no further net evolution is observed.

However, in general, the resulting state is multistriped. Multistripe states are only partially segregated, so that a clear tendency towards a fully segregated state with a

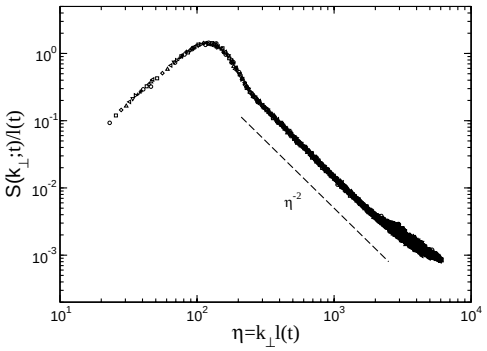

FIGURE 3. Scaling of the structure factor with time for a lattice $L_\perp \times L_\parallel = 256 \times 8$.

single stripe is generally observed in computer simulations. The stripe coarsening stage is characterized by a single typical length, $\ell_\perp(t) \equiv \ell(t)$, the mean stripe width, since the longitudinal length has reached the system limits. Assuming that the stripe coarsening process proceeds via effective diffusion (due to single particle events) and coalescence of stripes, it ensues that $\ell(t)$ obeys the following differential equation,[3]

$$\frac{\mathrm{d}\ell}{\mathrm{d}t} = L_\parallel^{-1}(\mu_{EC}\ell^{-3} + \mu_{HD}\ell^{-2}) \tag{1}$$

where μ_{EC} and μ_{HD} are parameters. The term ℓ^{-2} is associated to hole (particle) diffusion within particle (hole) stripes, while the term ℓ^{-3} is associated to the evaporation-condensation of particles and holes from stripes interfaces.[3] For large systems, eq. (1) predicts $\ell(t) \sim (t/L_\parallel)^{1/4}$ at early times and a crossover to $\ell(t) \sim (t/L_\parallel)^{1/3}$ for longer times. The crossover time is estimated as $\tau_{cross} \propto L_\parallel$. On the other hand, the time the system needs to reach the steady, single-striped state is $\tau_{ss} \propto L_\perp^3 L_\parallel[1 + \mathscr{O}(L_\perp^{-1})]$.[3] These two characteristic times, together with the time τ_{st} signaling the onset of the striped state, characterize the evolution. The different size and shape dependence of these three time scales, $\tau_{st}(L_\parallel)$, $\tau_{cross}(L_\parallel)$ and $\tau_{ss}(L_\perp, L_\parallel)$, defines different regions in the space $(L_\perp, L_\parallel)$, each characterized by a typical time evolution. In particular, one usually has $\tau_{cross}(L_\parallel) \ll \tau_{ss}(L_\perp, L_\parallel)$, so that $\ell(t) \sim (t/L_\parallel)^{1/3}$ is the most generally observed asymptotic behavior. However, for small enough values of $L_\perp$ and fixed $L_\parallel$, one has $\tau_{cross}(L_\parallel) > \tau_{ss}(L_\perp, L_\parallel)$ leading to $\ell(t) \sim (t/L_\parallel)^{1/4}$; this corresponds to a system that has reached the steady state before entering the asymptotic $t^{1/3}$ region. The time crossover between $1/4$ and $1/3$ behaviors, and the different size dependence of $\tau_{cross}(L_\parallel)$ and $\tau_{ss}(L_\perp, L_\parallel)$, induce a size crossover for the observed long time growth law. It may also happen that $\tau_{st}(L_\parallel) > \tau_{cross}(L_\parallel)$ and hence, once the striped state is formed, pure $t^{1/3}$ behavior is observed without any $t^{1/4}$ precursor region.

The structure factor is an important tool for experimental analysis.[1] Given that the DLG shows a unique relevant length scale in the stripe coarsening stage, one should expect dynamical scaling on $S(k_\perp;t)$, namely, $S(k_\perp;t) \propto \ell(t)F[k_\perp \ell(t)]$.[2] This is con-

firmed in Fig. 3 for a lattice $L_\perp \times L_\parallel = 256 \times 8$. In equilibrium ($E = 0$), the scaling function $F[\eta]$ is predicted to decay, according to Porod's law, as η^{-3} (for $d = 2$) at large η. This is a consequence of the isotropic short scale structure of the equilibrium system, which is captured by the correlation function, $C(\vec{r},t)$. The anisotropic, striped geometry of DLG, however, implies that $F[\eta] \sim \eta^{-2}$ as an (anisotropic) extension of Porod's law to our driven non-equilibrium model.[3] This is fully confirmed in Fig. 3. Furthermore, a detailed analysis of $F[\eta]$ reveals that, as $L_\parallel$ is increased, the anisotropic behavior $F[\eta] \sim \eta^{-2}$ crosses over to $F[\eta] \sim \eta^{-3}$ for very large values of η. This reflect the existence of standard nearly-isotropic thermal fluctuations for short wavelengths.

Summing up, we studied the time evolution after a quench to low T of a nonequilibrium interacting-particle model under a large drive. Anisotropic grains form, coarsening in strings as time goes on, until well defined narrow stripes develop. During the grain-string stage, the degree of segregation of the driven system is smaller than its equilibrium counterpart. The stripes, characterized by its mean width $\ell(t)$, further coarsen with time in such a way that $\ell(t)$ generally grows as $t^{1/3}$ due to hole diffusion in the bulk. However one may also observe $t^{1/4}$ at early times (or for short $L_\perp$) due to surface evaporation-condensation processes. Perhaps these mechanisms ar of some relevance for related experimental situations; see [6] for instance. We also found time self-similarity of the structure factor. The resulting scaling function $F(\eta)$ decays as η^{-2} for large η, due to the singular geometry induced by the drive.

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