Anisotropic Domain Growth of ANNNI Model at Low Temperatures

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We investigate the ordering kinetics for axial next nearest neighbor Ising (ANNNI) model in one and two dimensions by the multi-spin heat bath dynamical simulation. This dynamics enables us to overcome the pinning effect and to observe the dynamical scaling law for domain growth in the ANNNI model at zero temperature. The domain growth exponent is 1/2 isotropically both in the ferromagnetic and the dry-(commensurate) antiphase. In the wet-(commensurate) antiphase, however, it is approximately 1/3 in the modulated direction, whereas it remains 1/2 in the non-modulated direction. We suggest that these exponent values are dictated by 3 and 4 body diffusion-reaction processes of domain walls.

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The phase ordering kinetics of systems quenched from a high temperature disordered phase to a low temperature ordered phase has been widely studied including the domain growth law and the dynamical scaling behavior of correlation functions [1–3]. It is generally accepted that the universal behavior of the domain growth depends on the presence of topological defects, the conservation law of the order parameter, and types of local energy barriers [2–4]. Virtually all the systems studied thus far including anisotropic models such as the axial next nearest neighbor Ising(ANNNI) model are believed to have self-similar domains and an isotropic domain growth law [2–4, 10]. While previous studies of the ANNNI model did observe somewhat anisotropic dynamic structure factors at low temperature [6–8], the conventional belief is that the exponents characterizing the growth are isotropic. The previous work used single spin update algorithms which cannot overcome the strong pinning effect at low temperature and leads to sluggish dynamical behavior. Also, in accord with the prior expectation of isotropic behavior, the total excess energy (in both direction) was used to find the growth exponent [6–8].

The principal theme of this paper is a careful numerical study of the dynamics of coarsening of the ANNNI model. Our results indicate isotropic growth at low temperature for a range of parameter values governing the competition between the nearest and the next nearest neighbor exchange interaction in complete accord with previous expectations. However, we find in another part of parameter space striking evidence for anisotropic domain growth of self-affine domains with the exponent values (1/2 and 1/3) along the different directions being controlled by diffusion-reaction processes of the domain walls (defects). These results are obtained using a new multi-spin heat bath dynamics(MHBD) algorithm which allows one to overcome the strong pinning effects even at zero temperature. Our work provides the first vivid demonstration of anisotropic scaling behavior in the coarsening problem and establishes the power of the MHBD algorithm for effective equilibration of this rich system.

The ANNNI model was first introduced to describe the equilibrium properties of spatially modulated structures in magnetic and ferroelectric materials where the commensurate-incommensurate (C-INC) transition exists [1–3]. The competing interactions in this model are ferromagnetic interactions (J1 > 0) of nearest neighbor spins in all directions and antiferromagnetic interactions (J2 < 0) of next nearest neighbor spins in the modulation direction and give rise to a rich phase diagram: at low temperatures, depending on the competition ratio κ = −J2/J1, the ferromagnetic phase exists for κ < 0.5 and the (commensurate) modulated antiphase (⋯↑↑↓↓↑↑⋯) for κ > 0.5. This antiphase consists of a wet (0.5 < κ < 1) and a dry phase (κ > 1), which are separated by a line of wetting transitions as the temperature increases. On introducing the effect of thermal entropy, the phase diagram shows a variety of structures such as an incommensurate phase and devil’s staircases.

Our MHBD algorithm considers a square block of 4 spins in 2D or a string of 4 spins in 1D, so that we update a spin-cluster conformation among the 16 possible states. Each state has its own probability in accordance with the Boltzmann weight in the heat bath algorithm. One of the 16 states is selected randomly according to their probability of occurrence and consequently a new configuration of the 4 spins is obtained. We first applied MHBD to the simple Ising model on a square lattice of linear size L=1000. Simulations were carried out at $T = 0.1 J/k_B$ up to $10^4$ Monte Carlo step (MCS), and averaged over 50 initial configurations. The expected scaling collapse of the correlation function is obtained and is very consistent with that obtained with single spin update algorithms. Moreover, the analysis from the excess energy, the defect density, and the correlation function provides a domain growth exponent of 1/2. Thus MHBD is confirmed to be an excellent approach for studying the ordering kinetics at low temperatures.

We now consider a quenching of the linear ANNNI model, where the modulation of (J1 > 0 and J2 < 0) interactions exists precisely along the axis , from high $T$
to $T = 0$ because an ordered state exists only at $T = 0$. Right after a nucleation stage from the random initial states when $\kappa > 1$, the system consists of 1(· · · $\uparrow\downarrow\uparrow\downarrow$, · · ·), 3(· · · $\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow$, · · ·), 4(· · · $\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$, · · ·), 5(· · · $\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$, · · ·), 6(· · · $\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$, · · ·)-mers of up or down spins in the sea of dimers. These 1, 3, 4, 5, 6-mers (called domain walls or defects) diffuse, annihilate and produce stable dimers by collisions as time elapses. Because the density of trimers would be higher than any other $k$-mer except for the stable dimer, most of the excess energy of this nonequilibrium state comes from trimers. When three trimers merge together (· · · $\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\downarrow\uparrow\downarrow$, · · ·), a monomer is produced with 4 stable dimers around (· · · $\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$, · · ·) and this monomer, when combined with a trimer, will result in two dimers eventually. This 3 body-collision and annihilation of trimers is the dominant decay processes of domain walls and predicts the domain growth law $L(t) \sim (t/\log t)^{1/2}$, where $L(t)$ is a characteristic length and the logarithmic correction originates from the fact that $D=1$ is the critical dimension for the 3 body diffusion-reaction process $[4, 5]$. However, for $0.5 < \kappa < 1$, the domain walls are strongly pinned if their motion is controlled by a single spin update and thus such 3 body annihilation or other decay processes of domain walls can never occur. But, applying MHBD with a string of 2, 3 or 4 spins, 4 body annihilation process of trimers can occur which then becomes the dominant decay process in this regime: (3333) becomes (2433), (2442), or (2622) with the same energy, and (2622) becomes 6 dimers with an associated energy decrease $\Delta E = 4J_1 + 8J_2 < 0$ for $0.5 < \kappa < 1$. So, the rate equation for the density $A(t)$ of trimers, \[
abla \frac{dA(t)}{dt} = -4A(t)^4,\] is obtained which immediately predicts the growth law $L(t) \sim A(t)^{-1} \sim t^{1/3}$ $[4]$.

When 3 or 4 body collision of trimers occur, 4-mer, 5-mer, and 6-mer can be considered as the resonance of two trimers, three trimers, and four trimers. When 3 body collision of trimers is the dominant decay process among that of $k$-mer domain walls, the density of $k$-mer domain walls will have a descending order by 3, 1, 4, 5, 6-mers, whereas when 4 body collision of trimers is the dominant decay process, it will have a descending order by 3, 4, 5, 6, 1-mers. Therefore, it is advantageous and important to look at the most and the next most dominant decay process of domain walls in the system, which predicts the domain growth law of either $t^{1/2}$ or $t^{1/3}$ directly.

We simulated a phase ordering of 1D-ANNNI model employing MHBD with blocks of either 2 or 4 spins for a system size 4000 up to $10^4$ MCS at $\kappa = 0.2$, 0.4, 0.49, 0.51, 0.6, 0.9, 1.0, 1.01, 1.1, 1.5, 2.0, 3.0, 5.0, and 10.0. The densities of $k$-mer domain walls, the excess energy as well as the correlation function are calculated at each time and all quantities are averaged over an ensemble of 2000 runs. Figure 1 shows the densities of $k$-mer domain walls at $\kappa = 0.9$ and $\kappa = 1.1$ in the (commensurate) antiphase. In the wet phase ($\kappa = 0.9$), the descending order in their densities are 3, 4, 5, 6, 1-mers and in the dry phase ($\kappa = 1.1$), they are 3, 1, 4, 5, 6-mers. Therefore, the former and the latter ought to have the domain growth law of $t^{1/3}$ and $t^{1/2}$, respectively. These results are self-consistently supported by our analysis of the two-point correlation function.

![FIG. 1. The densities $A_k(t)$ of $k$-mer domain walls for the 1D-ANNNI model (a) in the wet phase ($\kappa = 0.9$) : 3,4,5,6,1-mer from top and (b) in the dry phase ($\kappa = 1.1$) : 3,1,4,5,6-mer from top.](image1)

![FIG. 2. The scaled correlation functions of 1D-ANNNI model in the ferromagnetic($\kappa = 0.4$), the dry($\kappa = 1.1$), and the wet ($\kappa = 0.6$) phase from top, which are collapsed for different times $t = 80, 160, 320, 640, 1280, 2560, 5120, 10240$ MCS at each $\kappa$ values. Inset shows the growth exponents in each phases. The two point correlation function $C(r, t)$ is defined as $C(r, t) = \left< S_i \cdot S_{i+r} \cdot (-1)^r/2 \right>$ suitable for the antiphase, where $r$ is even number, and $C(r, t) = \left< S_i \cdot S_{i+r} \right>$ for the ferromagnetic phase. The growth exponent $n$ is evaluated by the decay of the excess energy or the defect density and by the scaling collapse of the correlation function $C(r/L(t))$, where $L(t)$ is obtained from $C(L(t), t) = 1/2$ (see Fig. 2). For the ferromagnetic phase ($\kappa < 0.5$), we obtain $n = 0.5$ by fitting to a power law $L(t) \sim t^n$. For the dry-antiphase ($\kappa > 1$), $n \approx 0.46$ on fitting to $L(t) \sim t^n$ while $n \approx 0.52$ on fitting to $L(t) \sim (t/\log t)^n$. In order to detect the logarithmic correction, more extensive simulations with system size $2 \times 10^4$ were performed up to $6.5 \times 10^9$ MCS at $\kappa = 0.9$ and 1.1 averaged over 300 samples. The log-log plot of $L(t)$ versus $t$ at $\kappa = 1.1$
is not a straight line at longer times but has an upward curvature. On the other hand, the log-log plot of $L(t)$ versus $t/\log(t)$ shows a nice straight line. This is fully consistent with the fact that $D=1$ is the critical dimension of 3 body diffusion-reaction processes [14,15]. For the wet-antiphase ($0.5 < \kappa \leq 1$), the growth exponent $n \simeq 0.35$ with a power law fitting, which is close to 1/3 and consistent with the theoretical prediction [16]. This is a rare realization of 4 body diffusion-reaction process whose dynamic scaling is first observed in our numerical simulations.

For a 2D-ANNNI model, the ground state in the antiphase has 4 degenerate states (A,B,C,D). If the ground state at two boundaries along the modulated ($y$) direction of the finite system is fixed by A-state at one end and D-state at the other end, B and C-states can exist in between at equilibrium in the wet phase ($0.5 < \kappa < 1$). In the dry phase ($\kappa > 1$), the A-state meets the D-state directly without the appearance of B and C-states. The domain patterns in the dry and the wet phases are quite different (see Fig. 3): For a dry phase, it looks like a typical domain growth pattern having 4 degenerate ground states. But, for a wet phase, it is elongated (growing faster) along the non-modulated ($x$) direction. At $T = 0$ the wetting transition, similar to that of liquid between air and substrate, occurs at $\kappa = 1.0$, and there exists a line of wetting transition as the temperature increases $\kappa$.

We performed MHBD simulations for ordering kinetics of the 2D-ANNNI model at $T = 0$ for several $\kappa$ values ($\kappa=0.2, 0.4, 0.6, 0.9, 1.0, 1.1, \text{and} 2.0$) taking 4 spins as a square block. The system size is 2048×2048 and 30 samples are accumulated up to $10^4$MCS. MHBD could remove the pinning effect for $\kappa < 1$ so that domains grow well in both the ferromagnetic and the antiphase. The two point correlation functions for the antiphase were defined separately by $C_x(x, t) = \langle S_i \cdot S_{i+x} \rangle$ in the non-modulated ($x$) direction and $C_y(y, t) = \langle S_i \cdot S_{i+y} \cdot (-1)^{y/2} \rangle$ in the modulated ($y$) direction. The excess energy and the length of domain walls (defects) are calculated separately for each direction. The densities of $k$-mers along the $y$-direction are also calculated as in the 1D case. The growth exponents are evaluated by $L_x(t) \sim t^{n_x}$ and $L_y(t) \sim t^{n_y}$ obtained from the scaling collapse of correlation functions and by the domain wall densities $\rho_x(t) \sim t^{-n_x}$ and $\rho_y(t) \sim t^{-n_y}$.

The growth exponents $n_x$ and $n_y$ are $1/2$ at $\kappa = 0.2$ and 0.4 (ferromagnetic phase) and also at $\kappa = 1.1$ and 2.0 (dry-antiphase). But, at $\kappa = 0.6, 0.9, 1.0$ (wet-antiphase), $n_x$ and $n_y$ are anisotropic: $n_x \sim 0.55$ and $n_y \sim 0.39$. One may wonder whether these values are transient and may both approach 1/2 (or 1/3 and 1/2 respectively) in the very long time limit. More simulations with the larger system size $4096 \times 4096$ were performed up to $2 \times 10^4$MCS at $\kappa = 0.8$ and 1.0. Further more, MHBD with $3 \times 3$ and $4 \times 4$ block cells were used under the same conditions. However, the exponents $n_x \simeq 0.55$ and $n_y \simeq 0.39$ do not change significantly [15]. Hence one may also expect that the correction term must be included in $L_x(t)$ and $L_y(t)$. We considered two kinds of corrections: The first is $\rho(t) \sim L(t) \sim t^\alpha (1 + t^{1-\alpha})$ and the second is $\sim t^\alpha (\log t)^\alpha$. The non-linear fitting of the former does not give consistent results for different time intervals and $\kappa$ values. However, the same fitting of the latter gives $n_x \simeq 1/2$, $\alpha \simeq 1/2$ and $n_y \simeq 1/3$, $\alpha \simeq 1/3$ for many different time intervals and $\kappa$ values. So, the anisotropic domain growth laws in the wet-antiphase are consistent with $L_x(t) \sim (t \log t)^{1/2}$ and $L_y(t) \sim (t \log t)^{1/3}$. Figure 4 shows the nice scaling collapse of correlation functions both for the non-modulated ($x$) direction and for the modulated ($y$) direction in the wet and dry phase. A similar collapse is observed for a plot of the domain wall density (not shown).

The result from the densities of $k$-mers along the $y$-
direction further supports and is consistent with the above remarkable result because their descending sequence is $3,4,5,6,1$ at $\kappa = 0.9$ and $3,1,4,5,6$ at $\kappa = 1.1$ in agreement with the 1D case (see Fig. 5). So, one may identify that the 4 (3) body diffusion-reaction process of domain walls is important, as in 1D, as the dominant decay process in the wet (dry) phase of 2D-ANNNI model, which results in the dominant domain growth law of $t^{1/3}$ ($t^{1/2}$).

One may actually consider that the domain growth at $T = 0$ is possible since MHBD is adopted. However, the simulation by a single spin update, Glauber dynamics, at $T = 0.4J_1/k_B$ in the wet phase gives the similar anisotropic growth exponents $n_x \approx 0.56$ and $n_y \approx 0.40$. The two point correlation function along the modulated ($y$) direction has also the same dip as that from using MHBD. Therefore, a single spin update dynamics can give the similar but less precise result for $T > 0$, since it severely suffers from the strong pinning effect at the low temperatures.

We have presented a summary of our results of detailed investigation of the ordering kinetics of the 1D and the 2D-ANNNI model at $T = 0$ using the multi-spin heat bath dynamical simulation to overcome the pinning effect. Our simulations show that the dominant domain growth exponent becomes 1/2 isotropically both in the ferromagnetic and dry-(commensurate) antiphase. In the wet-(commensurate) antiphase, however, it is approximately 1/3 for the modulated direction, whereas it remains 1/2 for the non-modulated direction. The exponent values are explained by 3 and 4 body diffusion-reaction processes of domain walls (defects). Contrary to conventional belief regarding universality, our data suggest an extremely unusual situation in which the very nature of the domain growth law critically depends on the ratio between the strength of competing interactions.

In the context of domain growth dynamics of experimentally relevant systems, the chemisorbed adsorbate systems such as O/Pd(110) and H/Fe(110) are of particular interest [16,19,20]. Both systems exhibit a wetting phenomena in the $(3 \times 1)$ phase. It will be worthwhile to probe a temporal evolution of structural factor for these systems experimentally, and compare with our results.

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\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig5}
\caption{The densities of $k$-mer for the 2D-ANNNI model. (a) $\kappa = 0.9$ (the wet phase) : $3,4,5,6,1$-mer from top. (b) $\kappa = 1.1$ (the dry phase) : $3,1,4,5,6$-mer from top.}
\end{figure}

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