$n=\frac{1}{4}$ domain-growth universality class: Crossover to the $n=\frac{1}{2}$ class

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The kinetic domain-growth exponent is studied by Monte Carlo simulation as a function of temperature for a nonconserved order-parameter model. In the limit of zero temperature, the model belongs to the $n=\frac{1}{4}$ slow-growth universality class. This is indicative of a temporal pinning in the domain-boundary network of mixed-, zero-, and finite-curvature boundaries. At finite temperature the growth kinetics is found to cross over to the Allen-Cahn exponent $n=\frac{1}{2}$. We obtain that the pinning time of the zero-curvature boundary decreases rapidly with increasing temperature.

Domain-growth kinetics is a fundamental problem in statistical mechanics of practical relevance in metallurgy,[1] surface science,[2] earth sciences,[3] and magnetism.[4] During the past few years, the search for universality aspects in growth of ordered domains as it takes place after a thermal quench below a phase-transition temperature has been the subject of continued work. In particular, numerical computer simulations of microscopic models[5-8] have provided an important insight into the problem.

When the order parameter, describing the transition, is a nonconserved quantity, the Allen-Cahn theory[9] predicts that the system reduces the excess energy contained in the domain boundaries $\Delta E(t)$ by reducing their curvature. If scaling holds, the time evolution for the total excess energy decays as a power law. That is, $\Delta E(t)=E(t)-E_T(t\rightarrow\infty)\sim t^{-n}$, where $E_T(t\rightarrow\infty)$ is the equilibrium energy at the temperature towards which the quench has been directed and n is an exponent with universal character.

It is now well established[6,8,10] that at least two universality classes, characterized by $n=\frac{1}{2}$ and $\frac{1}{4}$, have to be considered even for nonconserved order parameters. The exponent $n=\frac{1}{2}$ corresponds to a curvature-driven process when it proceeds under the normal conditions required in the theory.[9] The exponent $n=\frac{1}{4}$ corresponds to a singular case of the Allen-Cahn theory, namely when one of the curvatures is zero.

The $n=\frac{1}{4}$ universality class was first found by numerical computer simulations of certain anisotropic models described by continuous variables.[6,11] In spite of the extensive data supplied by Mouritsen,[6] clearly evidencing the exponent $n=\frac{1}{4}$, the discovering was disputed[12,13] in a reaction to the interpretation suggested by Mouritsen for the unexpected slow-growth behavior. He proposed that it indicated a breakdown of the basic assumptions in the Allen-Cahn theory at zero temperature due to the presence of broad (or "soft") walls which might screen the interaction between domains.[6] This interpretation is not correct. In two recent works, we presented extensive Monte Carlo simulations[8] as well as theoretical support[10] that give conclusive evidence for the new class and simultaneously show that the Allen-Cahn assumptions are fulfilled.

The magnetic model used was initially developed to describe a martensitic transformation.[14] The boundary structure consists of a mixture of interconnected broad, curved, and sharp, straight boundaries. The width of the broad boundaries is found not to be relevant. However, they can easily curve almost without energy cost relative to the energy involved in the generation of a kink along the sharp boundary.[8] This is the reason for the sharp boundary being straight and the broad being curved. The mixture is the cause for the slow time evolution with $n=\frac{1}{4}$ because of a hierarchical movement[10] of the boundaries, where the decrease in length of one kind of boundary (the broad) depends on the other (the sharp). This hierarchical movement of the boundaries is, in fact, present in the models where the $n=\frac{1}{4}$ behavior was first detected.[6]

In this paper we extend our previous low-temperature study of the $n=\frac{1}{4}$ universality class to quenches to higher temperatures. The results clearly show that, as the temperature increases, a crossover occurs to the Allen-Cahn exponent characterized by $n=\frac{1}{2}$, in agreement with recent results.[6] It is found that in the temperature-range of the crossover the mixture of walls of zero and finite curvature is still present and that the rules of the hierarchical movement of boundaries hold. The reason for the crossover is that the temporal pinning of the straight boundary rapidly disappears as the temperature increases. This allows the curved boundary to decrease in length independently.

Let us briefly summarize the model which is described in more detail elsewhere.[8,15] Consider a magnetic model with continuous spin variables restricted to the upper part of the x-z plane on a two-dimensional x-y lattice. We use

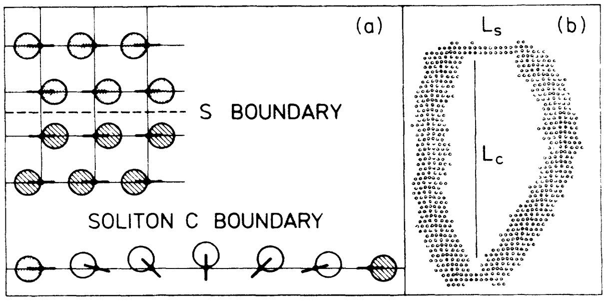

FIG. 1. (a) The upper part shows a sharp S boundary separating $+x$ (dotted) and $-x$ (dashed) domains. The circle indicates the displaced atom. The lower part shows a broad, solitonlike domain wall, a C boundary between $+x$ and $-x$ domains with the atomic displacement in the xz plane. However, for illustration purpose we show this displacement in the xy plane. A broad C boundary in (b) is a sequence of such solitons. (b) Typical domain showing two broad C boundaries connected by sharp S boundaries.

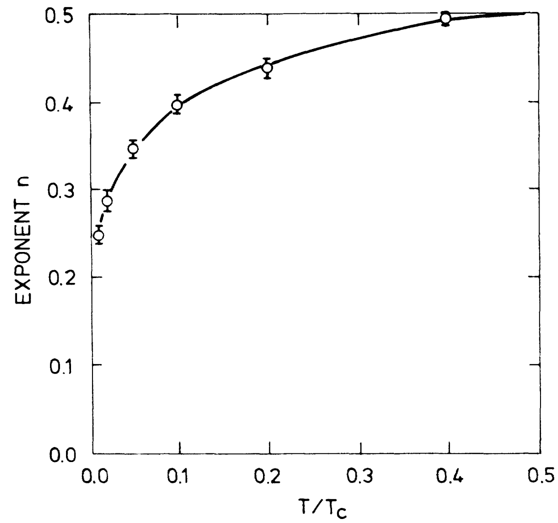

FIG. 2. The exponent n for quenches to various finite temperatures for a $N=100\times100$ system, averaged over fifteen Monte Carlo runs. A clear crossover from $n=\frac{1}{4}$ to $\frac{1}{2}$ is seen.

the Hamiltonian introduced recently for simulating martensitic transformations:[14]

$$H=\sum_{\langle ij\rangle}\{-KS_{iz}S_{jz}+J[\mathbf{S}_i\cdot\mathbf{S}_j-P(\hat{\mathbf{r}}_{ij}\cdot\mathbf{S}_i)(\hat{\mathbf{r}}_{ij}\cdot S_j)]\}$$
$$-D\sum_i(S_{ix}^4+S_{iy}^4)\,,$$

where $\hat{\mathbf{r}}_{ij}$ is a unit vector connecting nearest neighbors.

In Ref. 8 we made extensive Monte Carlo computer simulations on this simple restricted model (with $P=3$, $D=2J$, and $K=2.3J$) studying the domain growth after a rapid quench from $T=\infty$ to $T=0.02$ k_BT/J. We obtained that the total excess energy relaxes as $\Delta E(t)\sim t^{-n}$ with $n=\frac{1}{4}$.

In Fig. 1 we illustrate the two kinds of domain walls exhibited by the model [Fig. 1(a)], and the way they are connected forming the boundary structure [Fig. 1(b)]. The sharp, straight boundary, which we call the S boundary, is along the x direction, and the broad, curved boundary, called the C boundary (well modeled by a soliton function), is mainly along the y direction. The length of the S boundary L_s is measured in steps. The projected length of the C boundary on the y direction L_c is measured in solitons. It was found[8] that the number of solitons in the C boundary dominates the contribution to the total excess energy whereas the curvature energy is negligible.

Using standard Monte Carlo simulations techniques,[16] we have calculated the domain-growth kinetics after quenches from $T=\infty$ to different temperatures. The results have been obtained on a $N=100\times100$ lattice subject to periodic boundary conditions. At each temperature, the results were averaged over fifteen different runs. In

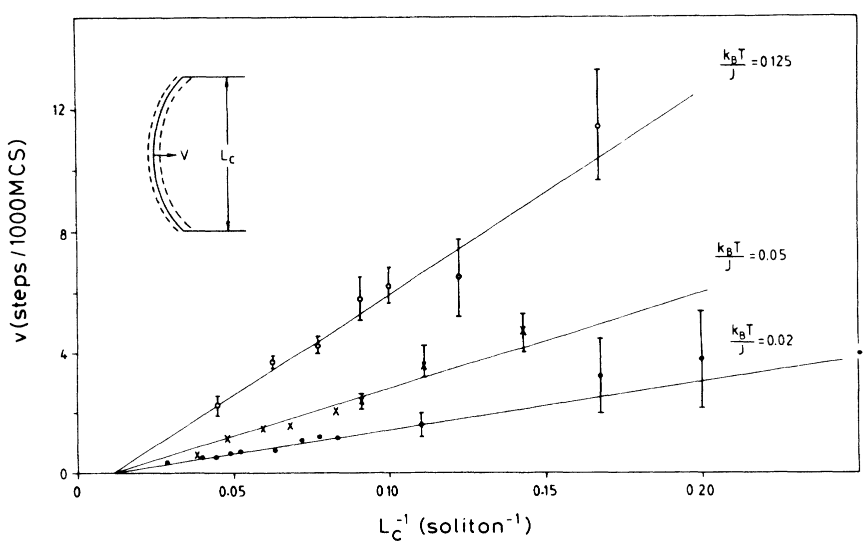

FIG. 3. Speed of the broad C boundary v vs the inverse length L_c^{-1} for different values of the temperature. v depends linearly on L_c^{-1} and increases with increasing temperature.

Fig. 2 we present the best exponent obtained by fitting the averaged excess energy to the expression $\Delta E(t) = t^{-n}$. The extremely long time necessary to complete the optimization process of the boundary widths at $T = 0$ K makes the determination of the exponent very difficult, at this temperature and much larger systems are required. Nevertheless, the results clearly show a crossover in the kinetic exponent value from $n = \frac{1}{4}$ to $\frac{1}{2}$ as a function of temperature. This is in agreement with recent results.[6]

Now we want to study the crossover region further. It is found that the mixture of straight and curved boundaries is still present. The C boundary moves with a constant velocity inversely proportional to its curvature. The velocity increases with increasing temperature. This can be seen in Fig. 3. We have plotted, for three different temperatures, the velocity of the C boundary as a function of $(L_c)^{-1}$ ($\sim$curvature). The points have been obtained from our simulations by following examples of domain-boundary patterns similar to the one shown in the inset. The length L_c does not change. This result evidences that the hierarchical movement of boundaries is present in the crossover region when the exponent increases and tends to the $n = \frac{1}{2}$ exponent.

The reason for the slow growth is that the C boundary has to wait for the S boundary to disappear before it can start to decrease. On the other hand, as the temperature increases, the speed of the C boundary increases and consequently the S-boundary length will disappear earlier, removing the pinning. To investigate this, we study the evolution of barrel-shaped domains with curved boundaries of various length L_c, but the same straight-boundary length L_s. The result is shown in Fig. 4. The pinning time t^* is defined as the time delay after which the elimination of the C-boundary length L_c starts. In Fig. 4 we have represented t^*/L_c versus the reduced temperature. Figure 4 shows that the pinning time decreases rapidly with increasing temperature. For $T > 0.25T_c$ one finds further that kinks are emitted onto the straight boundaries from the corners. This then allows L_c to decrease independently of the length L_s. Consequently, the heirarchical movement ceases.

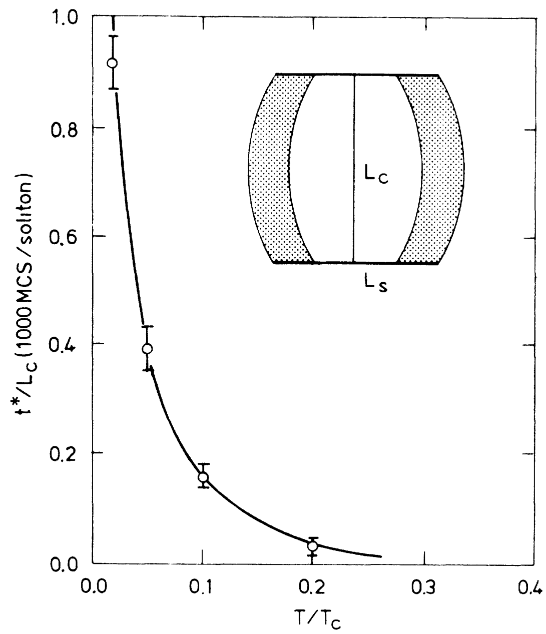

FIG. 4. The pinning time t^* of a barrel-shaped domain with curved walls of different L_c, but the same length L_s. The pinning time decreases with increasing temperature.

We conclude that the pinning of the straight boundary becomes irrelevant for the late time behavior at higher temperatures, and the system develops into a case corresponding to an all-curved-walls system. The scaling theory for this case gives the Allen-Cahn exponent $n = \frac{1}{2}$. The decrease in the pinning time is consistent with the crossover in the exponent shown in Fig. 4.

Finally, let us emphasize the fact that in order to obtain the algebraic growth laws it is imperative that the system has a scaling behavior. Therefore, the obtained results from the specific model are expected to have more validity and to shed light upon the general aspects of the new, unexpected slow-domain-growth universality class.

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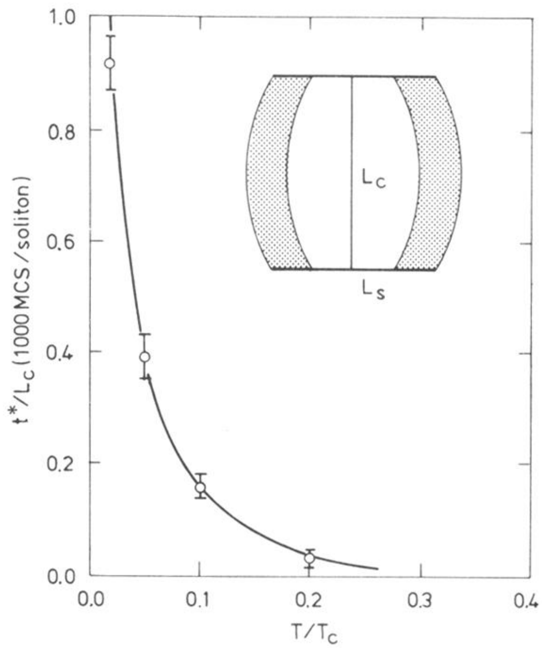

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