PHYSICAL REVIEW B VOLUME 15, NUMBER 11 1 JUNE 1977

Monte Carlo studies of the interface roughening transition*

Robert H. Swendsen†

Institut für Festkörperforschung der Kernforschungsanlage, Jülich, Germany

(Received 16 December 1976)

Monte Carlo simulations are used to study the roughening transition in the solid-on-solid and discrete Gaussian models of interfaces. It is demonstrated that very long simulation times are required to obtain a meaningful description of interface properties. Strong evidence is presented for the existence of the roughening transition, which is reflected in the thermodynamic properties of interfaces as well as the expected divergence of the interface width.

I. INTRODUCTION

In 1949, Burton and Cabrera[1] suggested that the interface between two phases in the three-dimensional (3D) Ising model should exhibit a "roughening" transition at a temperature T_R considerably below the bulk critical temperature T_c^{3D}(Ising). This transition is characterized by the interface becoming infinitely "rough" in the sense of a divergent interface width. The primary motivation for studying this transition comes from the theory of crystal growth, which uses the lattice-gas interpretation of the Ising model. As discussed in detail by Burton, Cabrera, and Frank,[2] interface roughening should play a basic role in determining growth rates and crystal perfection. Below T_R, growth only occurs by nucleation or by spiral growth in the presence of screw dislocations. Above T_R, the nucleation barrier is expected to vanish, giving a much higher growth rate that is linear in the chemical potential difference $\Delta\mu$.

The argument used by Burton and Cabrera[1] for the existence of the roughening transition was based on a mapping of the interface problem onto the two-dimensional spin-$\frac{1}{2}$ Ising model, which is valid at low temperatures. Consider a 3D simple-cubic Ising model with nearest-neighbor exchange J in the x and y directions and J' in the z direction. The interface is taken to be perpendicular to the z axis and is perfectly flat at $T=0$, with $S^z=-\frac{1}{2}$ for $z\geq 1$ and $S^z=+\frac{1}{2}$ for $z\leq 0$. In the lattice-gas interpretation, $S^z=+\frac{1}{2}$ represents a particle and $S^z=-\frac{1}{2}$ corresponds to a vacancy or hole. For small values of $T>0$, particles will appear on the surface ($S^z=+\frac{1}{2}$ spins in the x,y plane with $z=1$) with an energy $4J+J'-J'=4J$. The interactions within the x,y plane are just those of the two-dimensional (2D) Ising model with exchange constant J. Since the system is symmetric, the $z=0$ layer also maps onto a 2D Ising model. Burton and Cabrera then argued that since the 2D Ising model has a phase transition[3] at T_c^{2D}(Ising) $\approx(\frac{1}{2})T_c^{3D}$(Ising), at which the magnetization vanishes, the interface should also show a similar transition at about the same temperature, $T_R \approx T_c^{2D}$(Ising). This transition should be characterized by the particle concentration ($c_n=\langle S^z\rangle_n+\frac{1}{2}$, where the average is taken over the x,y plane with $z=n$) becoming the same in both layers. The gradient of the particle concentration then vanishes and the interface width diverges.

The difficulty with this argument is, of course, that before the interface width has become infinite, the mapping onto the 2D Ising model has broken down. The argument is, however, suggestive and also indicates that if the roughening transition does in fact exist, the value of J' should not be important. Most work on this problem has therefore concentrated on the solid-on-solid (SOS) limit, in which $J'\to\infty$ and the Hamiltonian can be written

$$\mathcal{H}(\mathrm{SOS})=\epsilon\sum_{i,j}\left(|h_{ij}-h_{i+1,j}|+|h_{ij}-h_{i,j+1}|\right), \tag{1}$$

where i and j denote the x and y coordinates, h_{ij} takes on integer values, and we have introduced $\epsilon=J$ to make contact with previous work.

In 1951, Burton, Cabrera, and Frank[2] extended the discussion to the three-and five-level versions of Eq. (1) in the Bethe approximation, but did not find any transition for these cases. They did find a maximum in the specific heat and made the rather unfortunate statement that it "can be interpreted as the transition temperature," but it is clear from the exact solution of the corresponding one-dimensional interface problem[3] that such an interpretation is not valid.

It might be supposed that the failure to find the roughening transition was due to the limitation to a finite number of layers, but in 1966 Temkin showed that this was not the case.[4] Temkin applied a Bragg-Williams approximation to the SOS model with an infinite number of layers. His results provided a good qualitative description of the thermodynamic properties, but still did not predict a roughening transition. This result cast considerable doubt on the existence of roughening, since Temkin's method, when applied to the 2D Ising model, reduces to the usual mean-field approximation with a phase transition. The problem posed by Temkin's results has recently been resolved by the identification of the essential correlations that had been neglected.[5] It was demonstrated that the roughening transition can be obtained from a mean-field treatment, reinforcing the belief that roughening does take place and is closely related to the phase transition in the 2D Ising model. However, the new mean-field approximation does not provide a good estimate for T_R, nor a rigorous upper bound. [A rigorous lower bound is available since van Beijeren[6] proved that $T_R \geq T_c^{2D}$(Ising) for arbitrary values of J'.]

The method of low-temperature series expansions has also been applied to this problem. Weeks *et al.*[7] and Gilmer *et al.*[8] have calculated the exact values of the first eight terms in the expansions of four properties of an interface in an isotropic Ising model ($J' = J$). Padé analysis of each series shows evidence of a singularity supporting the existence of roughening. Unfortunately, four different values of T_R are predicted. Three of the series represent different measures of the interface width and are related by exact inequalities.[9,10] These inequalities are violated by the predicted values of T_R. The predicted exponents describing the divergence of the various measures of the width also violate these inequalities if a single value of the roughening temperature is assumed. This means that these series are not long enough to show their true asymptotic behavior and we cannot rely on their predictions.

Leamy *et al.*[11] have also presented series predictions for the SOS model, but the exact inequalities are again violated. (The only available self-consistent set of roughening exponents are those given by the mean-field approximation.[5])

Monte Carlo simulations have also been performed in an attempt to clarify the situation.[12-14] Although they have contributed to our knowledge of the thermodynamics of interfaces, they have not been able to provide satisfactory evidence for the existence of the roughening transition. This has been primarily due to the use of short simulation times and the failure to study the size dependence and time dependence of the relevant properties.

The main purpose of this paper is to present the results of Monte Carlo simulations that do demonstrate the existence of the roughening transition and clarify its relationship to the phase transition in the 2D Ising model. We shall show that the roughening transition is reflected in a singularity in the specific heat and critical slowing down as well as in the expected divergence of the interface width.

We shall also present the results of what we believe to be the first Monte Carlo simulation of the closely related discrete-Gaussian (DG) model, described by the Hamiltonian

$$\mathcal{H}(\mathrm{DG}) = \epsilon \sum_{i,j} [(h_{ij} - h_{i+1,j})^2 + (h_{i,j} - h_{i,j+1})^2] . \qquad (2)$$

For height differences of 0 and ±1, Eqs. (1) and (2) give the same values of the energy. Since the average height difference for neighboring sites is about 0.25 at roughening, the transition is expected to be essentially the same in both models and to occur at approximately the same temperature. The DG model, however, is somewhat more tractable mathematically and has been mapped onto the 2D Coulomb gas by Chui and Weeks[15] and onto a sine-Gordon theory by Kroll, Müller-Krumbhaar, and Wagner.[16]

In Sec. II, we shall describe the relevant details of the Monte Carlo method. Sec. III contains the thermodynamic properties of the interface and Sec. IV has a discussion of the interface width. Time-dependent correlation functions in Sec. V demonstrate the presence of critical slowing down. The properties of a step in the interface also show the effects of roughening and are discussed in Sec. VI.

II. MONTE CARLO METHOD

Monte Carlo simulations of both SOS and DG models were carried out for a sequence of $N \times N$ square lattices with periodic boundary conditions, where $N = 5$, 10, 20, and 40. Runs were made both with and without a single (10)-step in the surface. The algorithm involved single-site processes that changed the height of the surface at a chosen site by one unit and did not conserve the total height (no particle conservation).

Two separate chains of pseudorandom numbers were used to generate the x and y coordinates of a site. A third chain was used to decide whether to attempt a creation or annihilation ($\Delta h_{ij} = +1$ or -1). If the proposed energy change was less than or equal to zero, it was carried out immediately; otherwise, the change was only carried out with a probability $\exp(-\beta \Delta E)$ as required by detailed balance. Separate chains were used for $\Delta h_{ij} = +1$ and -1. The five chains were broken by the use of a different random number generator and permuted every N^2 Monte Carlo step (that is, in intervals of one Monte Carlo step per site). System properties were recorded at intervals of one Monte Carlo step per site.

For each value of the temperature T and linear dimension N, a continuous simulation of 1.1×10^5 Monte Carlo steps per site was made (1.76×10^8 Monte Carlo steps for a 40×40 lattice), starting from a flat surface ($h_{ij}=0$). For the analysis, each simulation was divided into 11 groups (or runs) of 10^4. The first run was discarded and averages were taken over each of the remaining ten runs.

Errors proved to be larger than one would expect from simulations of this length, due to the long relaxation times discussed in Sec. V. (These long relaxation times prevented the study of larger lattices with the available computer time.) We believe that the most reliable error estimates are given by the spread in the values for each quantity obtained from each of the ten runs. The validity of this estimate depends primarily on the relaxation times being much less than 10^4 Monte Carlo steps per site, which is consistent with our results for the time-dependent correlation functions.

Direct integration of the measured time-dependent correlation functions[17] to obtain values of the effective correlation times resulted in error estimates that were somewhat erratic and generally more optimistic than those obtained by comparing different runs.

Consistency checks were made by repeating the entire calculation for a few values of T and N with different initial random numbers. These checks always agreed within the error estimates.

The common procedure of using different starting configurations, such as those generated at higher temperatures than one is interested in, was avoided in this calculation because of the possibility of freezing in metastable states with a double step in the surface.[18]

It is very difficult to be sure that a Monte Carlo simulation does not contain systematic errors. It is conceivable that an additional, very slow relaxation time (or even nonexponential decay) could cause such errors. We did look for a time dependence of the calculated quantities and made consistency checks on the time-dependent correlation functions. For the simulation times used, we did not find evidence of longer relaxation times or nonexponential decay. Tests with shorter runs ($\leq 10^3$ Monte Carlo steps per site) did contain systematic errors that led us to the longer simulations.

III. THERMODYNAMIC PROPERTIES

Throughout all simulations, the energy was monitored at time intervals of one Monte Carlo step per site. The averaged energy per site $\langle E\rangle$ (also denoted simply by E when no confusion can arise), was calculated, as well as the specific heat from the fluctuations

$$C=(\langle E^2\rangle-\langle E\rangle^2)(N^2/T^2). \tag{3}$$

Figure 1 shows the calculated energy as a function of temperature (in units of ϵ with $k_B=1$) for both SOS and DG models. The expected equivalence of the two models at low temperatures ($T\leq 0.8\epsilon$) is confirmed. Anticipating that we will find $T_R(\text{SOS})\approx 1.15\epsilon$ and $T_R(\text{DG})\approx 1.3\epsilon$, we see that the energies of the two models differ substantially in this temperature range. It is, however, interesting to note that the energy of each model at its roughening temperature is very nearly 0.5ϵ. The inflection points corresponding to the specific-heat maxima can be seen more clearly by viewing Fig. 1 at an angle. The statistical errors are somewhat smaller than the dots used for the SOS model.

Figure 2 plots the specific heat versus tempera-

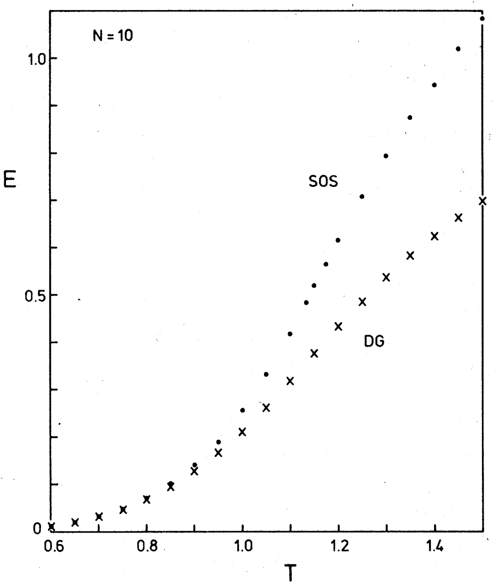

FIG. 1. Average energy per site E as a function of temperature T (in units of ϵ with $k_B=1$) for the SOS(•) and DG(✕) models with linear dimension $N=10$.

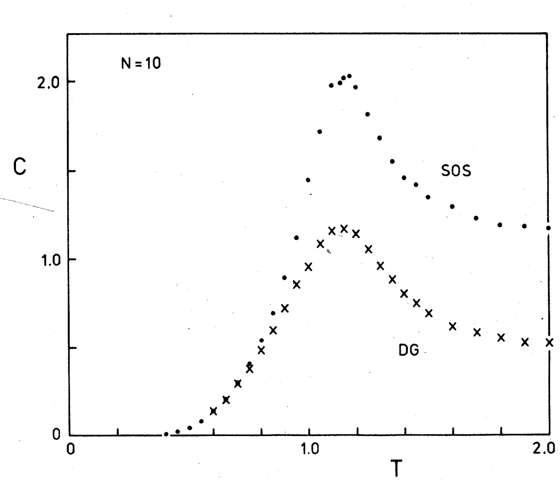

FIG. 2. Specific heat C vs T for the SOS(•) and DG(✕) models.

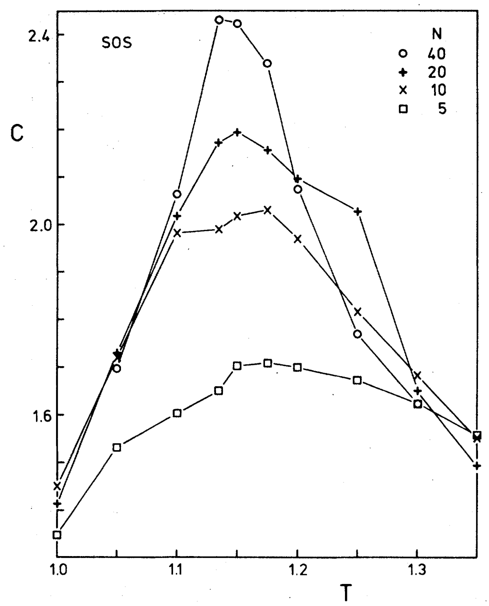

FIG. 3. C vs T for $N=5$, 10, 20, and 40 in the SOS model.

ture for both models. The errors are about twice the size of the crosses (~0.03) at and above the maximum and smaller at lower temperatures. The two models are again seen to be identical at low temperatures and qualitatively the same at higher temperatures, although the SOS specific heat is about a factor of two higher than that found for the DG model.

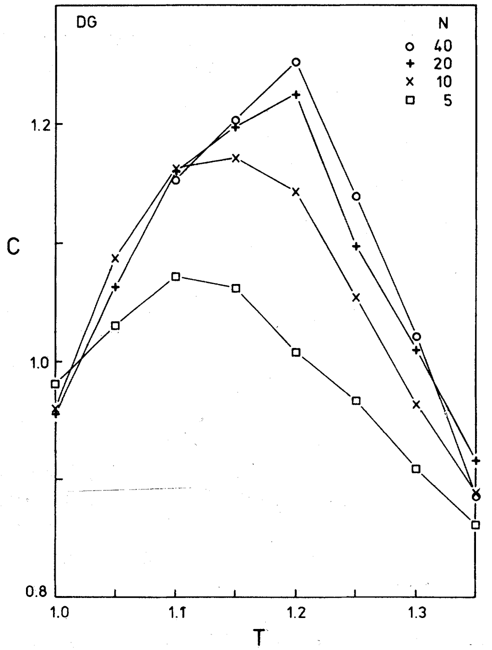

FIG. 4. C vs T for $N=5$, 10, 20, and 40 in the DG model.

A maximum in the specific heat does not, by itself, imply a phase transition and we must examine the size dependence to see if it turns into a singularity in the thermodynamic limit. This is done in Fig. 3 for the SOS model. For high and low temperatures, the specific heat is almost independent of N, but at intermediate temperatures, we find a significant N dependence. The peak shifts to lower temperatures and narrows as N increases, suggesting a singularity near $T=1.15\epsilon$ in the thermodynamic limit [recall that the rigorous lower bound for T_R is $T_c^{2D}(\text{Ising})=1.13459\epsilon$].[6]

The behavior of the peak in the specific heat for the DG model is rather different, as shown in Fig. 4. The size dependence is again only present at intermediate temperatures, but the peak does not show signs of narrowing and moves to higher temperatures as N increases. Since we do not have a rigorous upper bound for T_R, extrapolation is difficult. If T_R exists for the DG model, it is definitely higher than for the SOS model. However, it must be noted that the evidence for any singularity in the specific heat for the DG model is considerably weaker than for the SOS model.

IV. INTERFACE WIDTH

The width of the interface is not uniquely defined and many measures of it are conceivable.[7] One possibility is the maximum jump in layer concentration $(c_0 - c_1)$, which corresponds to the maximum density gradient in the continuum description. The reciprocal of this quantity gives a reasonable measure of the width, but it is unfortunately not an appropriate quantity to calculate in a simulation that does not conserve particle number.

The moments of the concentration profile are considerably easier to study and we have calculated both the second and fourth moments. The average value of the height was subtracted in each case, so that we computed

$$\begin{aligned}\langle n^2\rangle &= \sum_{n=-\infty}^{\infty} n^2(c_n - c_{n+1}) \\ &\quad - \left(\sum_{n=-\infty}^{\infty} n(c_n - c_{n+1})\right)^2 \\ &= \langle (h_{ij} - \langle h_{ij}\rangle)^2\rangle ,\end{aligned} \tag{4}$$

with a similar expression for $\langle n^4\rangle$.

Figure 5 shows $\langle n^2\rangle$ as a function of T for various values of N in the SOS model. The prediction of the Temkin approximation is shown for comparison. If the points for any finite value of N are examined, they are seen to lie on a smooth curve, which is qualitatively the same as that predicted by the Temkin approximation; no phase transition is evident. However, if the size dependence is

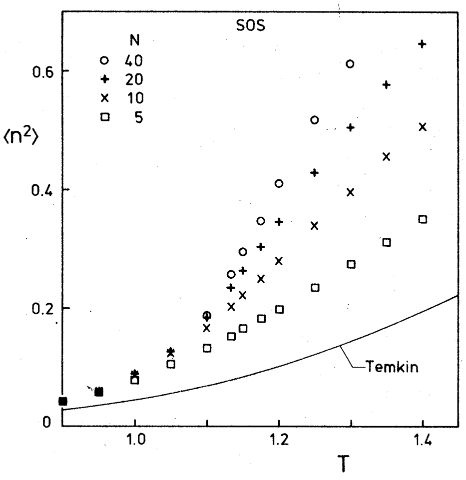

FIG. 5. Second moment of the concentration profile $\langle n^2\rangle$ [see Eq. (4)] vs T for several values of N in the SOS model. The solid line gives the prediction of the Temkin approximation.

taken into account, the width at higher temperatures does appear to be diverging as N increases.

The even spacing of the points and the analogy with the continuous Gaussian model[19] suggest plotting $\langle n^2\rangle$ vs $\ln(N)$ as shown in Fig. 6. For $T \leq 1.10\epsilon$, $\langle n^2\rangle$ reaches a limiting value and shows no sign of diverging. On the other hand, for $T \geq 1.20$, $\langle n^2\rangle$ is linear in $\ln(N)$ for $N \geq 10$ to within the accuracy of the calculation (about 1%), giving additional evidence that the singularity in the specific heat is indeed associated with roughening.

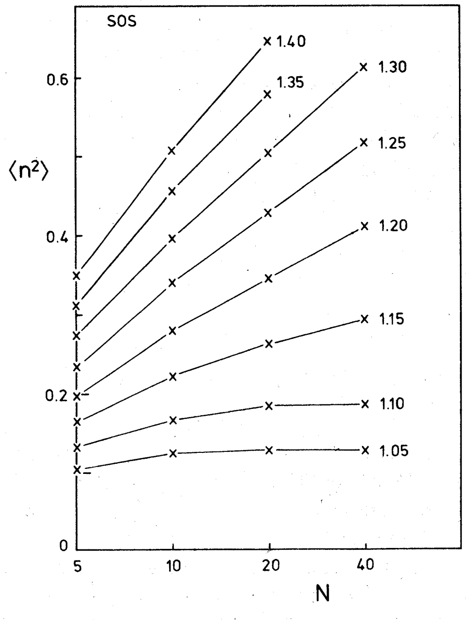

FIG. 6. $\langle n^2\rangle$ vs $\ln(N)$ for various temperatures in the SOS model.

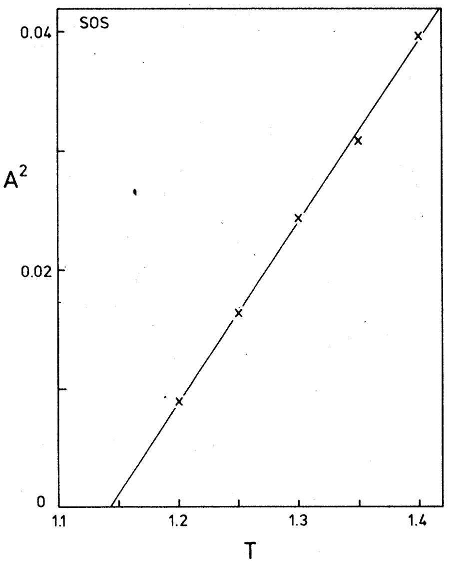

FIG. 7. A^2 as a function of temperature for the SOS model, where A is obtained by fitting Eq. (5) to the points in Fig. 6.

If we fit the linear regions to the form

$$\langle n^2\rangle = A\ln(N) + B\ , \tag{5}$$

and plot A^2 vs T, we find the straight line shown in Fig. 7. A least-squares fit of the points shown extrapolates to a roughening temperature of 1.14ϵ, which is consistent with the rest of the calculation and the rigorous lower bound.[6]

If we generalize Eq. (5) and assume that the various moments of the concentration profile take on the asymptotic forms

$$\langle |n|^k\rangle \sim (T-T_R)^{\zeta_k}\,[\ln(N)]^{\phi_k}\ , \tag{6}$$

then the Lapunov inequalities[9,10]

$$\langle |n|^k\rangle^{1/k} \leq \langle |n|^{k+1}\rangle^{1/k+1} \tag{7}$$

imply that

$$\zeta_k/k \geq \zeta_{k+1}/(k+1) \tag{8}$$

and

$$\phi_k/k \leq \phi_{k+1}/(k+1)\ . \tag{9}$$

This implies in turn that $\langle n^4\rangle$ should diverge at least as fast as $[\ln(N)]^2$. Unfortunately, the data do not support this prediction for the values of N used; $\langle n^4\rangle$ is better fit by $[\ln(N)]^{3/2}$. This means that either Eq. (6) is wrong or N is not large enough for $\langle n^4\rangle$ to show its true asymptotic behavior (or both). Actually, the ratio $\langle n^4\rangle/\langle n^2\rangle^2$ does satisfy inequality (7) and decreases monotonically with increasing N. Since unity is a lower bound for this ratio, $\langle n^4\rangle$ should be proportional to $\langle n^2\rangle^2$ for large

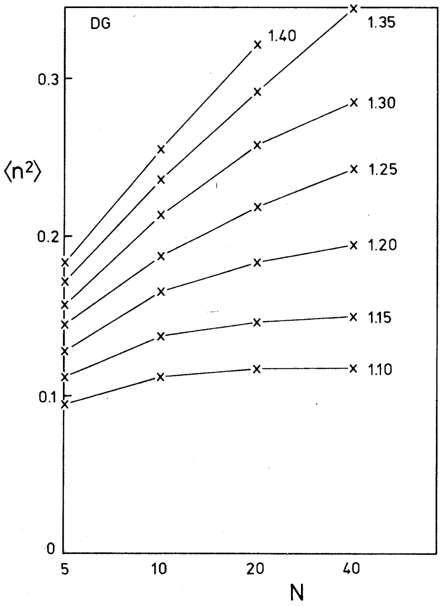

FIG. 8. $\langle n^2\rangle$ vs $\ln(N)$ for various temperatures in the DG model.

N. If Eq. (6) is correct, the exponent inequality (9) must then become an equality; $\phi_4=2\phi_2=2$.

Figure 8 shows a plot of $\langle n^2\rangle$ vs $\ln(N)$ for the DG model. Aside from the difference in scale with Fig. 6 (the DG values are smaller), no linear behavior is seen for $T\leq 1.30\epsilon$. The values for $T=1.35\epsilon$ and 1.40ϵ appear to be almost linear in $\ln(N)$, but more points are needed at higher temperatures to decide whether Eqs. (5) and (6) provide an appropriate description.

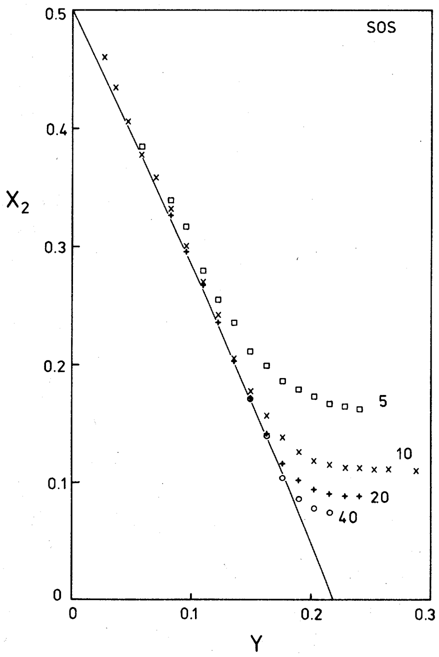

FIG. 9. $X_2=\exp(-4\beta\epsilon)/\langle n^2\rangle$ as a function of $Y=\exp(-2\beta\epsilon)$ for various values of N in the SOS model. The solid line represents the SOS prediction of the low-temperature expansion of Leamy *et al.* (Ref. 11).

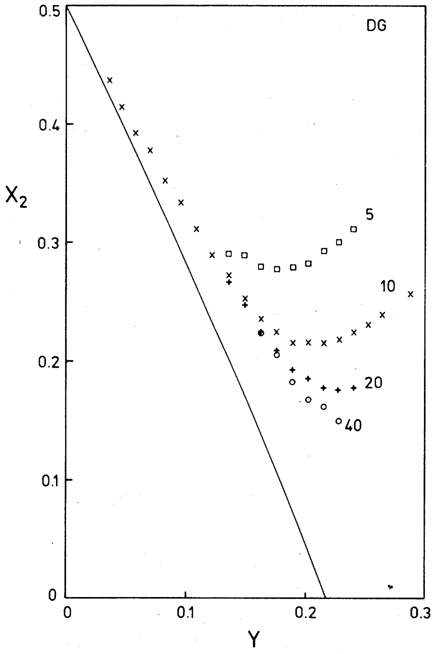

FIG. 10. Same as Fig. 9 for the DG model. The solid line is also the same as in Fig. 9 and represents the low-temperature expansion for the SOS model (Ref. 11).

Finally, it is interesting to compare our results directly with those obtained from low-temperature series expansions.[11] As mentioned in Sec. I, the roughening behavior predicted by these series shows certain inconsistencies,[9] indicating that they are not yet long enough to show their true asymptotic behavior. However, the series are still expected to give good predictions of the interface properties for temperatures sufficiently far below T_R.

Figure 9 shows a plot of $X_2=\exp(-4\beta\epsilon)/\langle n^2\rangle$ vs $Y=\exp(-2\beta\epsilon)$ for the SOS model with $N=5$, 10, 20, and 40. The solid line shows the predictions of the eight-term series.[11] At low temperatures, the size effect is magnified by this plot and shows the Monte Carlo points converging toward the series prediction as N increases. Thus, the Monte Carlo results confirm the series predictions at low temperatures. This is an important consistency check, since the Monte Carlo results do not agree with the roughening behavior extrapolated from low temperatures.[9,11] It should be noted that the Monte Carlo method involves only an extrapolation in system size and not in temperature.

Figure 10 shows the corresponding plot of X_2 vs Y for the DG model. The solid line is again the series prediction for the SOS model since DG series are not available. The plotted points lie considerably higher than those for the SOS model, corresponding to the smaller DG interface width. Figure 10 is also consistent with $T_R(\mathrm{DG}) > T_R(\mathrm{SOS})$, but the data are not sufficient for a direct extrapolation.

V. TIME-DEPENDENT CORRELATION FUNCTIONS

The dynamics of our interface models were studied through normalized, time-dependent correlation functions[17] of the form

$$f_A(t) = [\langle A(t)A(0)\rangle - \langle A\rangle^2]/(\langle A^2\rangle - \langle A\rangle^2)\ , \qquad (10)$$

where A was taken to be either the energy E or the second moment of the concentration profile $\langle n^2\rangle$. If $f_A(t)$ followed a simple exponential law, the relaxation time could be obtained from the inverse of the initial slope. Although $f_E(t)$ and $f_{n2}(t)$ are actually more complicated, we can still define an initial relaxation time characterizing the short-time decay of correlations. Since E and $\langle n^2\rangle$ were recorded at intervals of one Monte Carlo step per site, we used

$$\tau_A^I = -1/\ln[f_A(t=1)] \qquad (11)$$

for $A = E$ and $A = \langle n^2\rangle$.

Figure 11 shows τ_E^I vs T for various values of N in the SOS model.[20] For high and low temperatures, the size dependence is negligible. However, the maximum between $T = 1.1\epsilon$ and 1.2ϵ shows a definite size dependence, characteristic of critical slowing down. This behavior is quite similar to that seen in the 2D Ising model[21] and supports the link between the roughening transition and the usual second-order phase transitions.

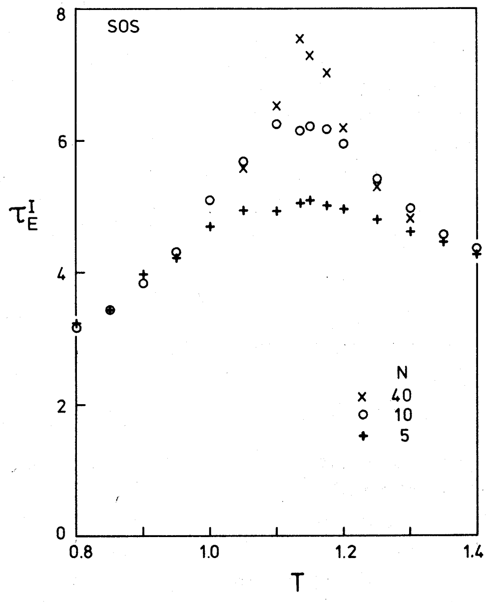

FIG. 11. Effective initial time constant, $\tau_E^I = -1/\ln[f_E(t=1)]$, as a function of temperature for the SOS model.

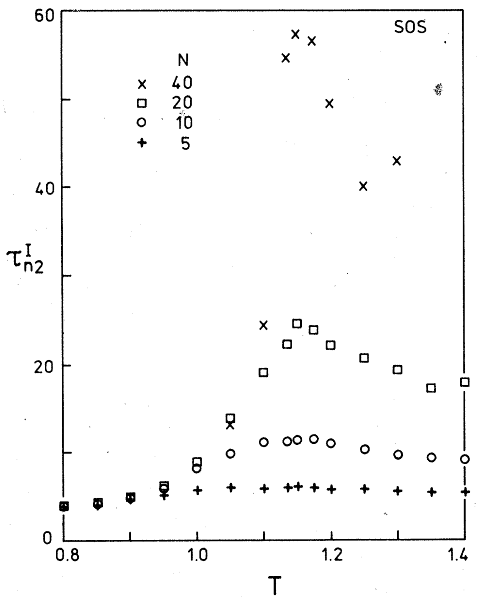

FIG. 12. Effective initial time constant τ_{n2}^I (from the second moment of the concentration profile), as a function of temperature for the SOS model.

The behavior of τ_{n2}^I, shown in Fig. 12, is considerably different. For low temperatures, τ_{n2}^I is essentially size independent and nearly equal to τ_E^I. However, it rises to a very high peak near $T = 1.15\epsilon$ (compare the scales in Figs. 11 and 12) and remains large for higher temperatures. This differs strongly from the usual critical slowing down, but it is consistent with the picture of an interface width dominated by large long-wavelength fluctuations.

Actually, both correlation functions show evidence of both long and short relaxation times, as shown in Fig. 13 for the SOS model, with $T = 1.15\epsilon$ and $N = 20$. Note that the long-time behavior of $f_{n2}(t)$ corresponds to a relaxation time of about 92, which is much longer than $\tau_{n2}^I \approx 24$ (both in units of one Monte Carlo step per site).

Critical slowing down is also seen in the DG model, as shown in Fig. 14, but τ_E^I is much farther from its asymptotic behavior than it is for the SOS model. τ_{n2}^I also exhibits critical slowing down for the DG model as seen in Fig. 15 and provides good evidence for the existence of roughening. However, it is not sufficient to locate the transition.

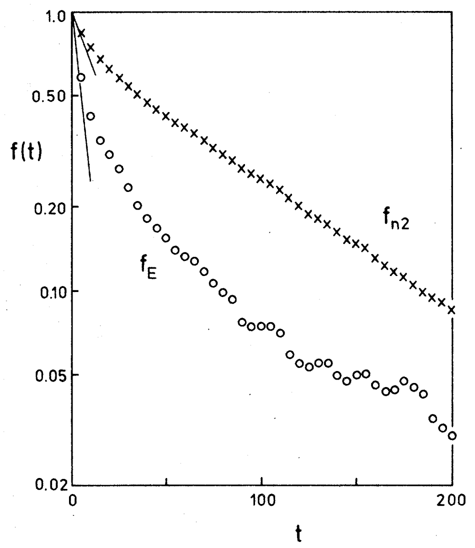

FIG. 13. Semilogarithmic plot of the normalized correlation functions $f_E(t)$ and $f_{n2}(t)$ as a function of time t (in units of one Monte Carlo step per site) for the SOS model ($T=1.15\epsilon$ and $N=20$).

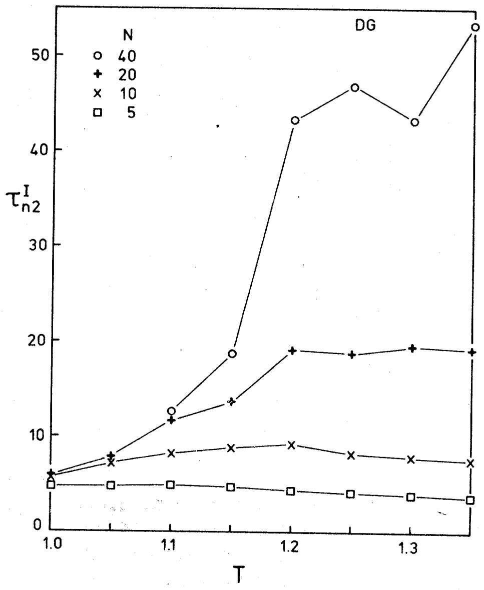

FIG. 15. Same as Fig. 12 for DG model.

VI. THERMODYNAMIC PROPERTIES OF STEPS

Recently, Leamy and Gilmer[14] made the interesting suggestion that the internal energy associated with a step should go exactly to zero at T_R. Unfortunately, confirmation of their suggestion turns out to be a difficult and somewhat subtle problem. First, it must be noted that very high accuracy is necessary for this calculation, since the Temkin approximation,[4,22] which does not predict roughening, does predict a rapid drop in the step energy. Leamy and Gilmer's Monte Carlo simulation times of 250 steps per site[14] were not sufficiently long to provide the required statistics. In addition, they only considered a 20×40 lattice with zero, two, four, and eight steps and defined their step energy as the linear term in a polynomial fit of the surface energy as a function of the number of steps for this particular lattice size. This is not equivalent to the asymptotic energy of a single step in the limit of infinite lattice size. The nonanalyticity they found seems to have been due to the use of different methods of fitting their data above and below what they believed to be the roughening temperature. The value for T_R they reported is about 10% too high.

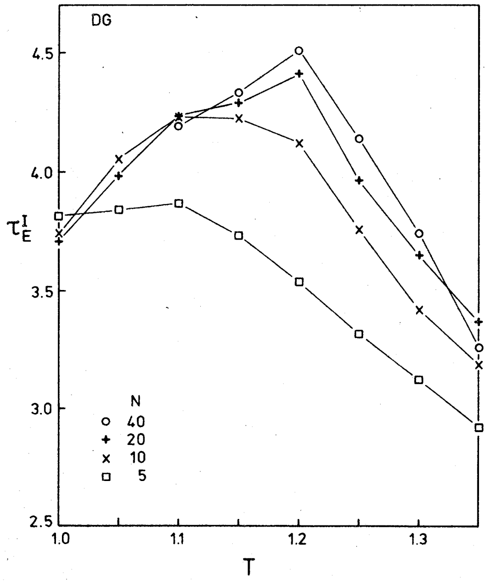

FIG. 14. Same as Fig. 11 for the DG model.

The method we used involved simulations for a series of $N\times N$ lattices with and without a single step as described in Sec. II. The step energy per unit length

$$E_{st}=N[E(1\text{ step})-E(\text{no steps})]\,, \qquad (12)$$

and the step specific heat from the energy fluctuations

$$C_{st}=N[C(1\text{ step})-C(\text{no steps})]\,, \qquad (13)$$

were thus obtained as functions of both T and N.

The basic behavior of E_{st} as a function of T is shown in Fig. 16 for both the SOS and DG models with $N=10$. The two models show similar behavior (identical at low temperatures), which is qualitatively the same as that predicted by the Temkin approximation.[22]

The exact result for a one-dimensional interface

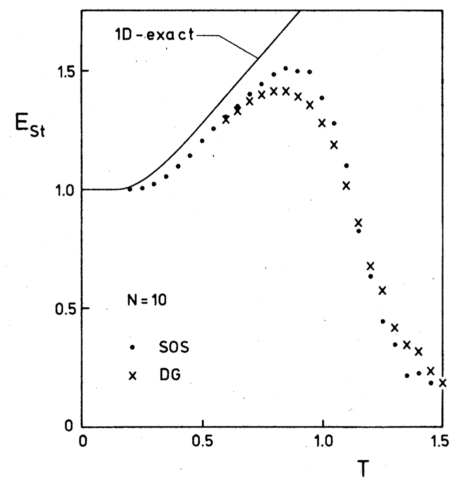

FIG. 16. Step energy per unit length E_{st} as a function of temperature for the SOS(•) and DG (**X**) models. The solid line represents the exact solution of the corresponding one-dimensional problem.

in a two-dimensional Ising model is shown for comparison. The Monte Carlo points lie well below this curve, even at fairly low temperatures. This is a well-known size effect[3] and as N is increased, E_{st} will also increase (for low temperatures) until it agrees with the curve. This size effect is clearly seen in Fig. 17, where E_{st} is plotted against $1/N$ for the SOS model. The plot also shows that E_{st} decreases for larger systems at higher temperatures, giving support to Leamy and Gilmer's suggestion. However, E_{st} probably goes to zero much more slowly than $1/N$ near T_R (if it does go to zero) and Fig. 17 does not provide conclusive evidence that it vanishes.

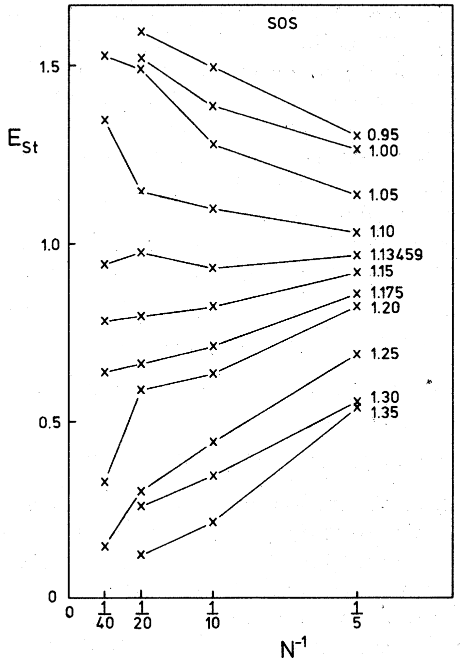

FIG. 17. E_{st} as a function of $1/N$ for various temperatures in the SOS model.

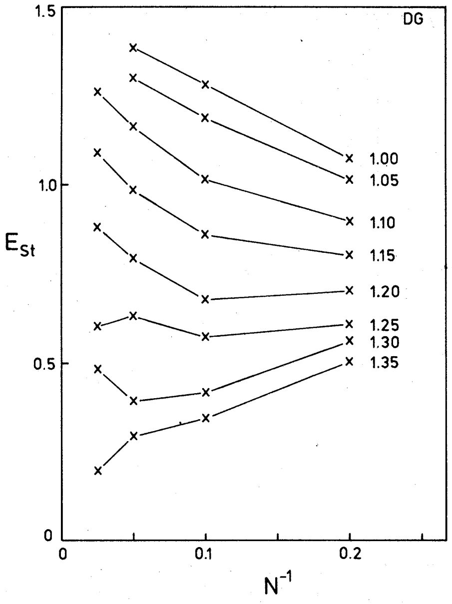

FIG. 18. Same as Fig. 17 for the DG model.

The situation is similar for the DG model, as shown in Fig. 18. Here, the plot of E_{st} vs $1/N$ suggests that the singularity, if present, lies near $T = 1.25\epsilon$ or 1.30ϵ.

More progress can be made by looking at the step specific heat. The basic temperature dependence is shown in Fig. 19 as a plot of C_{st} vs T for both SOS and DG models with $N = 10$. Again, the shape of both curves is qualitatively the same as that found in the Temkin approximation[22] and the size effect is again prominent at low temperatures.

Figure 20 shows the behavior of the negative peak in a plot of $(-C_{st})$ vs T for various values of N in the SOS model. The size dependence is very strong (note the change in scale from Fig. 19) and provides our best single piece of evidence for the value of T_R being $(1.15 \pm 0.05)\epsilon$, as opposed to the older predictions[7,8,11-14] centered about 1.28ϵ.

Figure 21 shows $(-C_{st})$ vs T for various lattice sizes in the DG model. The size dependence is also more pronounced than it was for the interface specific heat C (see Fig. 4), but it is still far from its asymptotic behavior. From this plot, the singularity appears to be developing about $T = 1.20\epsilon$ or 1.25ϵ, but since the peak is moving to higher temperatures with increasing lattice size, these values may be too low.

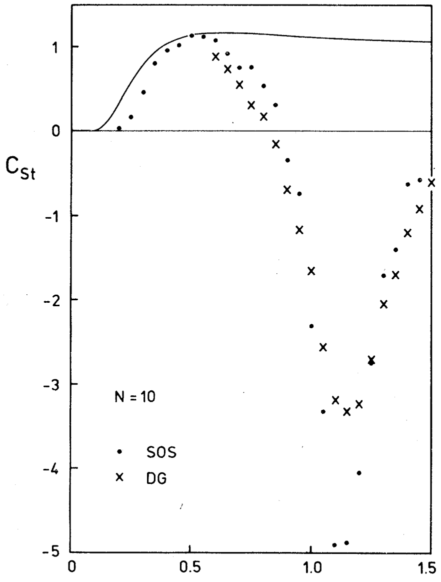

FIG. 19. Step specific heat C_{st} as a function of temperature for the SOS (•) and DG (×) models. The solid line represents the exact solution of the corresponding one-dimensional problem.

VII. CONCLUSION

One of the main purposes of this work was to determine whether the roughening transition does indeed exist. We believe that our Monte Carlo simulations have provided very strong evidence for its existence in the SOS model and good, although weaker evidence in the DG model.

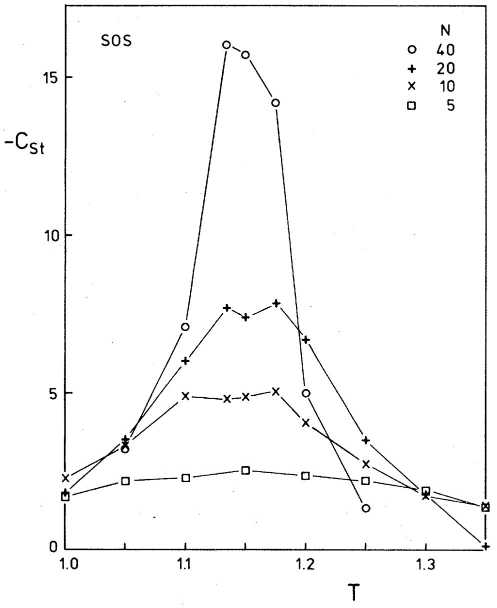

FIG. 20. Plot of the negative peak in the step specific heat ($-C_{st}$) as a function of temperature for various values of N in the SOS model.

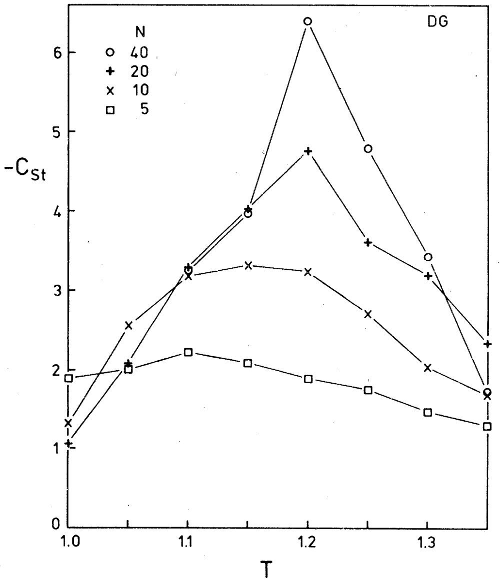

FIG. 21. Same as Fig. 20 for the DG model.

The singularity in the specific heat and the phenomenon of critical slowing down showed the relationship between the SOS model and the 2D Ising model to be closer than previous work on this problem had indicated. The value of the roughening temperature $T_R(\mathrm{SOS}) = (1.15 \pm 0.05)\epsilon$ found from these simulations is significantly lower than previously believed and is indistinguishable from the critical temperature of the 2D Ising model T_c^{2D} (Ising) $= 1.13459\epsilon$, which is known to be a rigorous lower bound [$T_R \geq T_c^{2D}$ (Ising)].

The DG model appears to have a roughening transition at a higher temperature than the SOS model. Because the peaks in the various quantities measured generally move to higher temperatures as N increases in the DG model, it is more difficult to locate the transition exactly. Our best estimate is $T_R(\mathrm{DG}) = (1.3 \pm 0.1)\epsilon$, which is consistent with the value of $(4/\pi)\epsilon = 1.273\,24\epsilon$ suggested by Kroll, Müller-Krumbhaar, and Wagner.[16]

It is hoped that the study of these two simple systems will serve as a guide to the expected phenomena and possible pitfalls to be encountered in future experimental and theoretical work on the properties of interfaces.

ACKNOWLEDGMENTS

I would like to thank Professor D. P. Landau and Dr. H. Müller-Krumbhaar for many interesting discussions and helpful suggestions.

*A preliminary report of some of the results contained in this paper was presented at the First European Conference on Crystal Growth, Sept. 12-17, 1976 (unpublished).

†Present address: Brookhaven National Laboratory, Upton, N. Y. 11973.

[1] W. K. Burton and N. Cabrera, Discuss. Faraday Soc. 5, 33 (1949).

[2] W. K. Burton, N. Cabrera, and F. C. Frank, Philos. Trans. R. Soc. Lond. 243, 299 (1951).

[3] L. Onsager, Phys. Rev. 65, 117 (1944).

[4] D. E. Temkin, in *Crystallization Processes*, edited by N. N. Sirota *et al.* (Consultants Bureau, New York, 1966).

[5] R. H. Swendsen, Phys. Rev. B 15, 689 (1977).

[6] H. van Beijeren, Commun. Math. Phys. 40, 1 (1975).

[7] J. D. Weeks, G. H. Gilmer, and H. J. Leamy, Phys. Rev. Lett. 31, 549 (1973).

[8] G. H. Gilmer, K. A. Jackson, H. J. Leamy, and J. D. Weeks, J. Phys. C 7, L123 (1974).

[9] R. H. Swendsen, Phys. Rev. Lett. 38, 615 (1977).

[10] A. M. Lapunov, Bull. Acad. Sci. St. Petersburg 13, 359 (1900).

[11] H. J. Leamy, G. H. Gilmer, and K. A. Jackson, in *Surface Physics of Crystalline Materials*, edited by J. M. Blakeley (Academic, New York, 1976).

[12] H. J. Leamy and K. A. Jackson, J. Appl. Phys. 42, 2121 (1971).

[13] G. H. Gilmer and P. Bennema, J. Appl. Phys. 43, 1347 (1972).

[14] H. J. Leamy and G. H. Gilmer, J. Cryst. Growth 24/25, 499 (1974).

[15] S. T. Chui and J. D. Weeks, Phys. Rev. B 14, 4978 (1976).

[16] D. Kroll, H. Müller-Krumbhaar, and H. Wagner (unpublished).

[17] H. Müller-Krumbhaar and K. Binder, J. Stat. Phys. 8, 1 (1973).

[18] P. Bennema and C. van Leeuwan (private communication).

[19] F. P. Buff, R. A. Lovett, and F. H. Stillinger, Phys. Rev. Lett. 15, 621 (1965).

[20] R.H. Swendsen, Phys. Rev. Lett. 37, 1478 (1976).

[21] E. Stoll, K. Binder, and T. Schneider, Phys. Rev. B 8, 3266 (1973).

[22] R. H. Swendsen, J. Cryst. Growth 36, 11 (1976).