Simulated healing of crystal surfaces

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We have studied the decay of one- and two-dimensional sinusoidal grooves on rough and smooth solid surfaces using Monte Carlo simulations of two-dimensional solid-on-solid models, employing both Glauber and Kawasaki dynamics. The dependence of the lifetime of the grooves on their wavelength and the time dependence of the average height (or amplitude) of the grooves are investigated. Where possible, the results are compared with theory and/or experiment.

I. INTRODUCTION

The roughening transition on crystal surfaces has been recognized and studied intensively in recent years.[1–3] It is understood that below the roughening temperature T_R the surface is smooth and facets can form,[2] while above T_R the surface becomes rough and is not faceted.

More recently, the effects of roughening on growth kinetics have also been studied experimentally,[4] theoretically,[5–7] the via computer simulations.[8] For example, the decay of sinusoidal-shaped grooves scored on a solid surface has been studied by Yamashita *et al.*[4] It is found that the grooves keep their sinusoidal shape when decaying at temperatures above T_R; below T_R, cusps develop in the profile. Phenomenological theories have been devised by several authors[5–7] in attempts to understand this behavior. The emphasis in the theoretical work is on how the lifetime of the grooves depends on their wavelength and, below the roughening transition, how the area of the developing flat (faceted) part of the surface grows with time. The same phenomenon has been examined by Selke and Oitmaa[8] in simulations on the discrete Gaussian model starting from an initial sinusoidally grooved (in one dimension) surface. These authors also study the dependence of the relaxation time on the temperature and on the wavelength of the grooves.

In this paper, we report results of Monte Carlo (MC) simulations using solid-on-solid (SOS) models with either Kawasaki or Glauber dynamics. The simulations are designed to study the decay of one- and two-dimensional sinusoidal-shaped grooves on both smooth and rough surfaces emphasizing (1) the dependence of the decay rate on the wavelength of the initial deformation and (2) the time dependence of the decay. The results are compared, where possible, to existing theoretical predictions and to experimental results.

The remainder of this paper consists of Sec. II, which contains a description of the model and Monte Carlo procedures along with a summary of related existing theoretical predictions; Sec. III, presenting the results and discussion; and Sec. IV, which is a summary.

II. MODEL AND THEORETICAL PREDICTIONS

We employ a SOS model with nearest-neighbor coupling J on a two-dimensional square lattice. Thus we are treating the surface of a three-dimensional solid. At each lattice site i there is a variable h_i which is the position or height of the interface at that site. Both the case of continuous h_i and that in which the h_i can be integers only have been simulated. The Hamiltonian is

$$H = J \sum_{\langle i,j \rangle} |h_i - h_j| + \sum_i \tfrac{1}{2} g h_i^2 , \tag{1}$$

where $\langle i,j \rangle$ denotes that the sum is over nearest-neighbor pairs of sites, and g represents the effect of a gravitational field. In this paper we report principally results using $g=0$; the case of $g \neq 0$ was investigated to a lesser extent. We anticipate reporting more fully on the latter in a future publication.

Simulations were done using two different orientations of the initial configuration of h_i's relative to the lattice. One orientation is such that, for one-dimensional (1D) grooves, lines of constant height are parallel to a $\{10\}$ direction. In this case the height at site (m,n) of the simple square lattice is given initially by

$$h(m,n) = h_0 \sin(2\pi m a/\lambda) ; \tag{2}$$

for 2D grooves it is given by

$$h(m,n) = h_0 \sin(2\pi m a/\lambda)\sin(2\pi n a/\lambda) ; \tag{3}$$

λ is the wavelength and a is the nearest-neighbor distance in the lattice. For the case of discrete heights, the values of $h(m,n)$ are rounded to the next lower (in magnitude) integer.

The second orientation is such that lines of constant height (for a 1D deformation) are parallel to a $\{11\}$ direction of the simple square lattice; the initial configuration of heights is

$$h(m,n) = h_0 \sin[2\pi(m+n)a/\sqrt{2}\lambda] ; \tag{4}$$

for 2D grooves it is

$$h(m,n)=h_0\sin[2\pi(m+n)a/\sqrt{2}\lambda]\times\sin[2\pi(m-n)a/\sqrt{2}\lambda]\ . \quad (5)$$

In the former case we use periodic boundary conditions on a simple square lattice measuring $L\times L$; in the latter case, we use periodic boundary conditions along $\{11\}$ directions; in order to do so conveniently we redefine the lattice as a centered square lattice measuring $L'\times L'$ having a square unit cell with a site at its center so that the total number of sites is $2L'^2$. Relative to the centered square lattice we employ periodic boundary conditions in the usual way, i.e., along $\{10\}$ directions. All of the results given in Sec. III were found using this second orientation of the grooves; the first one was employed in certain instances to check that the results do not depend qualitatively on orientation.

The time evolution of the system is simulated by standard MC methods with Glauber or Kawasaki dynamics corresponding to nonconserved and conserved material, respectively. We monitored the relaxation of the initial configuration by using both the average height of the nonuniformities, $\bar{h}(t)$, and the interface width, $w(t)$. These are defined as

$$\bar{h}(t)=\frac{1}{N}\sum_i |h_i(t)-z(t)| \quad (6)$$

and

$$w(t)=\left[\frac{1}{N}\sum_i [h_i^2(t)-z^2(t)]\right]^{1/2}, \quad (7)$$

where N is the total number of lattice sites, the sum is over all sites i of the lattice, and $z(t)$ is the instantaneous average position of the interface,

$$z(t)=\frac{1}{N}\sum_i h_i(t)\ . \quad (8)$$

For Glauber dynamics, $z(t)$ may deviate from zero because of fluctuations in the sum of the h_i's and so must be included in Eqs. (6) and (7). For Kawasaki dynamics it is always zero and therefore superfluous in these equations. A simple measure of the rate of relaxation, which we shall call the lifetime, may be obtained from either $\bar{h}(t)$ or $w(t)$ by defining

$$\bar{h}(\tau)-\bar{h}(\infty)\equiv f[\bar{h}(0)-\bar{h}(\infty)] \quad (9)$$

or

$$w(\tau)-w(\infty)\equiv f|[w(0)-w(\infty)]\ , \quad (10)$$

where f is some fraction such as $1/e$ ($e=2.7183\ldots$) and τ depends on f; $\bar{h}(\infty)$ and $w(\infty)$ are the equilibrium values of $\bar{h}$ and w, attained as $t\to\infty$. Our simulations show that the behaviors of $\bar{h}(t)$ and $w(t)$ are qualitatively the same, and therefore we have reported only results found from $w(t)$ in Sec. III.

In the simulations we use lattices ranging in size L' from 20×20 to 200×200. The system size is chosen so as to be commensurate with the initial value of λ. We ran numerous tests to determine the dependence of the results on system size. It was always possible to use sufficienty large lattices that the size dependence is so small as to be of no consequence for any quantity of interest with the exception of the equilibrium width of the interface at $T>T_R$. For $g=0$, this width is limited solely by the lattice size, being proportional to $\sqrt{\ln L'}$. Consequently, when determining τ from Eq. (10), one must use the value of $w(\infty)$ appropriate for the particular value of L' at which the simulation was done.

For Glauber dynamics, a Monte Carlo "move" consisted of an attempted change of the height at a site i by an amount δh_i chosen randomly on the interval $|\delta h_i|<0.5$ for continuously varying h_i and chosen as $\delta h_i=\pm1$ for discrete h_i. With Kawasaki dynamics, the attempted changes in h_i were accompanied by an equal and opposite change in the height at some neighboring site j. Relaxation is very slow in this case; therefore, to reduce the relaxation times, j was allowed to be as much as a third-neighbor site of i, necessitating the use of 18 sublattices in order to produce fully vectorizable code for running on the Ohio Supercomputer Center Cray.

In order to obtain reasonably smooth curves of $w(t)$ and $\bar{h}(t)$, as well as reliable values of τ, several MC runs, typically five to 20, were done for a given set of parameters. For $T>T_R$, separate runs were done to determine the equilibrium width $w(\infty)$ as a function of L'.

The kinetics of rough surfaces, i.e., $T>T_R$ have been studied in detail by Mullins.[9] He finds that, for $h_0\ll\lambda$, the lifetime of sinusoidal grooves will be proportional to λ^α, where $\alpha=2$ if the decay is dominated by the evaporation-condensation mechanism, and $\alpha=4$ if it is dominated by the surface diffusion mechanism. In our simulations these mechanisms correspond, respectively, to Glauber dynamics and to Kawasaki dynamics.

Mullins' predictions are in agreement with those from a critical dynamics study of the discrete Gaussian model[9–11] if there is a single mode dominating the relaxation process and if noise is not included. The condition of a single mode is the same as requiring that the groove keep the sinusoidal shape and a fixed wavelength throughout the relaxation process. Moreover, the height or width of the groove is predicted to decrease as an exponential function of the time in this case.

Simple arguments from critical dynamics theory[10] also allow the determination of gravitational effects on the lifetime of the grooves in the case of $T>T_R$. For the specific case of the discrete Gaussian model with nearest-neighbor interactions, it is predicted[10] that

$$\tau\sim\frac{1}{J'q^2+g} \quad (11)$$

for Glauber dynamics, and

$$\tau\sim\frac{1}{q^2(J'q^2+g)} \quad (12)$$

for Kawasaki dynamics; $q=2\pi/\lambda$; J' is the intercolumn interaction (in the discrete Gaussian model), and g is as in Eq. (1).

If $T<T_R$, the sinusoidal shape of the groove is no

longer stable. An increasing number of modes play a role during the dynamical evolution of the system toward equilibrium, leading to the development of cusps in the profile. Consequently, the theories mentioned above are invalid. Phenomenological theories considering the interaction and diffusion of steps and kinks have been developed for this relaxation in the case of conserved surface material.[5,6] There is a prediction that, for the particular case of $g \neq 0$, the relaxation time is proportional to λ^3/g for 2D grooves; for 1D grooves there are no predictions, to the best of our knowledge.

Also for $T < T_R$, in the late stages of the relaxation process, many modes are playing a role. The process is characterized by a broad distribution of relaxation times, and, as a consequence, the time dependence of $w(t)$ is expected to have the stretched-exponential form[12]

$$w(t)-w(\infty)\sim\exp[-(t/\tau)^x] \tag{13}$$

with exponent $x<1$. If τ is extracted from the behavior at sufficiently long times, it is expected to have a simple power-law dependence on the initial wavelength λ, $\tau\sim\lambda^\gamma$, in the limit $\lambda\rightarrow\infty$.

III. RESULTS AND DISCUSSION

We present first our results for $T > T_R$. We have done simulations using continuous h_i so that the surface is rough[10] at any $T>0$. In Fig. 1, we show in a log-log plot the wavelength dependence of the lifetime for both 1D and 2D grooves with Glauber dynamics at $T=0.4J/k$, and $h_0=4$. Times are measured in Monte Carlo steps per site (mcs). The lifetimes shown in the figure are extracted from $w(t)$ by Eq. (10) with $f=0.67$ and 0.47 for 1D and 2D grooves, respectively. It is clear that τ scales very nearly as λ^2 in agreement with theoretical predictions. We also extracted τ from other values of f; all choices lead to the same result, i.e., $\alpha=2$. More generally, for λ large enough in comparison with the initial amplitude of the grooves, $w(t)$ obeys a scaling relation of the form

$$w_{\rm red}(t)=F(t/\lambda^2)\ , \tag{14}$$

where $w_{\rm red}(t)\equiv[w(t)-w(\infty)]/[w(0)-w(\infty)]$. In Fig. 2, $\ln(w_{\rm red})$ is plotted against $2ta^2/\lambda^2$ with $\lambda/\sqrt{2}a=75$ and 100 for 1D grooves and with $\lambda/\sqrt{2}a=60$ and 100 for 2D grooves; h_0 and T are as in Fig. 1. The curves are roughly linear over a considerable range of time, displaying the essentially exponential character of the decay. We had expected *a priori*, on the basis of the theoretical predictions described in the previous section, that $w_{\rm red}(t)$ would be more nearly an exponential, i.e., that the curves in Fig. 1 would be closer to straight lines. We did additional simulations (results not shown) to test whether the deviation could be a size effect, a consequence of not being sufficiently in the limit $\lambda \gg h_0$, or the result of having allowed a maximum $|\delta h_i|=0.5$ which is too large in comparison with h_0 itself. None of these appears to be the explanation; we are unsure what is the reason for the deviation from simple exponential behavior, although it could simply be that the underlying theories are mean-field approximations (when noise is neglected in the critical dynamics calculation) and that fluctuations are re-

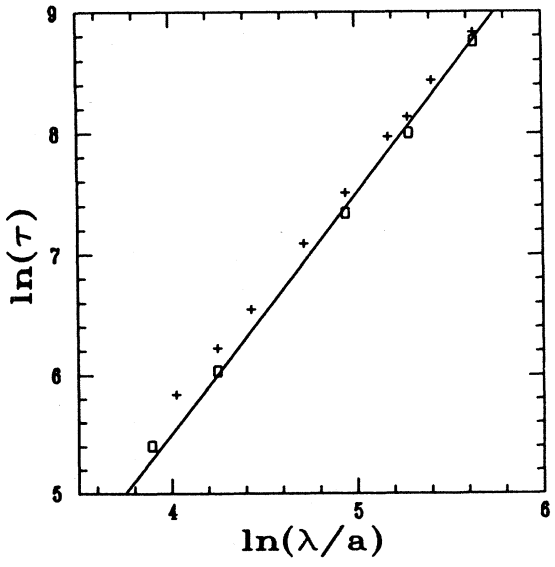

FIG. 1. The logarithm of τ (mcs) is plotted against that of λ/a for the case of Glauber dynamics, continuous height variables, and $T=0.4J/k$ ($T>T_R$), and both one-dimensional (+) and two-dimensional (□) grooves with $h_0=4.0$. The lifetime is determined using $f=0.67$ for $d=1$ and $f=0.47$ for $d=2$. The straight line has a slope of 2.

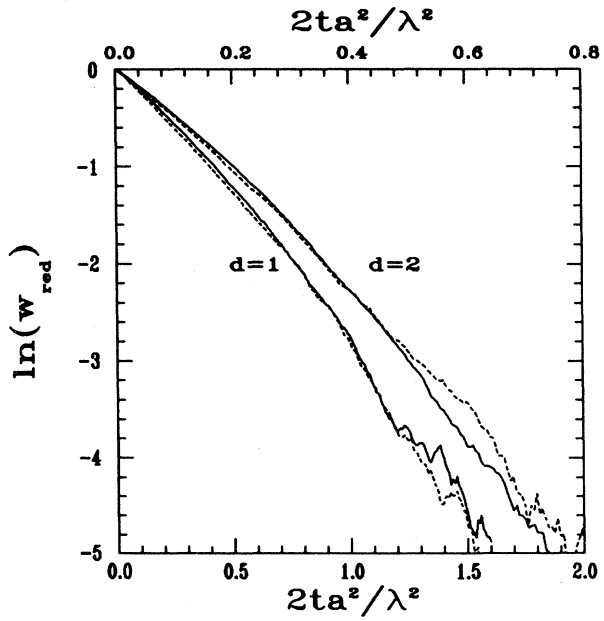

FIG. 2. For Glauber dynamics, continuous height variables, and $T=0.4J/k$ ($T>T_R$), the logarithm of $w_{\rm red}$ is plotted against $2ta^2/\lambda^2$ using 1D and 2D grooves with $h_0=4.0$. For one-dimensional Grooves, $\lambda/\sqrt{2}a=75$ (solid line) and 100 (dotted line); for two-dimensional grooves, $\lambda/\sqrt{2}a=60$ (solid line) and 100 (dotted line).

sponsible for the deviation from simple exponential behavior in our results. As for the scaling law expressed by Eq. (14), it is supported by the fact that in Fig. 2, the curves for different wavelengths but the same groove dimension are very nearly superposed except where $w(t)$ is close to $w(\infty)$; here the effect of small fluctuations in $w(t)$ is considerable; also $w(\infty)$ is known only approximately from our simulations.

For Kawasaki dynamics and continuous heights, we find again that $\tau \sim \lambda^{\alpha}$, this time with α quite accurately equal to 4 for both 1D and 2D grooves. Figure 3 is a log-log plot of τ versus λ/a for one- and two-dimensional grooves using $f=0.67$ and 0.70, respectively; $T=0.4J/k$ and $h_0=4.0$. Figure 4 shows $\ln(w_{\rm red})$ versus $4ta^4/\lambda^4$ for both one- and two-dimensional grooves with $\lambda/\sqrt{2}a=24$ and 30. Also, T and h_0 are as in Fig. 3; from this plot the scaling is clear (except again at long times where fluctuations make accurate comparison difficult); also, one sees that, as we found for Glauber dynamics, the relaxation is more or less, but certainly not precisely, exponential.

We turn next to presentation of our results at temperatures $T < T_R$ for which the height variables h_i are necessarily discrete. For our system, $T_R \approx 1.24J/k$ and for all practical purposes, relative to the results of interest, the equilibrium surface is flat, i.e., $w(\infty) \approx 0$; for example, at $T=0.4J/k$ where most of the simulations have been done, the equilibrium value of w is about 0.009 layers. Both Glauber and Kawasaki dynamics have been employed, and in both cases, $w(t)$ is far from a simple exponential function. In particular, in the case of conserved material (Kawasaki dynamics), $w(t)$ falls off very slowly at long times for both one- and two-dimensional grooves. One way to think of the reason for this behavior is that, in order for the surface to become flat on the atomic scale, every "particle" above the surface has to find a "hole" into which it can go. At long times, there are still some leftover particles and holes at different locations on the surface, and they must diffuse and find each

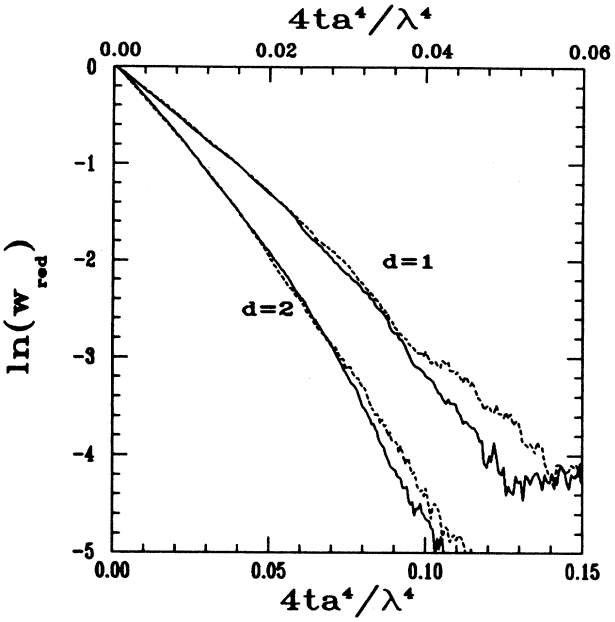

FIG. 4. For Kawasaki dynamics, continuous height variables, and $T=0.4J/k$ ($T > T_R$), the logarithm of $w_{\rm red}$ is plotted against $4ta^4/\lambda^4$ using 1D and 2D grooves with $h_0=4.0$; $\lambda/\sqrt{2}a=24$ (dotted line) and 30 (solid line) in both cases.

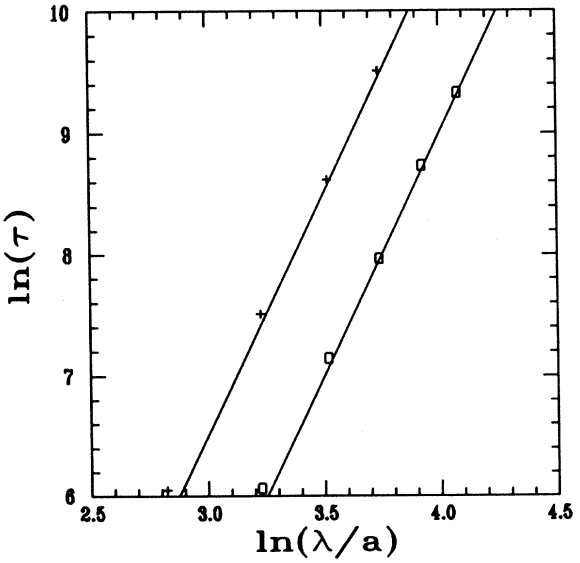

FIG. 3. The same as Fig. 1 except using Kawasaki dynamics and $f=0.67$ for 1D (+) and 0.70 for 2D (□) grooves. The straight lines have slopes of 4.

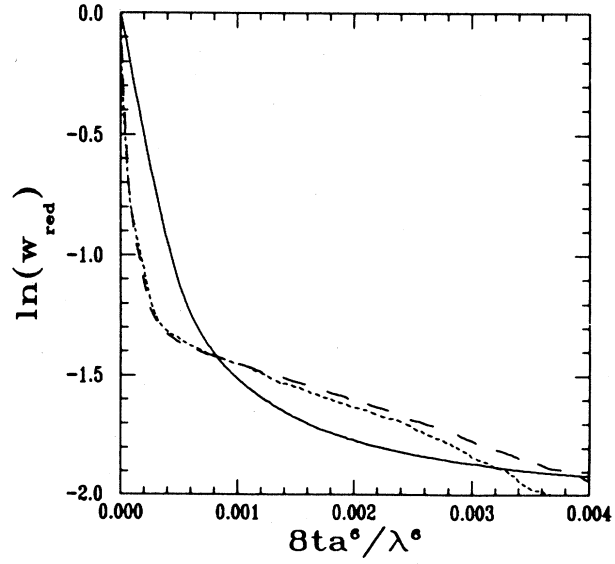

FIG. 5. For Kawasaki dynamics, discrete height variables, and $T=0.4J/k$ ($T < T_R$), the logarithm of $w_{\rm red}$ is plotted against $8ta^6/\lambda^6$ using 2D grooves and $h_0=5.5$; $\lambda/\sqrt{2}a=6$ (solid line), 12 (dashed line), and 15 (dotted line).

other in order to "annihilate." The situation in this limit is not unlike that of having two species of particles, A and B, which can diffuse and which react to give an inert object when they come into contact with each other.[13] We are currently involved in simulations of this phenomenon in a somewhat different context; details will be published elsewhere.[14] In the case of nonconserved materials, the situation is different and is equivalent to having particles A and B which can be both created and annihilated individually. As far as we know, there are no predictions of the time dependence of the densities of A and B in this case.

Figure 5 presents $\ln[w_{\rm red}(t)]$ versus $8ta^6/\lambda^6$ for conserved order-parameter dynamics, 2D grooves, $T=0.4J/k$, $h_0=5.5$, and $\lambda/\sqrt{2}a$ equal to 6, 12, and 15. For the two larger wavelengths in particular, the curves are roughly superposed, suggesting that the relaxation times scale approximately as λ^6 for large enough wavelength. The shape of the curves in these two cases indicates a crossover from an initial exponential regime to a long-time stretched-exponential behavior as more modes enter into the relaxation. Constraints on computer resources preclude our making any very quantitative statements and, in particular, from extensive study of the behavior at much longer times and/or larger wavelengths. We did look at one particular wavelength, $\lambda=12\sqrt{2}a$, at considerably longer times than what is shown in Fig. 5. Figure 6 shows $\ln[-\ln(w_{\rm red})]$ versus $ln\,(8ta^6/\lambda^6)$; at the longest times the curve approximates a straight line with a slope x between $\frac{1}{4}$ and $\frac{1}{3}$, consistent with stretched-exponential behavior, $w\sim\exp(-at^x)$. The deviation from straight-line behavior in the long-time regime is most likely a size effect; the simulations were done on a system with $L'=48$.

Figure 7 shows the same as Fig. 5 but for 1D grooves and $\lambda/\sqrt{2}a=6$, 12, and 18. There appears to be quite a bit of structure in the decay for the larger wavelengths; perhaps this is evidence for the introduction of more and more contributing modes. For long times, we see again behavior consistent with stretched-exponential decay with τ scaling approximately as λ^6.

Using nonconserved order parameter, discrete h_i, and $T<T_R$, we find that for two-dimensional grooves the decay appears to be a function of t/λ^2, but only at relatively short times. In Fig. 8 we show the logarithm of $w_{\rm red}$ as a function of $2ta^2/\lambda^2$ at $T=0.4J/k$, $h_0=5.5$, and $\lambda/\sqrt{2}a=60$, 90, and 120. The decay is clearly not a simple exponential and the curves superpose well only at short times. Additional short-time simulations were done using $T=0.4J/k$, $h_0=5.0$, and wavelengths between $20\sqrt{2}a$ and $200\sqrt{2}a$. Figure 9 is a log-log plot of τ, with $w_{\rm red}(\tau)=0.3$, versus λ/a; the data tend to fall on a line of slope 2 which is also shown. Hence we may infer that the relaxation time scales as λ^2 in the relatively short-time regime.

Quite different behavior arises at long times in particular for 1D grooves, nonconserved order parameter, and $T<T_R$. Whereas the relaxation of w in the $d=2$ case "speeds up" at longer times in some sense as shown by Fig. 8, we find that for $d=1$, it slows down, producing a

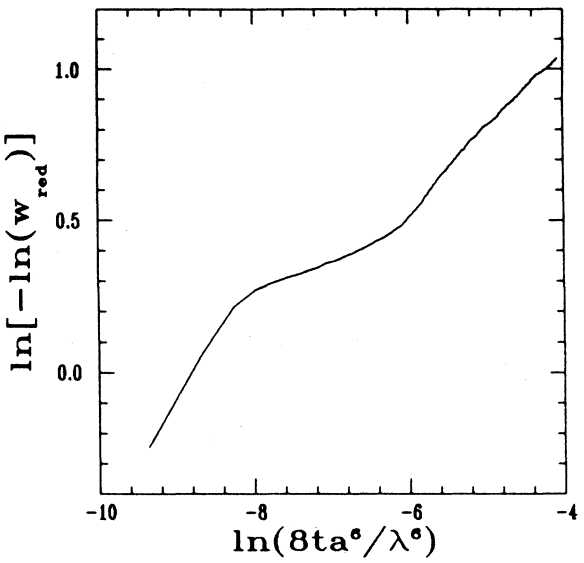

FIG. 6. For Kawasaki dynamics, discrete height variables, and $T=0.4J/k$ ($T<T_R$), we show $\ln[-\ln(w_{\rm red})]$ vs $\ln(8ta^6/\lambda^6)$ using $\lambda/\sqrt{2}a=12$, 2D grooves, and $h_0=5.5$

tail in $w_{\rm red}(t)$ reminiscent of the results for conserved order parameter, cf. Figs. 5 and 7. In Fig. 10 we show the logarithm of $w_{\rm red}$ as a function of $4ta^4/\lambda^4$ for $T=0.4J/k$, $h_0=5.5$, and $\lambda/\sqrt{2}a=20$ and 40. There is some evidence, from these results and further simulations with other wavelengths, that at short times the relaxation time scales as λ^3. The shape of the curves in Fig. 10 presumably signals the importance of multiple modes in the relaxation process.

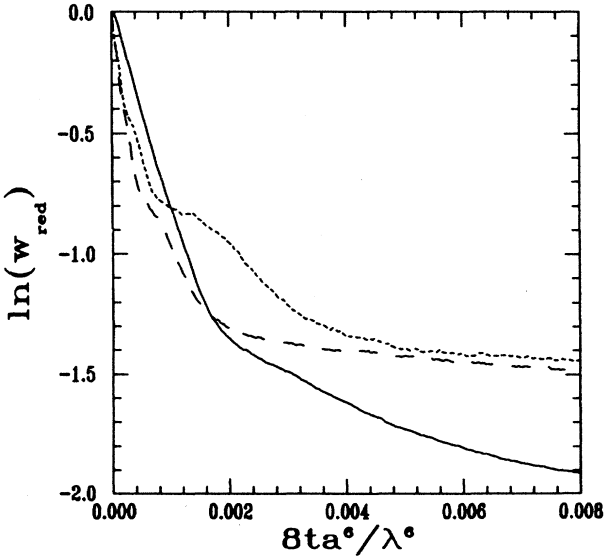

FIG. 7. The same as Fig. 5 except for 1D grooves with $\lambda/\sqrt{2}a=6$ (solid line), 12 (dashed line), and 18 (dotted line).

Finally, we have also done some simulations employing discrete h_i and temperatures well above the roughening temperature. The results are unexceptionally consistent with those using continuous h_i (described above) provided the initial amplitude h_0 is much smaller than λ.

Less attention was paid to the shapes of the decaying profiles in our work than to the behavior of the lifetime. We did examine profiles in some specific cases both above and below the roughening temperature. The results were consistent with extant published results from simulations[8] and theory.[7] That is, the profiles tend to remain roughly sinusoidal for $T > T_R$ and develop terraces for $T < T_R$, at least at relatively short times. At longer times, fluctuations destroy the initial simple periodic character of the grooves.

In the presence of a gravitational field, we have, for $T > T_R$, the predictions of Eqs. (11) and (12) for Glauber and Kawasaki dynamics. These suggest that one plot, respectively, τ^{-1} and $\lambda^2\tau^{-1}$ against λ^{-2} with $g \neq 0$ and see whether the result is a straight line. This is done in Fig. 11 with appropriate scaling of τ and λ. For all cases shown, $T = 0.4J/k$ and $h_0 = 4.0$. The results for nonconserved material are at $d=1$, $g = 0.02J$, and $f = 0.67$, and at $d=2$, $g = 0.03J$, and $f = 0.47$; those for conserved material are at $d=1$, $g = 1.0J$, and $f = 0.75$, and at $d=2$, $g = 1.0J$, and $f = 0.70$. The simulation results fit straight lines quite well at the larger values of λ in each case, consistent with expectations based on theory. We have also done limited simulations at $T < T_R$ (i.e., discrete h_i and $T = 0.4J/k$) with $g \neq 0$. We plan to pursue this work and report on it when we have a more complete picture and a better understanding of the relevant underlying physics.

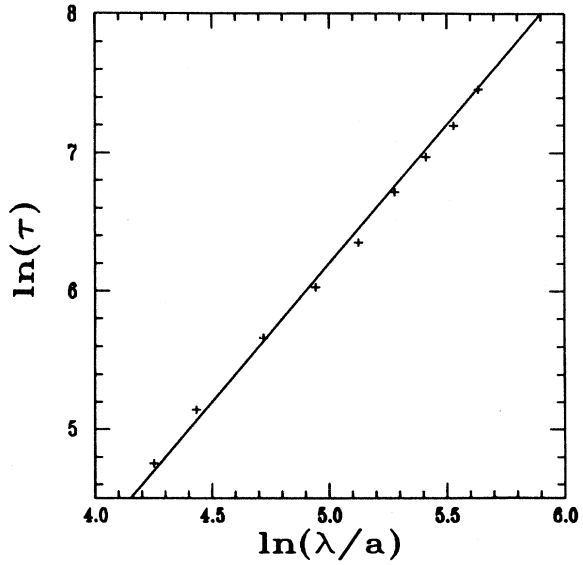

FIG. 9. For Glauber dynamics, discrete height variables, and $T = 0.4J/k$ ($T < T_R$), the logarithm of τ is plotted against that of λ/a using $h_0 = 5.5$ and 2D grooves; τ is determined using $f = 0.3$.

IV. SUMMARY

In this paper we have presented results for the healing of scratched solid surfaces using Monte Carlo simulations of a two-dimensional SOS model. We have used both conserved and nonconserved order-parameter dynamics corresponding, respectively, to surface diffusion and

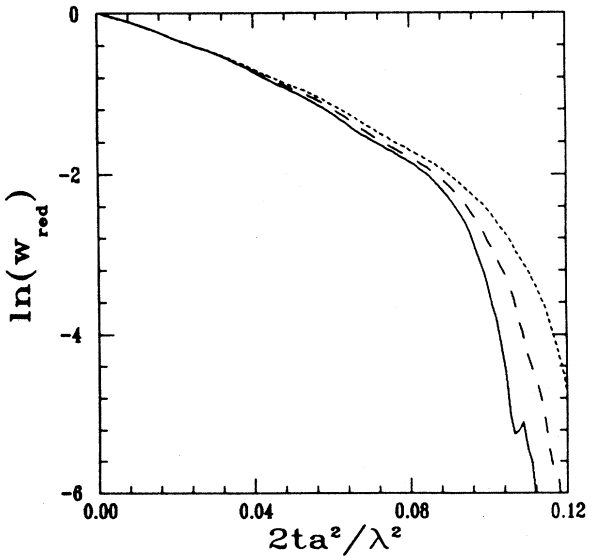

FIG. 8. For Glauber dynamics, discrete height variables, $T = 0.4J/k$ ($T < T_R$), the logarithm of w_{red} is plotted against $2ta^2/\lambda^2$ using 2D grooves and $h_0 = 5.5$; $\lambda = \sqrt{2}a = 60$ (dotted line), 90 (dashed line), and 120 (solid line).

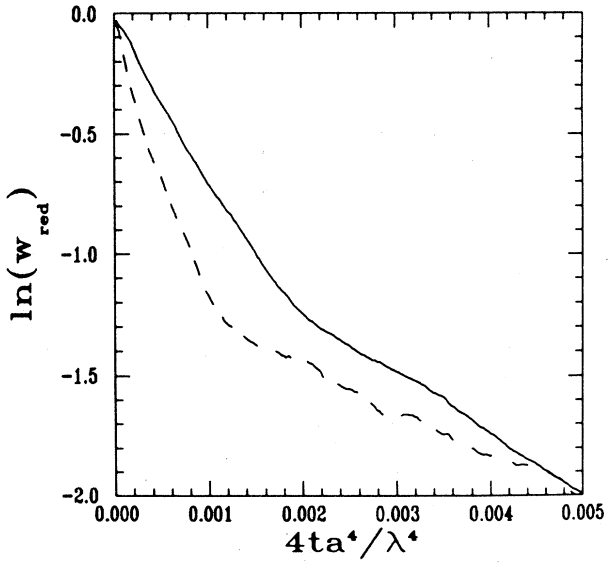

FIG. 10. For Glauber dynamics, discrete height variables, and $T = 0.4J/k$ ($T < T_R$), the logarithm of w_{red} is plotted against $4ta^4/\lambda^4$ for 1D grooves and $h_0 = 5.5$; $\lambda/\sqrt{2}a = 20$ (solid line) and 40 (dashed line).

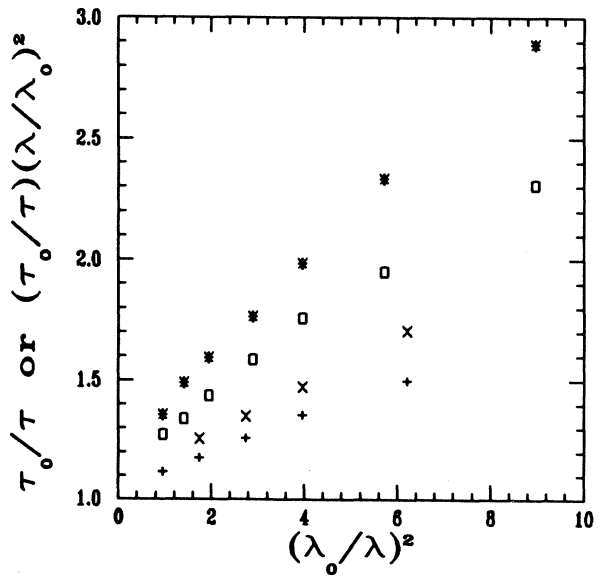

FIG. 11. Scaled inverse relaxation times (for Glauber dynamics) or scaled inverse relaxation times multiplied by scaled wavelength squared (for Kawasaki dynamics) are plotted against the scaled inverse wavelength squared for several cases with applied gravitational fields. In every case, continuous height variables ($h_0=4.0$) and $T=0.4J/k$ ($T>T_R$) are employed so that $T>T_R$. The specific cases are 1D grooves (+), $g=0.02J$, $f=0.67$, Glauber dynamics, $\tau_0=500$ mcs, $\lambda_0/\sqrt{2}a=200$; 2D grooves (×), $g=0.03J$, $f=0.47$, Glauber dynamics, $\tau_0=600$ mcs, $\lambda_0/\sqrt{2}a=200$; 1D grooves (□), $g=1.0J$, $f=0.75$, Kawasaki dynamics, $\tau_0=8000$ mcs, $\lambda_0/\sqrt{2}a=72$; and 2D grooves (*), $g=1.0J$, $f=0.70$, Kawasaki dynamics, $\tau_0=5000$ mcs, $\lambda_0/\sqrt{2}a=72$.

evaporation-condensation mechanisms, and have done simulations both above and below the roughening temperature of the surface. In the case of $T>T_R$, we have let the height variables of the model vary continuously so that $T_R=0$.

At $T>T_R$, we find that for initial configurations of either one- or two-dimensional sinusoidal-shaped grooves, the relaxation is predominantly, but not precisely, exponential in character with a lifetime proportional to λ^2 for nonconserved order parameter and to λ^4 for conserved order parameter. These conclusions are consistent with the predictions of Mullins[9] and of critical dynamics theory. The deviations from simple exponential behavior are ascribed to fluctuations present in the simulations but not in the theories. Our results are summarized by Figs. 1–4.

For $T<T_R$, the situation is considerably more complex. With conserved order-parameter dynamics, relaxation is very slow for both $d=1$ and $d=2$ grooves and the rate of relaxation appears to scale roughly as λ^6 for the largest times and wavelengths that we were able to treat. We should include a caveat that these were not large enough to be conclusive. There is ample evidence that multiple relaxation modes are playing important roles, which may lead to behavior of $w_{\rm red}(t)$ that is often referred to as a "stretched exponential". A characteristic property of this relaxation is a long tail in $w_{\rm red}(t)$ at large times. This behavior may be seen in Figs. 5–7. With nonconserved order-parameter dynamics and one-dimensional grooves, the behavior is similar in that there is a long tail in $w_{\rm red}(t)$ and evidence for the importance of more than one decay mode, as shown by Fig. 10. We note that Selke and Oitmaa[8] report exponential decay of their profiles below T_R. However, they study the decay of a particular Fourier coefficient of the profile, i.e., of a single mode, rather than of some average of all modes (as we do); we believe this is the source of the difference between our respective results.

Furthermore, for $d=2$ grooves and nonconserved order parameter, we do not find a long-time tail on $w_{\rm red}(t)$. Rather, the logarithm of $w_{\rm red}$ falls more precipitously at larger times than small ones and so the relaxation is relatively rapid. At the shorter times, the relaxation rate scales as λ^2, the same as for nonconserved order parameter and $T>T_R$. These conclusions may be extracted from Figs. 8 and 9.

We have also considered the effect of a gravitational field on the relaxation rates. For $T>T_R$, one has an explicit prediction from critical dynamics theory that the relaxation time should behave according to Eqs. (11) and (12). Our simulation results for this case, summarized in Fig. 11, are consistent with the predictions for the larger values of the wavelength. The deviations at shorter λ are probably a consequence of the discrete lattice and also of the fact that the theory is valid only for $h_0 \ll \lambda$.

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