Damage-spreading phase and damage-frozen phase in a solid-on-solid model

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Based on the recently suggested scaling ansatz [Phys. Rev. E **62**, 3376 (2000)] for damage spreading in the surface roughening phenomenon, the characteristics of the damage-spreading phase and damage-frozen phase in a two-dimensional solid-on-solid model that has a roughening transition at $T=T_R$ are studied. In the damage-spreading phase, which exists for $T>T_R$, the average vertical damage-spreading distance $\overline{d_\perp}(d_\parallel=0,L,T)$ and the average lateral damage-spreading distance $D_{||}(L,T)$ are shown to satisfy $\overline{d_\perp}(d_{||}=0,L,T)\simeq \ln L$ and $D_\parallel(L,T)\simeq L$, respectively. In the damage-frozen phase, which exists for $T<T_R$, it is shown that $d_\perp(d_\parallel=0,L\to\infty,T)\simeq$finite and $D_\parallel(L\to\infty,T)\simeq$finite. From these results it is concluded that the damage-spreading phase describes the surface roughening phase well and the damage-frozen phase describe the smooth phase well.

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By "damage spreading" (DS) [1], it is meant that two identical dynamical systems, which are initially the same as each other except for a small subset of the system, are simulated by the same sequence of random numbers to observe how the differences (damage) between two systems spread during dynamical evolution by detailed comparison of the two systems. The DS concept has been applied to analyses of dynamical systems such as biological systems [2], cellular automata [3], kinetic Ising models [4–10], and spin glass systems [11]. Recently, a scaling ansatz [16] based on a previous study [12] was suggested for damage spreading in the surface growth model [13,15] and the essential dynamical scaling properties of kinetic surface roughening were obtained from the scaling ansatz.

The suggested scaling ansatz [16] is briefly summarized as follows. Consider two systems A and B of growth. In system A growth begins with a flat surface, i.e., $h^A(r,0)=0$ for any r on the substrate, whereas growth in system B begins with $h^B(r,0)=0$ except at one point r_0, where $h^B(r_0,0)=1$. The surfaces in A and B are allowed to grow under the same growth rule and under the same sequence of random numbers. A damaged column at t is defined by the r at which $h^A(r,t)\neq h^B(r,t)$. If a column at r_d is damaged, the lateral damage-spreading distance $d_{||}$ and the vertical damage-spreading distance $d_\perp$ of the column are defined by $d_{||}\equiv|r_d-r_0|$ and $d_\perp\equiv|h^B(r_d,t)-\langle h^B\rangle|$, where $\langle h^B\rangle$ means the average surface height in system B. Then it has been shown that $\overline{d_\perp}(d_{||},t)$, the average of $d_\perp$ over the surviving damages that exist at the lateral distance $d_{||}$ (or at $r_d=r_0\pm d_{||}$), satisfies the dynamical scaling relation

$$\overline{d_\perp}=L^\alpha f_\perp\left(\frac{t-cd_{||}^z}{L^z}\right), \tag{1}$$

where $\overline{d_\perp}(d_{||},L,L)\simeq(t-cd_{||}^z)^\beta$ for $t-cd_{||}^z\ll L^z$ and $\overline{d_\perp}(d_{||},L,t)\simeq L^\alpha$ for $t-cd_{||}^z\gg L^z$. Of course the exponents α, β, and z in Eq. (1) are exactly the same exponents as in the usual scaling relation of dynamical surface roughening [13], $W(L,t)=L^\alpha(t/L^z)$, where $W(L,t)$ is the surface width of a given growth model with substrate size L at time t. As can be seen from Eq. (1), $\overline{d_\perp}$ of the column to which the initial damage is assigned (at $d_{||}=0$ or at r_0) faithfully reproduces the dynamical scaling relation $W(L,t)$ as

$$\overline{d_\perp}(d_{||}=0,t)(\equiv d_\perp^0)=L^\alpha f_\perp\left(\frac{t}{L^z}\right). \tag{2}$$

Another important scaling relation [16] for damage spreading in surface growth dynamics is the relation for the average lateral damage-spreading distance $D_{||}\equiv\langle d_{||}\rangle$ given by

$$D_{||}(L,t)=Lf_{||}(L/t^{1/z})\simeq\begin{cases} t^{1/z} & \text{if} \quad 1\ll t\ll L^z \\ L & \text{if} \quad t\gg L^z. \end{cases} \tag{3}$$

This relation is physically important [16], not only because $D_{||}(L,t)$ faithfully reproduces the correlation length ξ [13] of the kinetic roughening phenomenon but also because the sample-sized lateral DS distance (or $D_{||}\simeq L$) in the saturation regime ($t\gg L^z$) guarantees the self-affinity or anisotropy of the DS distances as $d_\perp^0\simeq L^\alpha\simeq D_{||}^\alpha$.

In this Brief Report we want to study how the damage-spreading concept can explain the thermal roughening transition. The model we consider in this report is a solid-on-solid (SOS) model [17] with the Hamiltonian

$$H=-J\sum_{\langle ij\rangle}|h(r_i)-h(r_j)| \quad (J>0), \tag{4}$$

where $\Sigma_{\langle ij\rangle}$ means the sum over nearest neighbor pairs only. The choice of the SOS model [17] is based on the fact that the model is well known to have the essential features of a typical thermal roughening transition even though it is very simple. The essential features of the roughening transition in the SOS model can be briefly summarized as follows. In the substrate dimension $d=1$ the surface is always rough except

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for $T=0$. Here the surface roughening in $d=1$ means that $W(L,t\rightarrow\infty,T)\simeq L^{\alpha}$ ($\alpha=1/2$), where $t\rightarrow\infty$ means the saturation regime (or $t\gg L^{z}$) in the kinetic roughening phenomenon [13] starting from the flat surface, and the surface state in the saturation regime is believed to be in thermal equilibrium at T. In $d=2$, there exists a roughening transition. In $d=2$ the interface for T above the roughening transition temperature T_R (or $T>T_R$) is in the roughening phase or $W(L,t\rightarrow\infty,T)\simeq\ln L(\alpha=0)$. For $T<T_R$ the surface is in the smooth phase or $W(L,t\rightarrow\infty,T)\rightarrow$ finite as $L\rightarrow\infty$.

In this report we want to find out if there exists a phase transition from the damage-spreading phase to the damage-frozen (DF) phase in the $d=2$ SOS model. In the DS phase, which we think describes the roughening phase, well (or the phase for $T>T_R$), $d_{\perp}^{0}$ and $D_{||}$ should satisfy

$$d_{\perp}^{0}(L,t\rightarrow\infty,T)\simeq\begin{cases}L^{\alpha}, & \alpha=1/2\ \ (d=1)\\ \ln L, & \alpha=0\ \ (d=2),\end{cases} \tag{5}$$

$$D_{\|}(L,t\rightarrow\infty,T)\simeq L. \tag{6}$$

These conjectures are expected from the scaling ansatz [16] for DS in kinetic surface growth models. In contrast it should hold that

$$d_{\perp}^{0}(L\rightarrow\infty,t\rightarrow\infty,T)\rightarrow\text{finite}, \tag{7}$$

$$D_{\|}(L\rightarrow\infty,t\rightarrow\infty,T)\rightarrow\text{finite} \tag{8}$$

in the DF phase, which we think describes the smooth phase well (or the phase for $T<T_R$) in $d=2$.

To prove our theoretical conjectures about the DS and DF phases, we have done simulations in order to see how initial damage propagates in the SOS model [17]. The simulation starts from a flat surface [or $h(r_i,t=0)=0$] and the periodic boundary condition is used in the lateral direction. The unit operation that is repeated in the simulation is as follows. Choose a column randomly and assume that the chosen column is at r_j. The change of $h(r_j,t)$ in the next Monte Carlo step is dependent upon the following probability assignments. Calculate the energy differences $\Delta E_{+}=H(h(r_j)+1)-H(h(r_j)),\Delta E_{-}=H(h(r_j)-1)-H(h(r_j))$ using the Hamiltonian (4), where $H(h(r_j)+1)$ is the energy of the system when the height at r_j is increased by a lattice unit and $H(h(r_j)-1)$ is that when the height is decreased by a lattice unit. The probabilities P_{+} for the process $h(r_j)\rightarrow h(r_j)+1$, P_0 for $h(r_j)\rightarrow h(r_j)$, and P_{-} for $h(r_j)\rightarrow h(r_j)-1$ are assigned as

$$P_{+}=\exp(-\Delta E_{+}/k_BT)/[\exp(-\Delta E_{+}/k_BT)+1+\exp(-\Delta E_{-}/k_BT)], \tag{9}$$

$$P_0=1/[\exp(-\Delta E_{+}/k_BT)+1+\exp(-\Delta E_{-}/k_BT)], \tag{10}$$

$$P_{-}=1-P_{+}-P_0. \tag{11}$$

All the numerical data in this report are taken after averaging over more than 100 independent runs.

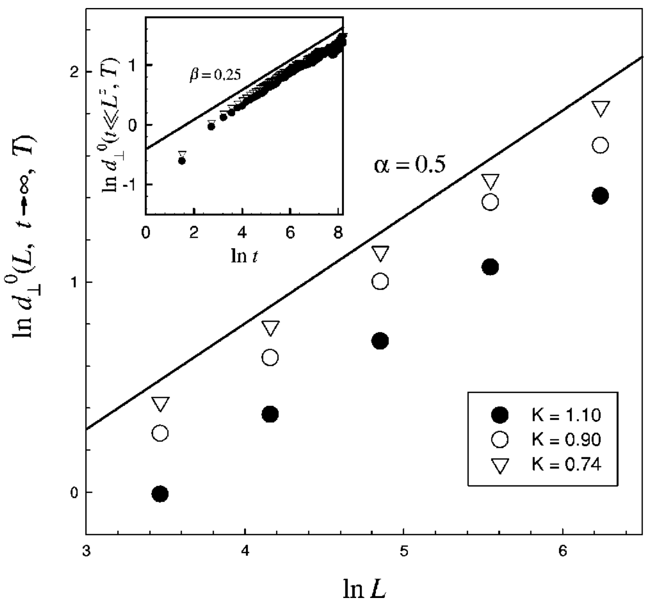

FIG. 1. Ln-ln plot of $d_{\perp}^{0}(L,t\rightarrow\infty,T)$ against L with the substrate sizes $L=32,64,128,256,512$ for the one-dimensional SOS model. The data were taken for $K=J/k_BT=1.10,0.90,0.74$. The solid line represents the relation $d_{\perp}^{0}(L,t\rightarrow\infty,T)\simeq L^{\alpha}$ ($\alpha=1/2$). The inset shows the time dependence of $d_{\perp}^{0}(t\ll L^{z},T)$ with $L=1024$. The solid line in the inset denotes the relation $d_{\perp}^{0}(t\ll L^{z},T)\simeq t^{\beta}\times(\beta=1/4)$.

We first report the one-dimensional simulation results. In the $d=1$ SOS model the surface is always rough except for $T=0$. If our conjecture is right, then there exists only the damage-spreading phase. This means that $d_{\perp}^{0}$ and $D_{||}$ satisfy Eq. (5) and Eq. (6), respectively, for any T. Our simulations for DS dynamics in the $d=1$ SOS model have been done for a variety of T's. In Figs. 1 and 2 the simulation results in $d=1$ are shown when $K(\equiv J/k_BT)=0.74$, $K=0.90$, and $K=1.1$. In Fig. 1, we show the data for $d_{\perp}^{0}$ in the saturation regime or in equilibrium, i.e., for $d_{\perp}^{0}(L,t\rightarrow\infty,T)$, with the substrate sizes $L=32,64,128,256,512$. As one can see from Fig. 1, $d_{\perp}^{0}(L,t\rightarrow\infty,T)$ satisfies Eq. (5) well. From the fit of the data to the formula $d_{\perp}^{0}(L,t\rightarrow\infty,T)\simeq L^{\alpha}$ we obtained $\alpha=0.50\pm0.01$ for $K=0.74$, $\alpha=0.50\pm0.02$ for $K=0.90$, and $\alpha=0.50\pm0.02$ for $K=1.10$. The inset of Fig. 1 shows the data for $d_{\perp}^{0}(t\ll L^{z},T)$ with $L=1024$ and the fit of the data to the relation $d_{\perp}^{0}(t\ll L^{z},T)\simeq t^{\beta}$ gives $\beta\simeq0.25$ regardless of the value of K. We have done simulations for a variety of T's in $d=1$ and obtained similar results to those in Fig. 1. From these simulation results it is concluded that $d_{\perp}^{0}$ in $d=1$ satisfies Eq. (5), or the characteristics of the damage-spreading phase. Furthermore, $d_{\perp}^{0}$ is critically the same as W, because the criticality of the $d=1$ SOS model dynamically belongs to the Edward-Wilkinson (EW) universality [13–15] with $\alpha=1/2$ and $\beta=1/4$.

In Fig. 2, the data for $D_{||}$ in the saturation regime or in equilibrium [or $D_{||}(L,t\rightarrow\infty,T)$] with $L=32,64,128,256,512$ are shown. All the lateral DS distances satisfy $D_{||}(L,t\rightarrow\infty,T)=aL$ excellently regardless of K. This result also means that the one-dimensional SOS model has only the

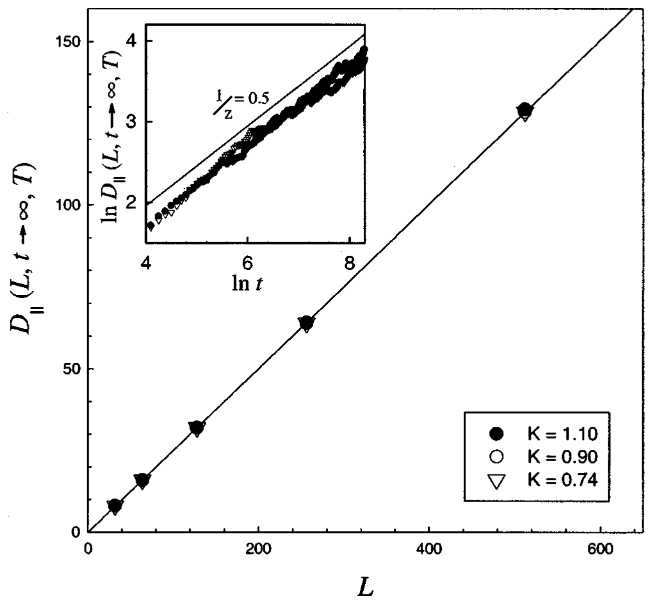

FIG. 2. Plot of $D_{||}(L,t\rightarrow\infty,T)$ against L for the one-dimensional SOS model. The values of L and K used are the same as those in Fig. 1. The solid line shows that the data satisfy the relation $D_{||}(L,t\rightarrow\infty,T)=aL$ excellently. The inset shows the time dependence of $D_{||}(t\ll L^z,T)$ with $L=1024$. The solid line in the inset denotes the relation $D_{||}(t\ll L^z,T)\simeq t^{1/z}$ $(z=1/2)$.

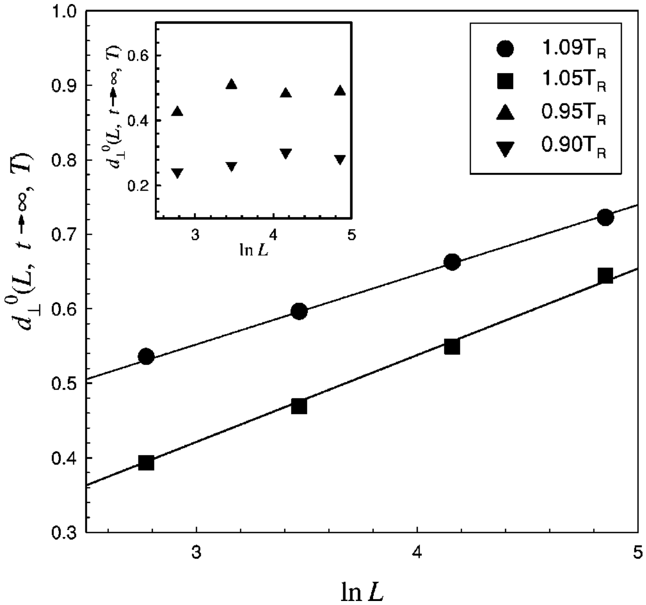

FIG. 3. The plot of $d_{\perp}^{0}(L,t\rightarrow\infty,T)$ against $\ln L$ for $T=1.05T_R$ and $T=1.09T_R$ in $d=2$. Substrate sizes used are $L\times L=16\times16,32\times32,64\times64$, and 128×128. Solid lines represent the relation $d_{\perp}^{0}(L,t\rightarrow\infty,T)=a\ln L$. Inset shows the same plot for $T=0.95T_R$ and $T=0.90T_R$.

damage-spreading phase (or only the roughening phase). Furthermore, the results in Fig. 2 tell us the physically important fact that only the sample-sized equilibrium lateral DS distance $(D_{||}\simeq L)$ guarantees the self-affinity of the damage-spreading phase and thus the existence of the damage-spreading phase can be checked solely by studying the lateral DS distance. The inset of Fig. 2 shows the data for $D_{||}(t\ll L^z,T)$ with $L=1024$ and the fit of the data to $D_{||}(t\ll L^z,T)\simeq t^{1/z}$ gives $z\simeq2$ regardless of the value of K. This is also consistent with the results $\alpha\simeq1/2$ and $\beta\simeq1/4$ that are obtained from Fig. 1, because $z=\alpha/\beta$.

The two-dimensional simulation results are displayed in Figs. 3 and 4. The two-dimensional SOS model has a phase transition from the roughening phase to the smooth phase. The transition temperature T_R is known to satisfy $K_R=J/k_BT_R=0.8061$ [17]. If our conjecture is right, then the damage-spreading phases exist for $T>T_R$ $(K<K_R)$, whereas the damage-frozen phases exist for $T<T_R$ $(K>K_R)$. Our simulations for DS dynamics in the $d=2$ SOS model were done for $T=1.09T_R$, $1.05T_R$, $0.95T_R$, and $0.90T_R$. In Fig. 3 we show the data for $d_{\perp}^{0}$ for the saturation regime or in equilibrium, i.e., for $d_{\perp}^{0}(L,t\rightarrow\infty,T)$, with the substrate sizes $L\times L=16\times16,32\times32,64\times64$, and 128×128. As is shown in Fig. 3, $T=1.09T_R$ and $T=1.05T_R$ satisfy the relation $d_{\perp}^{0}(L,t\rightarrow\infty,T)\simeq\ln L$ well. This result means that the phases for $T=1.09T_R$ and $T=1.05T_R$ are the damage-spreading phases as we expected. In contrast as is shown in the inset of Fig. 3, $d_{\perp}^{0}(L,t\rightarrow\infty,T)$ for $T=0.95T_R$ and $T=0.90T_R$ does not increase as L increases, and does not have any trend. Instead $d_{\perp}^{0}(L,t\rightarrow\infty,T)$ for $T=0.95T_R$ and $T=0.90T_R$ are sure to satisfy the relation $d_{\perp}^{0}(L\rightarrow\infty,t\rightarrow\infty,T)\simeq$finite. This result means that the phases for $T=0.95T_R$ and $T=0.90T_R$ are the damage-frozen phases as we expected. It is thus concluded from studying the vertical DS distances that the damage-spreading phases should exist for $T>T_R$, whereas the damage-frozen phases should exist for $T<T_R$. We have also studied the time dependence of $d_{\perp}^{0}(t\ll L^z,T)$ with the substrate size $L\times L=256\times256$ and have found that $d_{\perp}^{0}(t$

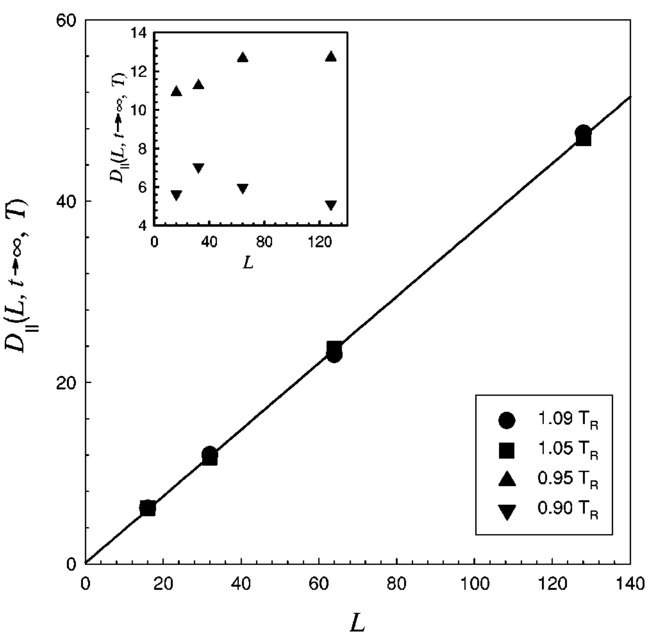

FIG. 4. Plot of $D_{||}(L,t\rightarrow\infty,T)$ against L for $T=1.05T_R$ and $T=1.09T_R$ in $d=2$. The sizes of substrates are the same as those in Fig. 3. The solid line shows that the data satisfy the relation $D_{||}(L,t\rightarrow\infty,T)=aL$ excellently as in Fig. 2. The inset shows the same plot for $T=0.95T_R$ and $T=0.90T_R$.

$\ll L^z,T)$ for $T=1.05T_R$ and $T=1.09T_R$ satisfies the relation $d_\perp^0(t\ll L^z,T)\simeq \ln t$. This result also supports the conclusion that the phases for $T=1.09T_R$ and $T=1.05T_R$ are the damage-spreading phases.

In Fig. 4 we show the data for $D_{||}$ in the saturation regime or in equilibrium, i.e., for $D_{||}(L,t\to\infty,T)$, with the same substrate sizes as in Fig. 3. As is shown in Fig. 4, $T=1.09T_R$ and $T=1.05T_R$ satisfy the relation $D_{||}(L,t\to\infty,T)=aL$ very well. This result also means that the phases for $T=1.09T_R$ and $T=1.05T_R$ are the damage-spreading phases as is concluded from the result in Fig. 3. Furthermore, it means that only the sample-sized lateral DS distance (or $D_{||}\simeq L$) guarantees the damage-spreading phase. In contrast, as is shown in the inset of Fig. 4, $D_{||}(L,t\to\infty,T)$ for $T=0.95T_R$ and $T=0.90T_R$ does not increase as L increases and does not have any trend. $D_{||}(L,t\to\infty,T)$ for $T=0.95T_R$ and $T=0.90T_R$ are sure to satisfy the relation $D_{||}(L\to\infty,t\to\infty,T)\simeq$ finite. This result also means that the phases for $T=0.95T_R$ and $T=0.90T_R$ are the damage-frozen phases as we concluded from the result in the inset of Fig. 3. We also studied the time dependence of $D_{||}(t\ll L^z,T)$ with the substrate size $L\times L=256\times 256$ and found that $D_{||}(t\ll L^z,T)$ for $T=1.05T_R$ and $T=1.09T_R$ satisfies the relation $D_{||}(t\ll L^z,T)\simeq t^{1/z}$ $(z=2)$. This result also supports the conclusion that the phases for $T=1.09T_R$ and $T=1.05T_R$ are the damage-spreading phases. Furthermore, $z=2$ in $d=2$ as well as in $d=1$ tells us that the damage-spreading phase of the SOS model belongs to the EW universality class as expected.

To summarize, we have shown that the two-dimensional SOS model has a transition from the damage-spreading phase to the damage-frozen phase. In the damage-spreading phase, which exists for $T>T_R$, $d_\perp^0$ and $D_{||}$ satisfy Eqs. (5) and (6), respectively, very well. Furthermore the damage-spreading phase describes the roughening phase (disordered phase) well, because the dynamical criticality or exponents for the damage-spreading phase agree well with those of the surface-roughening phase (or EW universality). The damage-frozen phase is well characterized by Eqs. (7) and (8) and thus describes the smooth phase (ordered phase) well. We have also demonstrated that the lateral DS distance $D_{||}$ can discriminate the damage-spreading (roughening) phase from the damage-frozen (smooth) phase, because only a sample-sized lateral DS distance (or $D_{||}\simeq L$) guarantees the self-affinity of the damage-spreading phase.

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