Time-reversed dielectric-breakdown model for erosion phenomena

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A time-reversed dielectric-breakdown model in which the annihilating probability of a particle on the surface site (x,h) depends on Laplacian field $\phi(x,h,t)$ as $P(x,h,t)=|\nabla\phi(x,h,t)|^{\kappa}/\Sigma_{x,h}|\nabla\phi(x,h,t)|^{\kappa}$ is suggested. This model is shown to be a theoretical model that covers a variety of eroding surfaces from the linear phenomena with dynamic exponent $z=1$ to those showing nonlinear behavior. $\phi(\mathbf{x},t)$ is defined to satisfy the Laplace equation $\nabla^2\phi=0$ with the boundary condition $\phi=0$ on the material and $\phi=1$ far from the material. The model with $0.5 \lesssim \kappa \lesssim 2$ is found to follow the linear growth equation with $z=1$ as the diffusion-limited erosion, which is also a time-reversed version of diffusion-limited deposition. For small κ, the dynamical scaling property of the eroding surface belongs to the Kardar-Parisi-Zhang universal class as the time-reversed Eden model. The model with $\kappa>2.5$ does not show any surface roughening behavior.

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I. INTRODUCTION

It is important to understand the dynamics of the surface eroded by reactions of particles from outside with particles in the material, because such evolution can be the key process for diverse phenomena such as electrolytic polishing, corrosion, etching, stable fluid invasion [1–5], chemical processes mediated by a catalytic particle [6,7], etc. Even though various theoretical scenarios [3,8] for growing surfaces such as the Kardar-Parisi-Zhang (KPZ) equation [9], conserved KPZ equation [10–13], linear growth equation [14], and growth models with quenched disorder [15–17] can be used to analyze eroding surfaces such as etched Si surfaces [5], these models were suggested mainly for growing or standing surfaces. Since the erosion processes are not merely the time-reversed processes of growth and the eroding surfaces cannot simply be understood from the models for growing surfaces, comprehensive models for the eroding surfaces are needed. However, there have been only a few theoretical models [2,3,6] suggested solely for such eroding surfaces. Among them, one of the most important models is the diffusion-limited erosion (DLE), which is the time-reversed process of the diffusion-limited deposition (DLD) [18].

DLE has been proved to follow the linear evolution equation [2,3]

$$\frac{\partial h_{\mathbf{q}}(t)}{\partial t}=-\nu|\mathbf{q}|h_{\mathbf{q}}(t)+\eta_{\mathbf{q}}(t), \tag{1}$$

$$\frac{\partial h(\mathbf{x},t)}{\partial t}=\nu|\nabla^2|^{1/2}h(\mathbf{x},t)+\eta(\mathbf{x},t), \tag{2}$$

where $h_{\mathbf{q}}(t)$ is the Fourier component of surface height $h(\mathbf{x},t)$, and $\eta_{\mathbf{q}}(t)$ is the Fourier component of Gaussian white noise $\eta(\mathbf{x},t)$ with $\langle\eta_{\mathbf{q}}(t)\rangle=0$ and $\langle\eta_{\mathbf{q}}(t)\eta_{\mathbf{q}'}(t)\rangle=\Delta\,\delta_{\mathbf{q}\mathbf{q}'}\,\delta(t-t')$. In DLE a particle starting far from the material undergoes a random walk before it touches the material. In DLE, both the incoming particle and the material particle, which the incoming particle first encounters, disappear through a reaction. This random walking property makes the incoming particle have more chance to contact the protruded part of the surface than the flat part. This nonlocality from the random-walk-like noise makes the fluctuation of surface follow Eq. (1) and make DLE a good model for the stable Laplacian front and for other eroding surfaces [2].

Although DLE is a good model for a sort of eroding surfaces, it is restricted to the limited applicability. If the incoming particle is attractively biased to the material, the eroding surface follows ballistic erosion [19], which is based on a local theory. Furthermore real eroding surfaces can have various nonlinear or hydrodynamic effects [2,3]. In this work, we want to suggest an extensive and powerful model as a paradigm for the evolution of eroding surfaces. As we shall see, our model explains not only the nonlocal eroding phenomena as DLE, but also the local or nonlinear KPZ-type eroding phenomena by a unified scheme.

We now want to briefly explain the theoretical background of our model. The space-time dependence of the density $\phi(\mathbf{x},t)$ of the random walkers in DLE or DLD follows the diffusion equation $\partial\phi/\partial t=D\nabla^2\phi$. In DLD the number of random walkers is always 1, because a new random walker is assumed to start only after the preceding walker sticks to the cluster. The growth process is thus very slow and the density of walkers at any time is very low, so that the growing process is nearly close to a steady state. From this fact the density field $\phi(\mathbf{x},t)$ of the walkers is expected to satisfy the Laplace equation

$$\nabla^2\phi=0, \tag{3}$$

with the following boundary condition: $\phi=1$ at the starting place of a walker and $\phi(\mathbf{x},t)=0$ on the cluster. This observation explains why the dielectric-breakdown model (DBM) [20] with a tuned parameter makes nearly the same ramified cluster as the DLD cluster. In DBM the Laplace equation (3) with the specified boundary condition is first numerically solved. Then the selection probability of a growth site is

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assigned to be proportional to $|\nabla\phi|^{\kappa}$, where $|\nabla\phi|$ is proportional to the particle flux to the site. Next choose a growth site based on the probability assignment and make the site belong to the cluster. The exponent κ in DBM was introduced to describe the relation between the local field and the growth probability. The structure of clusters as well as the fractal dimension d_f of the DBM model with $\kappa=1$ has been shown to be nearly the same as that of DLD. However, DBM is more powerful than DLD because of the physically important parameter κ. κ is a relevant parameter from the point of view that d_f varies as κ varies. From this fact DBM can be a model for a more wider class of the growth processes. The case with $\kappa=0$ corresponds to the case in which the growth probability is independent of ϕ and is equal to a type of Eden model [21] with $d_f=2$. A similar growth mechanism based on the gradient of density field was also used to describe dendrite growing problems [22].

In this work we want to suggest a paradigm for the evolution of eroding surfaces based on the time-reversed processes of DBM. DLE [2] was also a time-reversed process of DLD [18]. However, DLE was not a marginal extension of DLD but a decisive model for a sort of the eroding surfaces. We also want to show that TDBM is not a marginal extension of DBM but the model for the wider variety of eroding surfaces than DLE. Even though DLE was shown to be a model for the stable Laplacian front, TDBM with $\kappa=1$ is a more clear model that faithfully reproduces the circumstance for the derivation that the dynamical behavior of the stable Laplacian front follows Eq. (1). Furthermore, TDBM also covers a variety of the erosion processes including two extreme time-reversed random and irreversible growth models, i.e., the time-reversed Eden model and the time-reversed DLD (DLE) in a systematic and unified way. The unified way is by the variation of parameter κ, as κ in DBM makes the model cover from the needle crystal to the Eden model [20]. TDBM is a kind of the surface evolution model with both the deterministic and stochastic characters, because of the numerical solution of the Laplace equation. TDBM is also a nonlocal evolution model because of the Laplace equation. However, TDBM can also have the local nonlinearity by the variation of the parameter κ. For small κ, the model shows the nonlinear effects, so that it follows the nonlinear equation such as the KPZ equation [8,9]. This nonlinearity could also be related to the nonlinear effects from the relatively large attractive bias for the incoming particles in DLE [2].

II. MODEL

We now explain TDBM on a two-dimensional (2D) square lattice in detail. TDBM on a higher-dimensional hypercubic lattice can easily be obtained from the 2D definition. The evolution algorithm in TDBM has the following three steps (see Fig. 1).

(i) Set $\phi(x,y,t)=0$ at the sites occupied by the material particles and set $\phi(x,y=h_{max}+y_b,t)=1$, where h_{max} is the maximal surface height and y_b is a preassigned distance. The periodic boundary condition is imposed in the lateral direction.

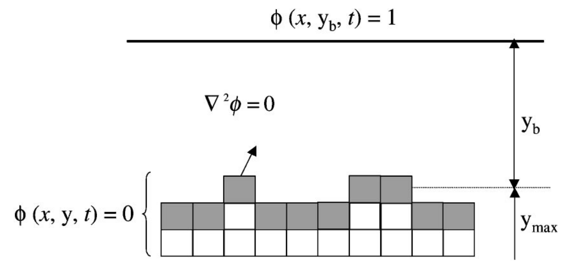

FIG. 1. The schematic diagram for the unit evolution process in the time-reversed dielectric-breakdown model in a 2D lattice. The shaded sites denote the surface sites for annihilation. Field $\phi(x,y,t)$ is assigned as $\phi(x,y,t)=0$ on the occupied sites and $\phi(x,h_{max}+y_b,t)=1$ on the line $y=h_{max}+y_b$. At the sites between the occupied sites and $y=h_{max}+y_b$, $\nabla^2\phi(x,y,t)=0$ holds. The annihilating probability of a surface site is determined by Eq. (5).

(ii) Solve the Laplace equation $\nabla^2\phi=0$ numerically with the boundary condition defined in step (i). $\nabla^2\phi=0$ is solved by the Gauss-Seidel over-relaxation method using the following lattice version of the Laplace equation:

$$\phi^{k+1}(x,y)=\phi^k(x,y)+\omega\Bigg[\frac{1}{4}\{\phi^k(x-1,y)+\phi^k(x+1,y)+\phi^k(x,y-1)+\phi^k(x,y+1)\}-\phi^k(x,y)\Bigg], \tag{4}$$

where ω is an over-relaxation parameter.

(iii) Using the numerical solution for $\phi(x,y)$ from step (ii), the annihilation probability $P(x,h(x,t))$ of a particle at a surface site $(x,h(x,t))$ is determined by

$$P(x,h(x,t))=\frac{|\nabla\phi(x,h,t)|^{\kappa}}{\sum_{x,h}|\nabla\phi(x,h,t)|^{\kappa}}. \tag{5}$$

Based on probability assignment (5), a surface site is chosen. Annihilate the particle at the chosen site. Then go back to step (i).

The numerical calculations start from the flat surface $h(x,t=0)=y_s$. We set $y_b\geqslant 20$. All the data for W are obtained by averaging over more than 100 independent runs, where W is the root mean square fluctuations of surface heights $\{h(x,t)\}$.

III. RESULTS

We first discuss results for TDBM with $\kappa=1$. The dependence of W for $\kappa=1$ on the Monte Carlo time t is shown in the inset of Fig. 2. Lateral sizes of the sample were $L=32,64,128,256,512,1024$. Solid curves in the inset show that each $W(L,t)$ fits very well to the analytic result from the linear equation (1) [2,3],

$$W^2=W_\infty^2+C\left\{\ln\left[1-\exp\left(\frac{-4\pi\nu t}{L}\right)\right]\right\}=W_\infty^2+f(t/L), \tag{6}$$

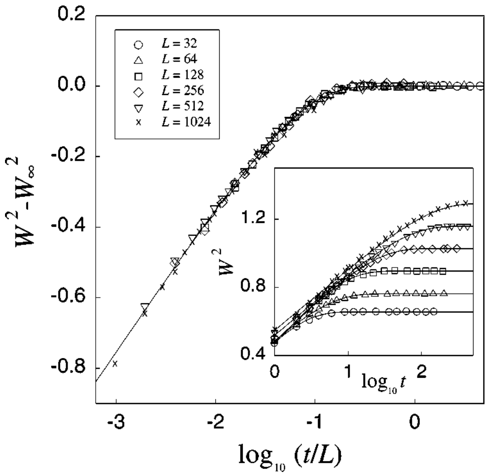

FIG. 2. Plot of W^2 of TDBM with $\kappa=1$ for the samples of various lateral sizes (L's). The inset shows the plot of the raw data of W^2 against $\log_{10}t$ and the solid curves in the inset show that W^2 for the different L satisfies relation (6) well. The main plot shows that the plot of $W^2-W_\infty^2$ for the different L against $\log_{10}(t/L)$ collapses well to one curve based on the scaling relation (6) with $z=1$.

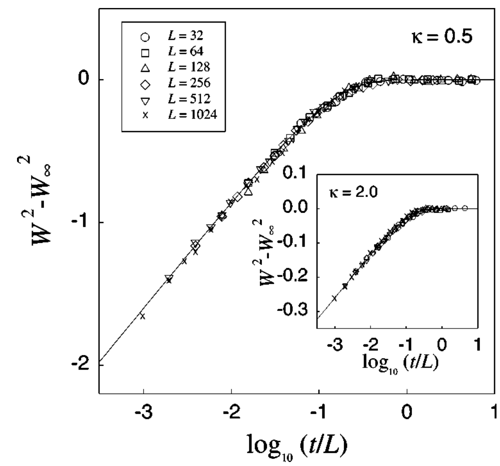

FIG. 3. Plot of $W^2-W_\infty^2$ for the different L in the cases $\kappa=0.5$ and $\kappa=2.0$ (inset). The plot shows W^2 for both cases collapses well to one curve based on the scaling relation (6) with $z=1$ as in Fig. 2.

where $W_\infty=W(L,t=\infty)$ and C is a constant. The main plot of Fig. 2 shows $W(L,t)$ for various L and t collapses well to one curve that represents the scaling plot based on Eq. (6). Normally the dynamic exponent z is defined through the relation $t_c\simeq L^z$, where t_c is the characteristic time or relaxation time t_c of the given dynamical behavior. Therefore, the results in Fig. 2 show that the dynamical behavior for $\kappa=1$ is that with $z=1$. The results in Fig. 2 also mean that TDBM with $\kappa=1$ follows Eq. (1) very well as DLE. This also means that the dynamic scaling property of DLE is the same as that of TDBM with $\kappa=1$ as the property of DLD is the same as that of DBM.

For the relevancy test of parameter κ, we also study TDBM with $\kappa\neq 1$. We first show for what values of κ W still follows Eq. (6) or the model follows Eq. (1). In Fig. 3, W in cases $\kappa=0.5$ and $\kappa=2.0$ is shown to satisfy the scaling property (6) well. As may be noticed from Fig. 3, it is confirmed that W of the model with the range $0.5\lesssim\kappa\lesssim 2$ satisfies the scaling property (6) well. This means that the nonlocality of the Laplace equation (3) is still dominant for $0.5\lesssim\kappa\lesssim 2$ and TDBM has the same scaling property as that with $\kappa=1$.

Another interesting case is in the limit $\kappa\to 0$. When $\kappa=0$, the annihilating probabilities on the surface sites become independent of field $\phi(x,t)$. This case becomes the time-reversed process of an Eden model [8,21]. The time-reversed Eden (TR-Eden) model (i.e., TDBM with $\kappa=0$) is exactly identical to the original Eden model if all the occupied (vacant) sites in the TR-Eden model are mapped to the vacant (occupied) sites. We thus expect that W for $\kappa=0$ satisfies the usual scaling relation

$$W=L^\alpha f(t/L^z) \tag{7}$$

with the KPZ exponents, i.e., roughness exponent $\alpha=1/2$, growth exponent $\beta=1/3$, and dynamic exponent $z=\alpha/\beta=3/2$ on a 1D substrate [8]. We confirm this expectation numerically. This result physically means that κ in TDBM can induce a nonlinear term such as the KPZ term $|\nabla h|^2$ if κ becomes small. To see the range of κ in which KPZ behavior is dominant, we study TDBM with small κ. We display the scaling behavior of TDBM with $\kappa=0.01$ in Fig. 4, in which we can clearly see the KPZ behavior with $\alpha=0.48$ and exponent $\beta=0.33$. However, we find that W does not show the KPZ behavior for $\kappa>0.02$. For $0.03\lesssim\kappa\lesssim 0.4$ we confirm that W shows the dynamic scaling behavior as in Eq. (7), but exponents α and β decrease from KPZ values as κ increases. The typical algebraic behavior of the model with $0.03\lesssim\kappa\lesssim 0.4$ is that shown in Fig. 5. In Fig. 5 we show that the dynamical behavior of the model with $\kappa=0.1$ satisfies the same scaling behavior as in Eq. (7) with $\alpha=0.3$ and β

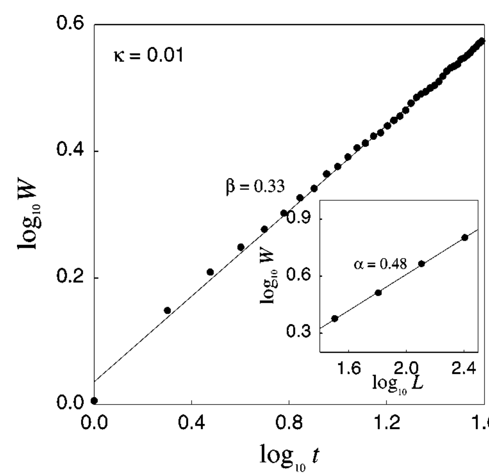

FIG. 4. The dynamical behavior of TDBM with $\kappa=0.01$ (or very small κ). The main plot shows the early time behavior of W or W for $t\ll L^z$. The solid line shows that the data fit well to the relation $W\simeq t^\beta(\beta=0.33)$. The inset shows that W in the saturation regime (or $t\gg L^z$) satisfies the relation $W\simeq L^\alpha(\alpha=0.48)$ well. This result shows that TDBM with a very small κ has the KPZ nonlinearity as the TR-Eden model when $\kappa=0$.

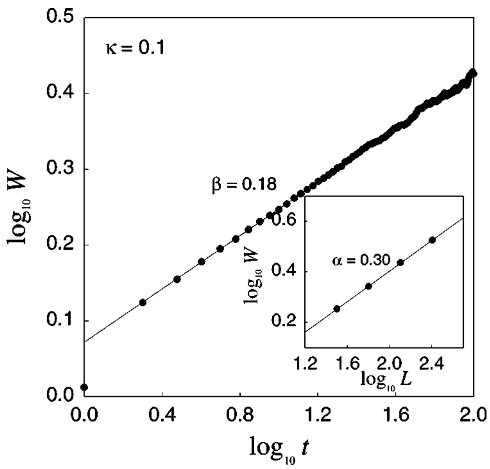

FIG. 5. The dynamical behavior of TDBM with $\kappa=0.1$. The main plot shows the early time behavior of W or W for $t \ll L^z$. The solid line shows that the data fit well to the relation $W \simeq t^{\beta}(\beta=0.18)$. The inset shows that W in the saturation regime (or $t \gg L^z$) satisfies the relation $W \simeq L^{\alpha}(\alpha=0.30)$ well. This result shows that the scaling behavior of TDBM with a moderately small κ is the same as Eq. (7), but the values of α and β decrease from the KPZ values as κ increases.

$=0.18$. The results in Figs. 4 and 5 mean that TDBM with $\kappa \lesssim 0.4$ shows the scaling behavior as in Eq. (7) with varying α and β unless κ becomes very small or $\kappa \lesssim 0.02$.

If $\kappa \to \infty$, we can expect that the nonlocality of the Laplace equation makes the annihilating probability at the protruded part of the surface enormously large and the surface becomes unroughened. We confirm that models with $\kappa > 2.5$ do not show any roughening behavior.

IV. SUMMARY AND DISCUSSION

In summary we have introduced a dynamical model for the eroding surfaces based on the nonlocality of the Laplace equation. This model naturally explains the dynamic scaling behavior of the so-called Laplacian front when $\kappa=1$. Furthermore the scaling behavior with $z=1$ exists in the rather broad range of κ, $0.5 \lesssim \kappa \lesssim 2$, where the nonlocality of the Laplace equation is still the important factor to decide the scaling property of TDBM. For small κ (or $\kappa \lesssim 0.4$), W shows the normal dynamical scaling behavior as in Eq. (7) with varying α and z. For the KPZ-like nonlinear behavior as in the TR-Eden model with $\kappa=0$, κ must become very small (or $\kappa \lesssim 0.02$). For the models with large κ (or $\kappa > 2.5$), the surface shows no roughening behavior.

We now want to add two final comments. One is on the crossover behavior from a regime to another when κ varies. The crossover behaviors we found are not sharp, but broad. Because we did not analyze the finite size effects using a sound theory, we cannot argue that the broad crossover comes from either the intrinsic character of the model or the finite size effects. This is partly due to the relatively long computing time to solve the Laplace equation. In the original DBM model [20] the existence of the several regimes of the model was shown, but the crossover behavior was not discussed, either. The reason for that is also believed to come from the same computing time problem.

The second comment is on the KPZ nonlinearity. As discussed previously, nonlinearity becomes important when κ becomes very small or the nonlocal behavior of the model becomes smeared out. Another way to make such localness is to give the incoming particle a drift velocity to the material in DLE or to make the particle undergo ballistic motion. According to a theoretical analysis [2] for the drift velocity effects on the Laplacian front, the bias can make the KPZ nonlinearity. In contrast, the scaling behavior of the eroding surface was shown to follow the Edwards-Wilkinson behavior with $z=2$ [8,23] when the incoming particle in DLE undergoes a biased random walk to the material [19]. It may be thus very interesting to study the algebraic behavior of TDBM more exactly in future studies.

ACKNOWLEDGMENT

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