

Anomalous scaling behavior in a solid-on-solid model for epitaxial growth

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We study the correlation function in a solid-on-solid model for epitaxial growth on one-dimensional substrates. In the transient regime, we find an anomalous situation that the roughness exponent ($\alpha \approx 1$) obtained from the surface width is different from that ($\alpha' \approx 0.75$) of the correlation function, which is well described by the scaling hypotheses previously proposed by Schroeder *et al.* [M. Schroeder, M. Siegert, D. E. Wolf, J. D. Shore, and M. Plischke, *Europhys. Lett.* **24**, 563 (1993)] and Das Sarma, Ghaisas, and Kim [S. Das Sarma, S. V. Ghaisas, and J. M. Kim, *Phys. Rev. E* **49**, 122 (1994)]. Few have been reported for anomalous scaling behaviors of the correlation function in growth models with $\alpha \leq 1$. We also measure the surface width for various ranges in a fixed size of system as in experiments. In case a surface width for a very small scale shows a power-law increase with time, the roughness exponent α' measured in experiments should be converted to α determining the universality classes. [S1063-651X(96)05407-4]

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I. INTRODUCTION

Recently, there has been much interest in kinetic roughening of growing surfaces. A great number of works to describe the surface roughness have been carried out by calculating the surface width and the correlation function in various kinetic growth models and continuum growth equations [1]. The surface width W , the root-mean-square value of the surface fluctuation for an initially flat surface, has been considered to obey the following scaling [2]:

$$W(L, t) \equiv [\langle (h - \langle h \rangle)^2 \rangle]^{1/2} \sim L^\alpha f(t/L^z), \quad (1)$$

where $h(\mathbf{x}, t)$ is the height of the surface in $d = d' + 1$ dimension (d' is the substrate dimension), L the lateral size of the substrate, t the growth time, α the roughness exponent describing a saturated surface, z the dynamic exponent, and the scaling function $f(x) \sim x^\beta$ (with the growth exponent $\beta = \alpha/z$) for $x \ll 1$ and $f(x) \rightarrow \text{constant}$ for $x \gg 1$. Here $\langle \dots \rangle$ denotes a spatial average. Thus the surface width W grows as $W(t) \sim t^\beta$ for $1 \ll t \ll L^z$ and $W(L) \sim L^\alpha$ for $t \gg L^z$. The critical exponents α and β determine the universality classes of growth models and continuum equations.

Another important quantity, the height-difference correlation function G has also been expected to scale as

$$G(\mathbf{r}, t) \equiv \langle [h(\mathbf{x} + \mathbf{r}, t) - h(\mathbf{x}, t)]^2 \rangle \sim r^{2\alpha} g(r/t^{1/z}), \quad (2)$$

where the scaling function $g(x) \rightarrow \text{constant}$ for $x \ll 1$ and $g(x) \sim x^{-2\alpha}$ for $x \gg 1$. Thus the correlation function G grows as $G(r) \sim r^{2\alpha}$ for $r \ll t^{1/z}$ and $G(t) \sim t^{2\beta}$ for $r \gg t^{1/z}$. For most models such as random deposition with surface diffusion [3] and ballistic deposition [4], one obtains the same critical exponents from the surface width W and the correlation function G . One can easily see that α obtained from G never

exceeds unity, with the help of a triangle with side lengths $|h(r+1) - h(r)|$, $|h(r) - h(r-1)|$, and $|h(r+1) - h(r-1)|$ [5].

More recently, in growth models for molecular beam epitaxy (MBE), there occurred an anomalous situation that the critical exponent α obtained from the surface width is different from that (α') from the correlation function [6,7]. In growth models proposed by Wolf and Villain (WV) [8] and Das Sarma and Tamborenea (DT) [9], the calculations of the surface width yielded $\alpha \sim 3/2$ while those of the correlation function did $\alpha' \sim 3/4$. To resolve this inconsistency, Schroeder *et al.* [10] and Das Sarma, Ghaisas, and Kim [11] proposed scaling hypotheses for the correlation function for surfaces with large local slopes or with $\alpha > 1$.

In addition to the WV and the DT models, various growth models have been proposed for describing epitaxial growth. In previous works [12,13], we studied a natural extension of the WV model, which is considered to be described by the continuum equation

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h - \nu_1 \nabla^4 h + \lambda_1 \nabla^2 (\nabla h)^2 + \eta, \quad (3)$$

where η is a white noise. This *extended* WV model shows the same crossover behavior as in the original WV model but in much smaller length and time scales. In $d' = 2$, we obtained the same results of the critical exponents from the surface width W and the correlation function G , which indicates that the conventional scaling [Eq. (2)] is satisfied in $d' = 2$. In contrast to the result in $d' = 2$, an anomalous scaling behavior is observed at initial stages in $d' = 1$. The calculation of $G(r, t)$ for small r yields $\alpha' \approx 3/4$ which is not consistent with $\alpha \approx 1$ for small L [14].

This work is mainly motivated by two points. First, we investigate an anomalous scaling behavior of the correlation function in a growth model with $\alpha = 1$. Few have been reported for anomalous scaling behaviors in growth models

with $\alpha \leq 1$ [15]. In Sec. III, we show an anomalous scaling behavior in the extended WV model in $d' = 1$, which is well described by the scaling hypotheses [10,11] previously proposed. We also confirm the results previously obtained from the surface width by the calculation of the correlation function. Second, in the presence of an anomalous scaling behavior, one can give rise to a question; “is the roughness exponent measured in experiments α or α' ?” In Sec. IV, we estimate the roughness exponent as in experiments. Finally Sec. V is devoted to a brief summary.

II. ANOMALOUS SCALING

In this section, we briefly summarize analytic and numerical results (in $d' = 1$) relevant to this work. In Eq. (3) describing a conservative growth without desorption and vacancies, the Edwards-Wilkinson (EW) term ($\nu \nabla^2 h$) produces $\alpha = 1/2$ and $\beta = 1/4$ and describes a growing surface in the presence of gravitation [16]. The $-\nu_1 \nabla^4 h$ term introduced by Herring and Mullins [17] yields $\alpha = 3/2$ and $\beta = 3/8$. Kim and Das Sarma [18] proposed a restricted-curvature (RC) model to be described by the $-\nu_1 \nabla^4 h$ term, where if $|\nabla^2 h| \leq N$ (N a restriction parameter), freshly landed atoms are deposited or evaporated, otherwise forbidden. The $\lambda_1 \nabla^2 (\nabla h)^2$ term was solved by Lai and Das Sarma (LD) [19] to yield $\alpha = 1$ and $\beta = 1/3$. Various growth models relevant to Eq. (3) are briefly mentioned in Ref. [13]. In a conservative growth, the critical exponents α and z satisfy a general relation $2\alpha + d' = z$ [8].

Anomalous scaling behaviors have been observed in the RC, DT, and WV models and expected to show up in growth models with power-law increases of $G(1,t)$. It has been considered that the DT and the WV models show the Herring-Mullins behavior at initial stages but crossover to other classes [20–22]. The calculations of the surface width in the RC model and in the DT and the WV models at initial stages yielded $\alpha \approx 3/2$ and $z \approx 4$, while those of the correlation function did not yield the same results [6,10,11,21]. To resolve these inconsistencies, Schroeder *et al.* [10] and Das Sarma, Ghaisas, and Kim (DGK) [11] investigated anomalous scaling behaviors.

Schroeder *et al.* noted the power-law increase of $G(1,t) = \langle (\nabla h)^2 \rangle = a^2(t)$ as a sign of an anomalous scaling behavior. While $G(1,t)$ is constant in conventional growth models, it increases as $t^{2\lambda}$ in the RC, DT, and WV models. They regarded the averaged step height $a(t)$ as a natural unit of measuring h and considered a characteristic time $b(t) \sim t^\mu$ associated with $a(t)$, where μ is set to 2λ for a conservative growth. Taking $G(1,t)$ into consideration, they proposed a scaling ansatz as

$$G(r,t) \sim G(1,t) r^{2\alpha'} \tilde{g}(r/t'^{1/z'}), \quad (4)$$

where $t' = t/b(t)$ and asymptotic behaviors of the scaling function $\tilde{g}(x)$ are the same as those of $g(x)$ in Eq. (2). They also obtained an alternative representation by subsuming the time dependence of $G(1,t)$ in a scaling function $\hat{g}(x)$;

$$G(r,t) \sim r^{2\alpha} \hat{g}(r/t^{1/z}), \quad (5)$$

with the scaling function $\hat{g}(x) \sim x^{-2(\alpha-\alpha')}$ for $x \ll 1$ and $\hat{g}(x) \sim x^{-2\alpha}$ for $x \gg 1$. A comparison of Eq. (4) with Eq. (5) in asymptotic regimes yields relations between the critical exponents (α , β , and z) from W and those (α' , β' , and z') from G as the following:

$$z = \frac{z'}{1-2\lambda}, \quad \alpha = \alpha' + z\lambda, \quad \text{and} \quad \beta = \beta'. \quad (6)$$

One can easily notice $\beta' \neq \alpha'/z'$ and $t^{1/z} = t'^{1/z'} \sim \xi$ where ξ is the correlation length. We note that the critical exponents α' and z' also satisfy the same relation as that between α and z

$$2\alpha' + d' = z'. \quad (7)$$

They obtained numerical results $\alpha' \approx 0.75$, $z' \approx 2.4$, and $2\lambda \approx 0.38$ in the WV model, which are consistent with Eq. (6).

On the other hand, the anomalous scaling ansatz of DGK is based on an analytic calculation of $G(r,t)$ in the continuum equation $\partial h/\partial t = -\nu_1 \nabla^4 h + \eta$ which yields $\alpha = 3/2$ and $z = 4$. The analytic calculation of $G(r,t)$ for $r \leq t^{1/z}$ yields $r^{2\alpha} (r/t^{1/z})^{-1}$. The power “ -1 ” of $r/t^{1/z}$ was generalized to a constant “ $-\kappa$ ” for a nonequilibrium surface with $\alpha > 1$. This scaling ansatz is the same to Eq. (5) with $\kappa = 2z\lambda$. They obtained $\alpha' \approx 1$ (0.7), $z' \approx 3$ (2.5), and $\kappa \approx 1$ (1.6), so that $2\lambda \approx 0.25$ (0.4) in the RC (DT) model [23]. They also obtained the same results in the WV model as in the DT model. In their work, it was also argued that in the case of $\alpha = 1$, one obtains $\kappa = 0$, that is, $G(1,t) \sim \ln t$, which was confirmed in a modification of the restricted solid-on-solid model [24]. In contrast to this, we obtain $G(1,t) \sim t^{0.2}$ and $\kappa \approx 0.6$ in the transient regime with $\alpha = 1$ in the extended WV model.

One can simply obtain $G(1,t) \sim t^{2(\alpha-1)/z}$ by a dimensional analysis. It is considered that the RC, a larger curvature [25], and the modification of the restricted solid-on-solid model follow the above scaling, while the DT, the WV, and the extended WV models do not [5]. In a recent work of Krug [22], multiscaling behavior of the q th-order correlation function was observed and a crossover to the LD behavior was discussed in the DT model. The crossover behaviors may affect the scaling of $G(1,t)$ in the DT, the WV, and the extended WV models.

III. ANOMALOUS SCALING IN THE EXTENDED WV MODEL

In the previous works [12,13], we investigated a natural extension of the WV model, where freshly landed atoms relax into local energy minima where the binding energy is calculated within next-nearest-neighbor approximation. The extended WV model shows the LD behavior in the transient regime and the EW behavior in the asymptotic regime. Beyond expectation, we could observe the crossover behavior in much smaller length and time scales than in the original WV model, both in $d' = 1$ and $d' = 2$. In $d' = 1$, the calculation of W yielded that α (β) changes from 1 (1/3) to 1/2 (1/4). The EW behavior in the asymptotic regime was also confirmed by the measurement of surface diffusion current.

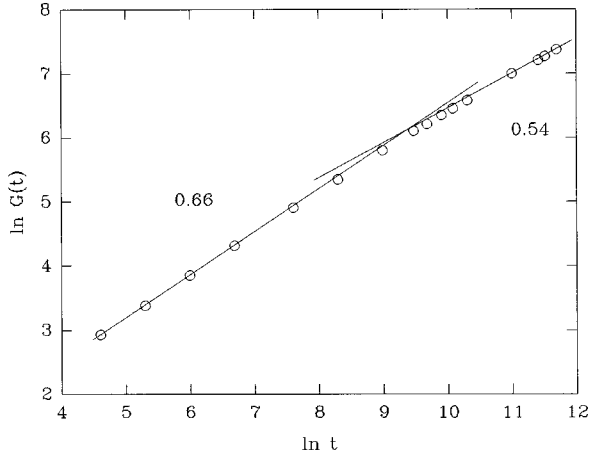


FIG. 1. The log-log plot of G vs t with $L=2000$ where 2β is given by the slopes. The extended WV model shows the Lai-Das Sarma behavior in the transient regime and the Edwards-Wilkinson behavior in the asymptotic regime. Statistical averages were taken over 300 samples.

In $d'=1$ [12], the presence of another nonlinear $\lambda_2 \nabla \cdot (\nabla h)^3$ term was reported. In view of the result in $d'=2$ [13], it is considered to be an artifact on one-dimensional substrates, owing to a very slow crossover from the LD to the EW behavior.

We calculate the correlation function G in $d'=1$ with periodic boundary condition. As seen in Fig. 1, the log-log plot of $G(t)$ vs t confirms the crossover behaviors of β mentioned above, where $G(t)$ was obtained from the saturation value of G in the plot of $G(r,t)$ vs r for several values of t . We have $\beta=0.333\pm 0.001$ at early growth times and 0.271 ± 0.004 for $t>35\,000$. From the results of the surface width, we estimated the crossover time $t_c\sim 13\,000$.

Next we calculate $G(1,t)$. As shown in Fig. 2, $G(1,t)$ grows as $t^{1/5}$ in the transient regime and saturates to constant

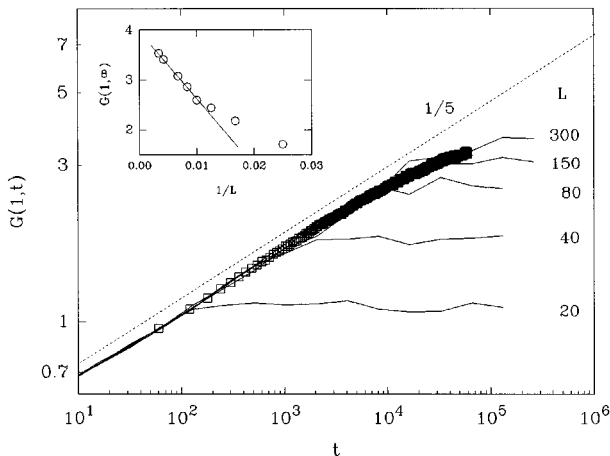


FIG. 2. The log-log plots of $G(1,t)$ vs t for various L . We obtained $G(1,t)\sim t^{0.2}$ for $L=1000$ (\square) in the transient regime. The inset shows the plot of $G(1,t)$ vs $1/L$ in the asymptotic regime. Statistical averages were taken over 500 samples.

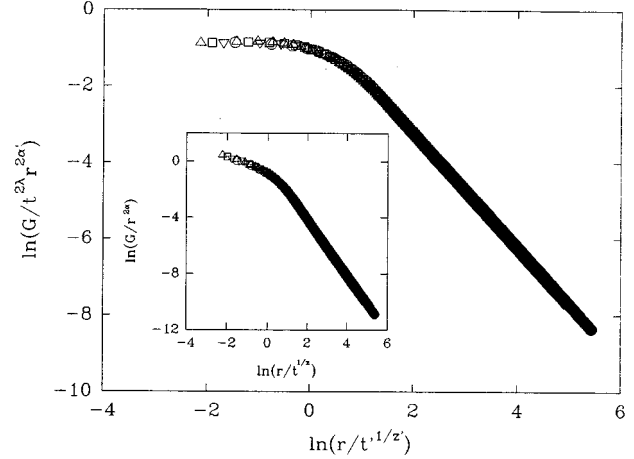


FIG. 3. The scaling plots of $G(r,t)$ by Eq. (4) for $t=100, 200, 400,$ and 800 with $L=2000$. We have $\alpha'=0.75$, $2\lambda=0.2$, and $z'=2.5$. The scaling plots of $G(r,t)$ by Eq. (5) are also shown in the inset where $\alpha=1$ and $z=3$. Statistical averages were taken over 300 samples.

values in the asymptotic regime. The constant saturated value of $G(1,t)$ has a correction of order $1/L$, as shown in the inset, which confirms the EW behavior in the asymptotic regime. In the original WV model, a crossover to EW class was manifested from the scaling behavior of $G(1,\infty)$ [26].

The power-law increase of $G(1,t)$ in the transient regime showing the LD behavior ($\alpha=1$ and $z=3$) indicates the presence of an anomalous scaling behavior in the extended WV model. We obtained $\alpha'\approx 0.75$ from the slope in the log-log plot of $G(r,t)$ vs r for small r . It is noted that $\alpha'\approx 0.75$ was also obtained in the regime showing the LD behavior in the original WV model [21]. With $z'\approx 2.5$ obtained from Eq. (7), we collapse the data of $G(r,t)$ according to Eq. (4) with $2\lambda\approx 0.2$, as seen in Fig. 3. We also collapse those according to Eq. (5), as shown in the inset. We obtain $\kappa=2z\lambda\approx 0.6$ for small values of $r/t^{1/z}$. Very good data collapses indicate that the anomalous scaling behavior in the transient regime is well described by the previously proposed anomalous scaling hypotheses.

Finally, we examine the correlation function in the asymptotic regime showing the EW behavior ($\alpha=1/2$ and $\beta=1/4$). For a large length ($L\gg L_c\sim t_c^{1/z}$) and time ($t\gg t_c$) scales, we expect that the correlation function $G(r,t)$ behaves as $G(r)\sim r^{3/2}$ for $r\ll L_c$, $G(r)\sim r$ for $L_c\ll r\ll \xi\sim t^{1/z}$, and $G(t)\sim t^{1/2}$ for $\xi\ll r$. To present this behavior, we show the log-log plots of $G(r,t)/t^{2\beta}$ as a function of $r/t^{1/z}$ for various $t>t_c$ in Fig. 4. We have $2\beta=0.54$ and $z=2$ corresponding to the EW behavior in the asymptotic regime. As shown in the figure, the correlation function G grows as $G(r,t)\sim r^{3/2}$ for small values of $r/t^{1/z}$ and the data of G fall into a single curve for large values of $r/t^{1/z}$. Since the crossover length $L_c\sim t_c^{1/z}$ is independent of t while the correlation length ξ is not, the curve is splitted for small values $r/t^{1/z}$. The data collapse shows that our understanding of $G(r,t)$ in the presence of a crossover behavior is correct.

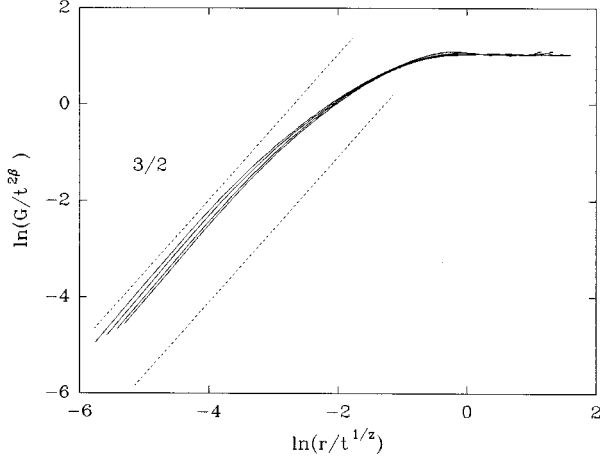


FIG. 4. The log-log plots of $G(r,t)/t^{2\beta}$ vs $r/t^{1/z}$ with $2\beta=0.54$ and $z=2$. We have $t=40\,000, 50\,000, 70\,000,$ and $100\,000$ (from right to left) and $L=2000$. Statistical averages were taken over 300 samples. The parallel dotted lines with the slope $3/2$ were merely drawn for a guide to the eye.

IV. ROUGHNESS EXPONENT IN EXPERIMENTS

As commented by Schroeder *et al.* [10], a surface width is usually measured in experiments as a function of r ($<L$) for a fixed L rather than as a function of L as calculated in numerical simulation. To make it clear whether the roughness exponent measured in experiments is α or α' , we calculate the surface width $W_e(r,t)$ in the transient regime as in experiments. In Fig. 5, we show the log-log plot of $W_e(r,t)$ vs r for various t . As expected, the roughness exponent measured in experiments is consistent with α' obtained from the correlation function. Using $W_e^2(2,t)=G(1,t)/4$, we apply the same ansatz as that of Schroeder *et al.*

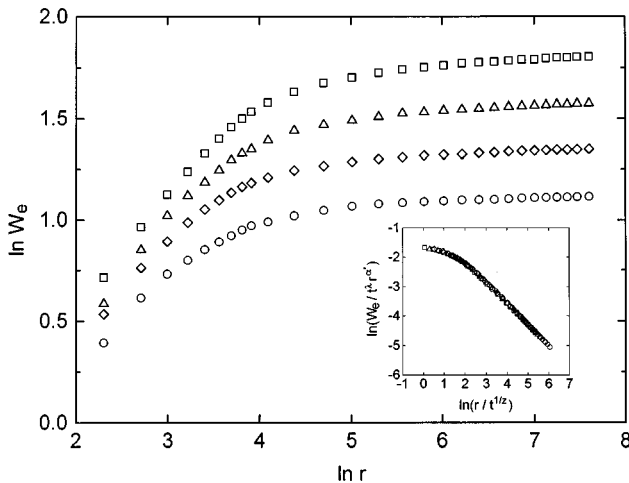


FIG. 5. The log-log plots of $W_e(r,t)$ vs r for $t=100$ (\circ), 200 (\diamond), 400 (\triangle), and 800 (\square) with $L=2000$. Statistical averages were taken over 500 samples. The inset shows the scaling plots of $W_e(r,t)$ by Eq. (8) where $\alpha'=0.75$, $2\lambda=0.2$, and $z=3$.

$$W_e^2(r,t) \equiv \langle \langle (h - \langle h \rangle_r)^2 \rangle_r \rangle \sim W^2(2,t) r^{2\alpha'} \tilde{f}(r/t^{1/z}), \quad (8)$$

where $\langle \dots \rangle_r$ denotes a spatial average over a region of size r , a scaling function $\tilde{f}(x) \rightarrow \text{constant}$ for $x \ll 1$ and $\tilde{f}(x) \sim x^{-2\alpha'}$ for $x \gg 1$. Here we used a relation $t^{1/z} = t'^{1/z'}$. The inset shows the data collapse of $W_e(r,t)$ as a function of $r/t^{1/z}$. The perfect data collapse shows that $W_e(r,t)$ behaves in the same way as $G(r,t)$. We also measured $W_e(r,t)$ in the WV model and in the random deposition with surface diffusion. As expected, $W_e(r,t)$ also shows an anomalous scaling behavior in the WV model. But in the random deposition with surface diffusion, $W(2,t)$ saturates to a constant immediately (so that, the data of $W_e(r,t)$ with different t coincide for small r) and both $W_e(r,t)$ and $W(L,t)$ yield the same roughness exponent $\alpha=1/2$. Finally we check the behavior of $W_e(L,t)$. Here, for simplicity, we do not consider a crossover to a regime with the conventional scaling. For $r=L$, we have $W_e^2(L,t) \sim W_e^2(2,t) L^{2\alpha'} \tilde{f}(L/t^{1/z})$. Since $W_e^2(2,t) \sim t^{2\lambda}$ for $t < L^z$ and $W_e^2(2,t) \sim L^{2z\lambda}$ for $t > L^z$, we obtain $W_e^2(L,t) \sim t^{2\beta}$ for $t < L^z$ and $W_e^2(L,t) \sim L^{2\alpha}$ for $t > L^z$ with the help of Eq. (6), so that we recovered the behavior of $W(L,t)$.

To our knowledge, an anomalous scaling behavior has not been observed in experiments. Moreover, in numerical simulations on two-dimensional substrates of real system in experiments, few have been reported for an anomalous scaling behavior except for the simulation of the WV model on a two-dimensional substrate by Šmilauer and Kotrla [21]. However, it is not sufficient to arrive at the conclusion whether an anomalous scaling behavior is simply an artifact on one-dimensional substrates or it can be observed in experiments. One can find similar figures to our Fig. 5 in experimental works, such as Fig. 3 of Ref. [27] and Fig. 2 of Ref. [28]. The scattered data for small scales in the figures may be due to anomalous scaling behaviors or simply due to a finite size effect. In Ref. [27], Tong *et al.* obtained the roughness exponent (α') as 0.84 ± 0.05 for the MBE growth of CuCl on CaF₂(111). If $W_e(r,t)$ for small r increases as a power law of t , the value of the roughness exponent is underestimated, so that the surface roughness is expected to be described by the Herring-Mullins behavior rather than by the LD behavior. We emphasize that *in the presence of power-law increase of the surface width for a very small scale*, the underestimated roughness exponent α' , measured in experiments, should be converted to α which determines the universality class.

V. SUMMARY

We have studied the correlation function in the extended WV model on one-dimensional substrates. In the transient regime showing the Lai-Das Sarma behavior, we have found that the roughness exponent $\alpha' \approx 0.75$ obtained from the correlation function is different from $\alpha \approx 1$ obtained from the surface width. Few have been reported for anomalous scaling behaviors of the correlation function in growth models with $\alpha \leq 1$. This anomalous behavior of the correlation function is well described by the previously proposed scaling hypotheses. It is considered that the anomalous scaling behavior stems out of the groove instability which was originally dis-

cussed by Amar, Lam, and Family [29] in various growth models; a macroscopic groove can be found in the saturated regime of a system with a size less than the crossover length. In the asymptotic regime showing the Edwards-Wilkinson behavior, the conventional scaling is satisfied. We also calculated the surface width as measured in experiments. The result shows that if a surface width for a very small scale shows a power-law increase with time, the measured roughness exponent should be modified according to Eq. (6) for a comparison with theoretical works.

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