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# Stochastic equation for the morphological evolution of heteroepitaxial thin films

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A stochastic partial differential equation for the morphological evolution of strained epitaxial films is derived from atomistic aggregation kinetics. The transition rules and rates are based on a model that incorporates the effects of strain through environment-dependent energy barriers to adatom detachment. Comparisons with previous approaches based on continuum elasticity provide an atomistic interpretation of the governing equation for heteroepitaxial thin films.

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Self-organization on strained epitaxial surfaces has been studied with many theoretical methods, including kinetic Monte Carlo (KMC) simulations,[1–10] molecular dynamics,[11–13] and continuum equations.[14–18] One of the "grand challenges" for computational materials science is the synthesis of such disparate descriptions into a multiscale theory of morphological evolution. The presence of strain relaxation, in particular, endows the rates of atomistic processes on strained surfaces with a dependence on nonlocal factors such as the height and lateral extent of a terrace above a substrate[4] and the presence of neighboring islands.[19] These effects are manifestations of elastic interactions, which find a natural expression within a continuum framework.

In this Rapid Communication we derive a stochastic differential equation for the morphological evolution of heteroepitaxial surfaces from an atomistic model[4] for coherent three-dimensional (3D) island formation. Our approach is based on first expressing the transition rules of this model as a lattice Langevin equation,[20] which is then regularized to obtain a stochastic partial differential equation. The deterministic part of this equation has the same form as that derived by Golovin *et al.*[17] from continuum elasticity, but with coefficients that have a direct relation to the underlying atomistic processes.

We first consider a one-dimensional (1D) substrate with $L$ sites on each site $i$ of which is a column of $H_i$ particles. Every surface configuration corresponds to an array $\mathbf{H}=\{H_1,H_2,\ldots,H_L\}$. The probability that the system has configuration $\mathbf{H}$ at time $t$ is $P(\mathbf{H},t)$, which is a solution of the master equation[21]

$$\frac{\partial P}{\partial t}=\int [W(\mathbf{H}-\mathbf{r};\mathbf{r})P(\mathbf{H}-\mathbf{r},t)-W(\mathbf{H};\mathbf{r})P(\mathbf{H},t)]d\mathbf{r}, \tag{1}$$

where $W(\mathbf{H};\mathbf{r})$ is the transition rate density from $\mathbf{H}$ to $\mathbf{H}+\mathbf{r}$, and $\mathbf{r}=\{r_1,r_2,\ldots,r_L\}$ is the array of jump lengths at each site. This equation can be transformed into a lattice Langevin equation for height fluctuations,[20]

$$\frac{dh_i}{d\tau}=K_i^{(1)}+\eta_i, \tag{2}$$

where $h_i=\Omega^{-1}H_i$ and $\tau=\Omega^{-1}t$ are continuous height and time variables rescaled by a "largeness" parameter $\Omega$, $\eta_i$ are Gaussian noises that have mean zero, $\langle\eta_i(\tau)\rangle=0$, and covariance

$$\langle\eta_i(\tau)\eta_j(\tau')\rangle=K_{ij}^{(2)}\delta(\tau-\tau'), \tag{3}$$

in which $\delta(x)$ is the Dirac $\delta$ function, and

$$K_i^{(1)}(\mathbf{h})=\int r_i W(\mathbf{h};\mathbf{r})d\mathbf{r}, \tag{4}$$

$$K_{ij}^{(2)}(\mathbf{h})=\int r_i r_j W(\mathbf{h};\mathbf{r})d\mathbf{r} \tag{5}$$

are the first and second moments of $W$. There is a direct correspondence between solutions of Eqs. (1) and (2) in the limit $\Omega\to\infty$.[20]

The processes in our model are random deposition and surface diffusion. For random deposition,

$$W_1(\mathbf{h};\mathbf{r})=\tau_0^{-1}\sum_i \delta(r_i-a_\perp)\prod_{k\neq i}\delta(r_k), \tag{6}$$

where $\tau_0^{-1}$ is the average deposition rate per site and $a_\perp$ is the vertical lattice spacing. The transition rate density for nearest-neighbor hopping is

$$W_2(\mathbf{h};\mathbf{r})=\sum_{ij} w_{ij}\delta(r_i+a_\perp)\delta(r_j-a_\perp)\prod_{k\neq i,j}\delta(r_k), \tag{7}$$

where $w_{ij}=\frac{1}{2}\Lambda_i(\delta_{i,j-1}+\delta_{i,j+1})$, $\delta_{i,j}$ is the Kronecker $\delta$, and the local hopping rate $\Lambda_i=\nu_0 e^{-\beta E_i}$, where $\nu_0\sim 10^{13}$ s$^{-1}$, $\beta=1/(k_BT)$, $k_B$ is Boltzmann's constant, $T$ is the absolute temperature, and $E_i$ is the hopping barrier from the $i$th site. The total transition rate density $W=W_1+W_2$, from which we obtain[20]

$$K_i^{(1)}=\frac{1}{2}a_\perp\Delta^2\Lambda_i+\frac{a_\perp}{\tau_0}, \tag{8}$$

$$K_{ij}^{(2)}=\frac{1}{2}a_\perp^2[\delta_{i,j}\Delta^2\Lambda_i-\Lambda_i\Delta^2\delta_{i,j}-\Delta^2(\Lambda_i\delta_{i,j})]+\delta_{i,j}\frac{a_\perp^2}{\tau_0}, \tag{9}$$

in which the second difference $\Delta^2 f_i=f_{i-1}-2f_i+f_{i+1}$ acts only on the index $i$ in Eq. (9).

A basic description of aggregation is obtained by setting[22–25] $E_i=E_S+n_iE_N$, where $E_S$ is the energy barrier from the substrate and $E_N$ the contribution from each of the $n_i$ lateral nearest neighbors. Ratsch *et al.*[4] used a Frenkel-Kontorova model to calculate the effect of strain relaxation at island boundaries on $E_N$. To lowest order, the interplay between strain relaxation and surface morphology is de-

 

scribed by the functional form $E_N=E_N[h_i,(\Delta h_i)^2,\Delta^2 h_i]$, where $(\Delta h_i)^2=\frac{1}{4}(h_{i-1}-h_{i+1})^2$, which accounts for the absolute height, slope, and curvature around the detaching atom. Including higher-order differences of $h_i$ in $E_N$ provides a more accurate description of the height environment, but does not alter the structure of the resulting coarse-grained equation. With this form of $E_N$ we have

$$\Lambda_i = \nu_0 e^{-\beta E_S}(\Theta_{i-1}\Theta_{i+1} + e^{-\beta E_N}\theta_{i-1}\Theta_{i+1} + e^{-\beta E_N}\Theta_{i-1}\theta_{i+1} + e^{-2\beta E_N}\theta_{i-1}\theta_{i+1}), \tag{10}$$

where $\Theta_{i\pm1}=1-\theta_{i\pm1}$, $\theta_{i\pm1}=\theta(h_{i\pm1}-h_i)$, and, for integer height differences $\Delta h=n$,

$$\theta(n) = \begin{cases} 1, & \text{if } n \geqslant 0; \\ 0, & \text{if } n < 0. \end{cases} \tag{11}$$

Equation (10) can be expressed more succinctly as

$$\Lambda_i = a_\perp^{-2} D_S[1-\gamma\theta(\Delta^+ h_i)][1-\gamma\theta(\Delta^- h_i)], \tag{12}$$

with $D_S=a_\perp^2\nu_0 e^{-\beta E_S}$, $\Delta^\pm h_i=h_{i\pm1}-h_i$, $\gamma=1-e^{-\beta E_N}$, and

$$\theta(\Delta h) = \max(a_\perp^{-1}\Delta h+1,0) - \max(a_\perp^{-1}\Delta h,0), \tag{13}$$

which generalizes the hopping rules of our model to continuous heights.[20] Equations (2) and (3), with Eqs. (8), (9), (12), and (13) embody the statistical properties of the original lattice model.[20]

The lattice equations (2) and (3) can be converted into a continuum stochastic equation by first regularizing the step function in Eq. (13). An analytic representation is

$$\theta(\Delta h;\delta) = \frac{1}{2}\int_{-\infty}^{a_\perp^{-1}\Delta h}\{\mathrm{erf}[(s+1)\delta] - \mathrm{erf}(s\delta)\}ds$$

$$= A(\delta) + \frac{B(\delta)}{a_\perp}\Delta h + \frac{C(\delta)}{a_\perp^2}(\Delta h)^2 + \cdots, \tag{14}$$

where $\delta>0$, $\mathrm{erf}(x)$ is the error function, and $A$, $B$, and $C$ are coefficients in the Taylor expansion of $\theta$ around $\Delta h=0$. We have that $\lim_{\delta\to\infty}\theta(\Delta h;\delta)=\theta(\Delta h)$ for all real $\Delta h$. The height function $h_i$ is now replaced by an analytic function $u(x,\tau)$ such that

$$h(i\pm k,\tau) = \sum_{n=0}^{\infty}\left(\frac{\partial^n u}{\partial x^n}\right)\Bigg|_{x=i}\frac{(\pm a_\parallel k)^n}{n!}, \tag{15}$$

where $a_\parallel$ is the lateral lattice spacing, and $\gamma$ is expanded around $[h,(\Delta h)^2,\Delta^2 h]=(0,0,0)$:

$$\gamma[h,(\Delta h)^2,\Delta^2 h] = \sum_{l,m,n=0}^{\infty}\frac{\gamma_{lmn}}{l!m!n!}\left(\frac{h}{a_\perp}\right)^l\left(\frac{\Delta h}{a_\perp}\right)^{2m}\left(\frac{\Delta^2 h}{a_\perp}\right)^n. \tag{16}$$

Substitution of these expansions into Eqs. (8) and (9) yields a convergent series with successively higher spatial derivatives of $u$. The value of $\delta$ in Eq. (14) determines if the regularized equation captures *all* of the properties of the lattice model (large $\delta$) or only *coarse-grained* features (small $\delta$).[26] Here, we choose $\delta\lesssim0.01$ to obtain the leading-order equation

TABLE I. Coefficients in the 1D equation (17). For $\delta\sim0.01$, $A\sim0.5$, $B\sim0.006$, and $C\sim-3\times10^{-7}$.

$$\nu_2 = -\frac{a_\parallel^2}{a_\perp^2}D_S A\gamma_{100}(1-A\gamma_{000})$$

$$\nu_4 = -\frac{a_\parallel^4}{2a_\perp^2}D_S(1-A\gamma_{000})\left(B\gamma_{000}+\frac{1}{6}A\gamma_{100}+2A\gamma_{001}\right)$$

$$\nu_6 = -\frac{a_\parallel^6}{360a_\perp^2}D_S(1-A\gamma_{000})(30B\gamma_{000}+A\gamma_{100}+60A\gamma_{001})$$

$$\lambda_1 = -\frac{a_\parallel^2}{2a_\perp^3}D_S A[\gamma_{200}(1-A\gamma_{000})-A\gamma_{100}^2]$$

$$\lambda_2 = -\frac{a_\parallel^4}{12a_\perp^3}D_S[6B^2\gamma_{000}^2+(12C\gamma_{000}+12A\gamma_{010}+A\gamma_{200})\times(1-A\gamma_{000})-A^2\gamma_{100}^2]$$

$$\lambda_3 = -\frac{a_\parallel^4}{12a_\perp^3}D_S[6B\gamma_{100}(1-2A\gamma_{000})+(12A\gamma_{101}+A\gamma_{200})\times(1-A\gamma_{000})-A^2\gamma_{100}(12\gamma_{001}+\gamma_{100})]$$

$$D_2 = \frac{a_\parallel^3}{2}D_S(1-A\gamma_{000})\left(1-A\gamma_{000}-\frac{2}{a_\perp}A\gamma_{100}u\right)$$

$$\frac{\partial u}{\partial\tau} = \nu_2\frac{\partial^2 u}{\partial x^2} + \nu_4\frac{\partial^4 u}{\partial x^4} + \nu_6\frac{\partial^6 u}{\partial x^6} + \frac{\partial^2}{\partial x^2}\left[\lambda_1 u^2 + \lambda_2\left(\frac{\partial u}{\partial x}\right)^2 + \lambda_3 u\frac{\partial^2 u}{\partial x^2}\right] + F + \xi, \tag{17}$$

where $F=a_\perp/\tau_0$ is the average deposition rate and the smoothed Gaussian noise $\xi$ has zero mean and covariance

$$\langle\xi(x,\tau)\xi(x',\tau')\rangle = 2\left(D_0 - \frac{\partial}{\partial x}D_2\frac{\partial}{\partial x}\right)\delta(x-x')\delta(\tau-\tau'), \tag{18}$$

where $D_0=a_\parallel a_\perp^2/(2\tau_0)$ is due to deposition and the remaining coefficients are compiled in Table I. The deterministic part of Eq. (17) has the same form as that derived by Golovin *et al.*[17] from continuum elasticity for a rigid substrate. The description of detachment kinetics solely in terms of short-range absolute height environments is also valid only where deformation of the substrate is neglected, as was indeed the case in Ref. 4. Morphological evolution on a deformable substrate produces nonlocal terms,[16,18] which reflect elastic interactions mediated by the substrate.

The atomistic ancestry of the coefficients in Eq. (17) allows us to relate this equation to specific materials and

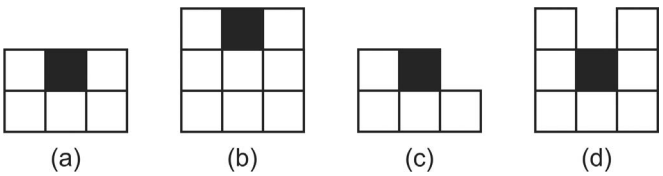


FIG. 1. For the indicated local configurations of the shaded particle, $E_N^{(a)}<E_N^{(b,c)}$ and $E_N^{(a)}>E_N^{(d)}$ for $E_N^{(1,0,0)}(0,0,0)>0$ and $E_N^{(0,0,1)}(0,0,0)<0$.

TABLE II. Coefficients in the 2D equation (19). The values of $A$, $B$, and $C$ are as in Table I.

$$\nu_2 = -\frac{a_\parallel^2}{a_\perp^2} D_S A \gamma_{100}(1-A\gamma_{000})^3$$

$$\nu_4 = -\frac{a_\parallel^4}{12a_\perp^2} D_S(1-A\gamma_{000})^3(3B\gamma_{000}+A\gamma_{100}+12A\gamma_{001})$$

$$\nu_4' = -\frac{a_\parallel^4}{2a_\perp^2} D_S(1-A\gamma_{000})^3(B\gamma_{000}+4A\gamma_{001})$$

$$\nu_6 = -\frac{a_\parallel^6}{360a_\perp^2} D_S(1-A\gamma_{000})^3(15B\gamma_{000}+A\gamma_{100}+60A\gamma_{001})$$

$$\nu_6' = -\frac{a_\parallel^6}{24a_\perp^2} D_S(1-A\gamma_{000})^3(B\gamma_{000}+4A\gamma_{001})$$

$$\lambda_1 = -\frac{a_\parallel^2}{2a_\perp^3} D_S A(1-A\gamma_{000})^2[\gamma_{200}(1-A\gamma_{000})-3A\gamma_{100}^2]$$

$$\lambda_2 = -\frac{a_\parallel^4}{12a_\perp^3} D_S(1-A\gamma_{000})^2[3B^2\gamma_{000}^2+(6C\gamma_{000}+12A\gamma_{010}+A\gamma_{200})(1-A\gamma_{000})-3A^2\gamma_{100}^2]$$

$$\lambda_2' = -\frac{a_\parallel^4}{8a_\perp^3} D_S(1-A\gamma_{000})^2[2B^2\gamma_{000}^2+(4C\gamma_{000}+8A\gamma_{010})(1-A\gamma_{000})]$$

$$\lambda_3 = -\frac{a_\parallel^4}{12a_\perp^3} D_S(1-A\gamma_{000})^2[3B\gamma_{100}(1-4A\gamma_{000})+(12A\gamma_{101}+A\gamma_{200})(1-A\gamma_{000})-3A^2\gamma_{100}(\gamma_{100}+12\gamma_{001})]$$

$$\lambda_3' = -\frac{a_\parallel^4}{4a_\perp^3} D_S(1-A\gamma_{000})^2[B\gamma_{100}(1-4A\gamma_{000})+4A\gamma_{101}(1-A\gamma_{000})-12A^2\gamma_{100}\gamma_{001}]$$

$$D_0 = \frac{a_\parallel^2 a_\perp^2}{2\tau_0}$$

$$D_2 = \frac{a_\parallel^4}{4} D_S(1-A\gamma_{000})^3\left(1-A\gamma_{000}-\frac{4}{a_\perp}A\gamma_{100}u\right)$$

growth scenarios. For $T>0$, we have $0<\gamma_{000}<1$ and, hence, the sign of $\nu_2$ is determined by the sign of $\gamma_{100}=[\beta E_N^{(1,0,0)}e^{-\beta E_N}]|_{(0,0,0)}$. The key quantity is $E_N^{(1,0,0)}(0,0,0)$, which is the rate of change of $E_N$ with the film height. Golovin *et al.*[17] considered situations where $\nu_2>0$, which corresponds to $E_N^{(1,0,0)}(0,0,0)<0$. Alternatively, the calculations in Ref. 4 suggest $E_N^{(1,0,0)}(0,0,0)>0$, i.e., $\nu_2<0$. The growth of 3D islands then results from the decreasing detachment rate with increasing height, as shown in Figs. 1(a) and 1(b). We focus on this case below.

The sign of $\nu_4$ is determined by the sign of $B\gamma_{000}+\frac{1}{6}A\gamma_{100}+2A\gamma_{001}$. Choosing[4] $E_N(0,0,0)=0.3$ eV, $E_N^{(1,0,0)}(0,0,0)\sim 0.01-0.05$ eV, and $T\lesssim 900$ K, the above quantity is positive for $E_N^{(0,0,1)}(0,0,0)\gtrsim -0.03$ eV, in which case $\nu_4<0$ and the sixth-order term in Eq. (17) can be omitted.[27] A negative $E_N^{(0,0,1)}(0,0,0)$ implies that strain is relieved more effectively by islands with larger numbers of lateral edge atoms[4] [Fig. 1(c)], but local depressions are suppressed [Fig. 1(d)]. For $E_N^{(0,0,1)}(0,0,0)\lesssim -0.03$ eV, we find $\nu_4>0$, which necessitates the inclusion of the sixth-order derivative, for which $\nu_6>0$, for stability.

Our procedure can be applied to obtain the equation for morphological evolution during heteroepitaxial growth on a two-dimensional (2D) substrate, with the result

$$\begin{aligned}\partial_\tau u = {} & \nu_2(\partial_x^2 u+\partial_y^2 u)+\nu_4(\partial_x^4 u+\partial_y^4 u)+\nu_4'\partial_x^2\partial_y^2 u+\nu_6(\partial_x^6 u+\partial_y^6 u)\\ & +\nu_6'(\partial_x^4\partial_y^2 u+\partial_x^2\partial_y^4 u)+\partial_x^2(\lambda_1 u^2+\lambda_2 u_x^2+\lambda_2' u_y^2+\lambda_3 u u_{xx}\\ & +\lambda_3' u u_{yy})+\partial_y^2(\lambda_1 u^2+\lambda_2 u_y^2+\lambda_2' u_x^2+\lambda_3 u u_{yy}+\lambda_3' u u_{xx})\\ & +F+\xi, \end{aligned} \tag{19}$$

where $\partial_x \equiv \partial u/\partial x \equiv u_x$, with a similar notation for other derivatives, $F=a_\perp/\tau_0$, and the smoothed Gaussian noise $\xi(x,y,\tau)$ has zero mean and covariance analogous to Eq. (18). This equation contains the same types of terms as Eq. (17), but in a form that respects the fourfold symmetry of the lattice. The coefficients are compiled in Table II. As for a 1D substrate, $\nu_2<0$ if $E_N^{(1,0,0)}(0,0,0)>0$. For $E_N^{(0,0,1)}(0,0,0)\gtrsim -0.02$ eV the linearized 2D equation is stabilized by negative $\nu_4$ and $\nu_4'$, and the sixth-order terms can be omitted.[27] But, for $E_N^{(0,0,1)}(0,0,0)\lesssim -0.02$ eV, $\nu_6$ and $\nu_6'$ must be included for stability.

In Fig. 2 we show morphologies and associated two-point correlation functions,

$$G(\mathbf{x},\tau)=\left\{\frac{1}{Na_\parallel^2}\int [u(\mathbf{x}+\mathbf{x}',\tau)-u(\mathbf{x}',\tau)]^2 d\mathbf{x}'\right\}^{1/2}, \tag{20}$$

where $\mathbf{x}=(x,y)$ and $Na_\parallel^2$ is the area of an $La_\parallel\times La_\parallel$ lattice, at 0.5 monolayers (ML) during growth at 0.1 ML/s obtained by integrating the linearized 2D equation (19) with periodic boundary conditions and only deposition noise. We use parameters consistent with the simulations in Ref. 4, which leads to a fourth-order equation. At $T=650$ K [Figs. 2(a) and 2(c)], there is scant evidence of structure. But the morphology at $T=750$ K [Figs. 2(b) and 2(d)], which corresponds to the simulated temperature in Ref. 4, clearly shows the development of locally ordered (i.e., self-organized) 3D islands. The most striking aspect of Fig. 2(b) is its similarity to the KMC simulations in Fig. 3 of Ref. 4 in terms of the size of the 3D islands, their density, and the time scale of their formation.

The trends in Fig. 2 can be further extended by solving, at least formally, the linearized versions of Eqs. (17) and (19) using Fourier transforms. Introducing the spatial transform

$$u(\mathbf{x},\tau)=\int \frac{d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{k}\cdot\mathbf{x}} u(\mathbf{k},\tau), \tag{21}$$

with an analogous expression for $\xi(\mathbf{k},\tau)$, and neglecting the difference between $\nu_4$ and $\nu_4'$, the solution to the linearized fourth-order equation with $u(\mathbf{k},0)=0$ can be written as

$$u(\mathbf{k},\tau) = \int_0^\tau [e^{(|\nu_2|k^2 - |\nu_4|k^4)(\tau - s)} \xi(\mathbf{k},s)] ds, \tag{22}$$

where the Gaussian noise $\xi$ has zero mean and covariance

$$\langle \xi(\mathbf{k},\tau)\xi(\mathbf{k}',\tau')\rangle = 2(2\pi)^d (D_0 + D_2 k^2)\delta(\mathbf{k}+\mathbf{k}')\delta(\tau - \tau'), \tag{23}$$

in which $D_2$ is taken to be a constant and $d$ is the substrate dimension. For $k > (D_0/D_2)^{1/2} \equiv k_D$ diffusion noise dominates over deposition noise. On the other hand, the deterministic terms in Eq. (22) imply a critical wave number $k_c = (\nu_2/\nu_4)^{1/2}$, below which all modes are unstable. Thus, if $k_c > k_D$, fluctuations due to deposition *and* diffusion "feed into" unstable modes, so the self-organization process is enhanced by diffusion noise. For the coefficients in Table II, diffusion fluctuations excite only a relatively narrow band of unstable modes at $T=650$ K, but at $T=750$ K this effect is dominant for $L \lesssim 200 a_\parallel$. However, since $E_N$ increases with height, $D_2$ decreases accordingly, so $k_D$ increases with height. Thus, for large enough terrace heights, diffusion noise only minimally perturbs the unstable modes, even for $T=750$ K, which supports the stabilization of island heights.

In summary, we have derived a stochastic differential equation for the morphological evolution of strained heteroepitaxial films from an atomistic model. The deterministic terms are the same as those obtained by Golovin *et al.*[17] from continuum elasticity. Two crucial differences from this earlier work are the presence of noise due to deposition and diffusion and the relation of the coefficients to the original atomistic processes. Since the parametrization of such atomistic processes is becoming available through density functional calculations,[28–30] our methodology offers the promise of a genuine multiscale atoms-to-continuum description of the morphological evolution of heteroepitaxial thin films.

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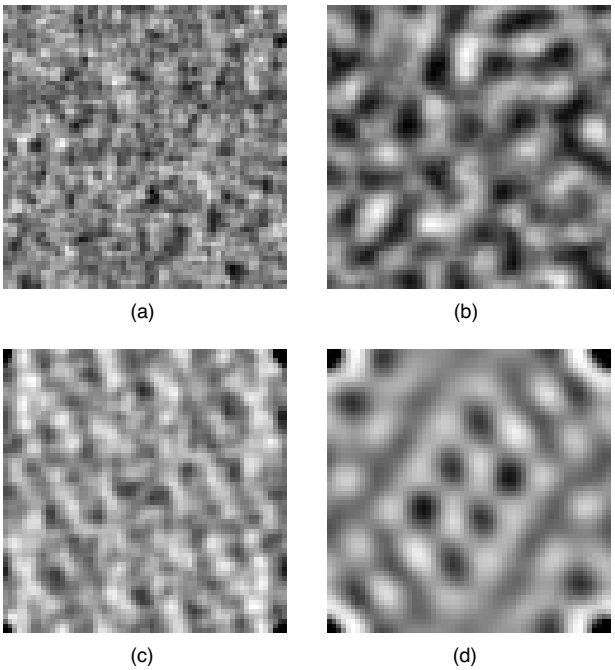


FIG. 2. Heights $u$ (a),(b) and two-point correlation functions $G$ (c),(d) obtained from the linearized fourth-order equation (19) at 0.5 ML for a system of size $60a_\parallel \times 60a_\parallel$ at $T=650$ K (a),(c) and $T=750$ K (b),(d) with $E_S=1.3$ eV, $E_N(0,0,0)=0.3$ eV, $E_N^{(1,0,0)}(0,0,0)=0.01$ eV, and $E_N^{(0,0,1)}(0,0,0)=-0.004$ eV. The ranges of $u$ and $G$, in units of $a_\perp$, are (a) $-0.6 \leqslant u \leqslant 1.5$, (b) $-0.3 \leqslant u \leqslant 1.5$, (c) $0 \leqslant G \leqslant 0.4$, and (d) $0 \leqslant G \leqslant 0.5$.

[1] A. Kobayashi and S. Das Sarma, Phys. Rev. B **37**, 1039 (1988).
[2] D. A. Faux *et al.*, Phys. Rev. B **42**, 2914 (1990).
[3] B. G. Orr *et al.*, Europhys. Lett. **19**, 33 (1992).
[4] C. Ratsch *et al.*, J. Phys. I **6**, 575 (1996).
[5] K. E. Khor and S. Das Sarma, Phys. Rev. B **62**, 16657 (2000).
[6] P.-M. Lam and S. Tan, Phys. Rev. B **64**, 035321 (2001).
[7] F. Much and M. Biehl, Europhys. Lett. **63**, 14 (2003).
[8] M. Meixner *et al.*, Phys. Rev. B **67**, 195301 (2003).
[9] M. T. Lung *et al.*, Phys. Rev. Lett. **95**, 086102 (2005).
[10] G. Russo and P. Smereka, J. Comput. Phys. **214**, 809 (2006).
[11] P. A. Taylor and B. W. Dodson, Phys. Rev. B **36**, 1355 (1987).
[12] W. Yu and A. Madhukar, Phys. Rev. Lett. **79**, 905 (1997).
[13] G. Capellini *et al.*, Phys. Rev. Lett. **96**, 106102 (2006).
[14] B. J. Spencer *et al.*, J. Appl. Phys. **73**, 4955 (1993).
[15] B. J. Spencer *et al.*, Phys. Rev. B **47**, 9760 (1993).
[16] Y. Xiang and W. E, J. Appl. Phys. **91**, 9414 (2002).
[17] A. A. Golovin *et al.*, Phys. Rev. E **68**, 056203 (2003).
[18] W. T. Tekalign and B. J. Spencer, J. Appl. Phys. **96**, 5505 (2004).
[19] H. M. Koduvely and A. Zangwill, Phys. Rev. B **60**, R2204 (1999).
[20] A. L.-S. Chua *et al.*, Phys. Rev. E **72**, 051103 (2005).
[21] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).
[22] M. C. Bartelt and J. W. Evans, Phys. Rev. B **46**, 12675 (1992).
[23] T. Shitara *et al.*, Phys. Rev. B **46**, 6815 (1992).
[24] J. G. Amar and F. Family, Phys. Rev. Lett. **74**, 2066 (1995).
[25] C. Ratsch *et al.*, Surf. Sci. **329**, L599 (1995).
[26] C. A. Haselwandter and D. D. Vvedensky (unpublished).
[27] In this case $\nu_6 < 0$, but overall stability of the equation is ensured by an eighth-order term. The dependence of these quantities on $\delta$ will be discussed in a future publication.
[28] E. Penev *et al.* Phys. Rev. B **64**, 085401 (2001).
[29] A. van de Walle *et al.*, Phys. Rev. B **67**, 041308(R) (2003).
[30] L. Huang *et al.*, Phys. Rev. B **70**, 155320 (2004).