

# Continuum model of surface roughening and epitaxial breakdown during low-temperature Ge(001) molecular beam epitaxy

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Numerical simulations based on a discrete model describing step edge motion are used to compute the surface morphological evolution of Ge(001) layers deposited by low-temperature ( $T_s = 45\text{--}230\text{ }^\circ\text{C}$ ) molecular beam epitaxy and to probe the relationship between surface roughening and the onset of epitaxial breakdown—the abrupt growth mode transition from epitaxial to amorphous—at temperature-dependent critical film thicknesses  $h_l(T_s)$ . Computed surface widths  $w$  and in-plane coherence lengths  $d$  as a function of layer thickness  $h$  exhibit good agreement with experimental values. Inspired by experimental results indicating that epitaxial breakdown is initiated at faceted interisland trenches as the surface roughness reaches a  $T_s$ -independent overall aspect ratio, we show that simulated data for  $w/d = 0.03$  correspond to thicknesses  $h_l \propto \exp(-E_l/kT_s)$  with  $E_l = 0.63\text{ eV}$ , a value equal to the Ge adatom diffusion activation energy on Ge(001). Simulated  $h_l$  values agree well with experimental data. Above a critical growth temperature of  $170\text{ }^\circ\text{C}$ , computed  $w/d$  values saturate at large film thicknesses, never reaching the critical aspect ratio  $w/d = 0.03$ . Thus, the model also predicts that epitaxial breakdown does not occur for  $T_s > 170\text{ }^\circ\text{C}$  as observed experimentally.

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## I. INTRODUCTION

The growth front during low-temperature (LT) homoepitaxy of group-IV (Refs. 1–10) and III-V (Refs. 3 and 11) semiconductors exhibits an abrupt structural breakdown once a critical film thickness is reached. This also occurs during LT heteroepitaxial growth, but the kinetics can be strongly mediated by strain.<sup>12–17</sup>

We have shown previously, using LT molecular beam epitaxy (MBE) of Ge/Ge(001), that epitaxial breakdown is a growth mode transition driven by kinetic surface roughening.<sup>10</sup> Ge(001) homoepitaxy in the low adatom mobility two-dimensional multilayer growth mode leads to the formation of a periodic array of self-organized mound structures preferentially bounded along  $\langle 100 \rangle$  directions.<sup>6,9,10</sup> Surface widths  $w$  and in-plane coherence lengths  $d$  increase monotonically with film thickness  $h$ . Ge(001) layers grown at temperatures  $T_s$  greater than a critical value  $T_c$  remain fully epitaxial, while deposition at  $T_s < T_c$  leads to a locally abrupt transition from epitaxial to amorphous growth.<sup>10</sup> This transition is initiated at a temperature-dependent critical thickness  $h_l(T_s)$  as the surface roughness reaches a critical aspect ratio  $w/d$  which is independent of  $T_s$ .<sup>10</sup>  $h_l(T_s)$  follows the relationship  $h_l \propto \exp(-E_l/kT_s)$ , where  $E_l = 0.63\text{ eV}$ .

An atomistic description of epitaxial breakdown during LT growth, based upon a combination of plan-view transmission electron microscopy (TEM), cross-sectional TEM (XTEM), and atomic force microscopy results, was proposed in Ref. 10 and is summarized here. During the early stages

of deposition, the surface remains smooth, with a roughness comparable to that of the substrate. However, low adatom mobilities combined with an attachment asymmetry due to the presence of a positive Ehrlich barrier<sup>18–22</sup> at down-steps, and/or preferential attachment at up-steps, soon lead to a divergence in adatom flux and, hence, increased nucleation on terraces. As growth continues and the multilevel islands coalesce, trenches are formed which become deeper and wider, i.e., the amplitude of the roughness increases, as deposition proceeds. Incomplete filling of terraces results in the development of deep cusps bounded by  $\{111\}$  facets, where  $l = 7, 5, 3$ , which eventually transform to low-energy  $\{111\}$  surfaces. Atomic shadowing in the cusps results in incomplete island coalescence and the subsequent formation of intercolumnar voids.

The transition from epitaxial to amorphous growth is initiated on  $\{111\}$  faceted cusps, where 111 stacking faults form due to double-positioning defects. The stacking faults quickly progress vertically and laterally along  $\{111\}$  facet planes. The initial transformation from crystalline to amorphous occurs in the cusps, with the regions between adjacent valleys still epitaxial. The growth mode transition is completed as 111 stacking faults at cusps on opposite corners or sides of individual islands intersect, resulting in a continuous epitaxial/amorphous interface which is globally rough but locally abrupt, as observed in XTEM images. In this description of LT epitaxial breakdown, the essential parameters, at a given  $T_s$ , are the adatom surface diffusion barrier  $E_m$ , the Ehrlich step-edge barrier  $E_b$ , and the vapor flux  $F$ .

Here, we use Villain's model of surface instabilities<sup>23,24</sup> to quantitatively describe the evolution of Ge(001) surface

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roughness  $w$  as a function of film thickness  $h$  and growth temperature  $T_s$  in order to probe the relationship between surface roughening and epitaxial breakdown and test the above picture of surface morphological evolution. Our simulation results accurately reproduce experimental observations.

## II. MODEL

Surface roughening is modeled following the approach of Elkinani and Villain<sup>23–26</sup> who derived continuum equations for the motion of step edges. The model involves two characteristic length scales: the nucleation length  $l_c$  and the Ehrlich length  $l_E$ .<sup>23,24</sup>  $l_c$  is the terrace width required to nucleate a new island, whereas  $l_E$  is defined such that if the terrace width  $l$  is smaller than  $l_E$ , atoms landing on this terrace migrate to, and are incorporated at, an up-step; however, if  $l \gg l_E$ , approximately half of the atoms that land on the terrace will migrate to the up step and half to the down step.

A schematic illustration of a typical growing (1+1)-dimensional crystal is presented in Fig. 1. The local step velocity is expressed as

$$v_n = f(l_n) + f(l_{n+1}), \quad (1)$$

where  $l_n$  and  $l_{n+1}$  are the widths of the terraces above and below the step edge, respectively.<sup>25</sup> For vicinal terraces,

$$f(l_n) = \frac{bFl_n}{2} \left( 1 - \frac{l_E}{l_n + l_E} \right) \quad (2)$$

and

$$f(l_{n+1}) = \frac{bFl_{n+1}}{2} \left( 1 + \frac{l_E}{l_{n+1} + l_E} \right). \quad (3)$$

When a terrace adjacent to the step edge is an island peak or valley, i.e. the local top (maximum) or bottom (minimum) terrace, the functions  $f(l_{n,n+1})$  are defined as

$$f(l_{n,n+1}) = \frac{bFl_{n,n+1}}{2}. \quad (4)$$

New islands are created on terraces of width  $l_{n,n+1}$  with a probability  $P_{\text{nuc}}(l_{n,n+1})$  per unit time

$$P_{\text{nuc}}(l_{n,n+1}) = \frac{F^2 l_{n,n+1}^4}{12D} \left( 1 + \frac{6l_E}{l_{n,n+1}} \right). \quad (5)$$

$P_{\text{nuc}}$  becomes unity when  $l_{n,n+1}$  becomes of order  $l_c$ . Adjacent step edges are limited to approaching within  $b/2$  of each other [2.0 Å for the Ge(001) surface] although, in reality, the actual value chosen for the minimum step edge separation is irrelevant since  $l_c$  and  $l_E$  can be rescaled to modify the step spacing.

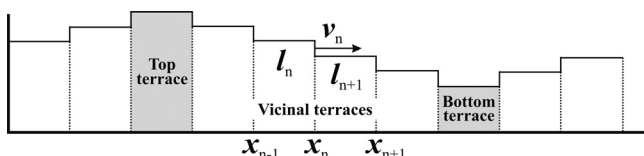


FIG. 1. Schematic surface profile during crystal growth.

Simulation input parameters include  $l_E$ ,  $l_c$ , and the number of monolayers deposited. The output is an array showing the position and height of individual step edges for each simulated film thickness. Surface roughness as a function of film thickness is quantified using the height-height correlation function  $H(\rho) = \langle h_i h_j \rangle$  and the height-difference correlation function  $G(\rho) = \langle |h_i - h_j|^2 \rangle$ , where  $h_{i,j}$  are the heights at positions  $i$  and  $j$  separated by a distance  $\rho$  and the brackets correspond to averages over the measured surface. The mean interisland separation  $d$  is extracted from the position of the first local maximum in  $H(\rho)$ . The correlation functions are related to the surface width  $w$ , which is equivalent to the root mean square roughness, through the relationship  $2w^2 = G(\rho) + 2H(\rho)$ .

We determine the numerical values for the nucleation and Ehrlich lengths  $l_c$  and  $l_E$  for homoepitaxial Ge(001) growth by LT-MBE as a function of  $T_s$  based upon analyses of published *in situ* scanning tunneling microscopy (STM) data obtained during the early stages of surface roughening, well before the onset of epitaxial breakdown.<sup>6,9</sup> The simulated samples were of length  $100l_c^2/l_E$  in order to maintain an equal number of islands at each temperature. The starting surface consists of terraces of length  $l_0 = 810$  Å, which is equivalent to the average terrace length on the  $\pm 0.1^\circ$  miscut Ge(001) substrates used in Refs. 6, 9, and 10.

Figure 2 is a plot of  $l_c$  and  $l_E$  values for LT-MBE Ge(001) as a function of  $T_s$ .<sup>6,9,27</sup>  $l_c$  and  $l_E$  were extracted from STM data at  $T_s = 60, 100, 155, 175,$  and  $230$  °C using the relationships  $l_c = n^{1/2}$  and  $l_E = (dw/dh)^{1/2} l_c$  where  $n$  is the island density at a coverage of 0.3 ML and  $dw/dh$  is the roughening rate. As  $T_s$  is increased from 60 to 230 °C,  $l_c$  increases from 20 to 100 Å while corresponding  $l_E$  values remain nearly constant (approximately equal to the surface lattice spacing), decreasing slightly from 4.5 to 3.9 Å. The best fit to  $l_c$  vs  $T_s$  is shown by the dashed line which corresponds to

$$l_c = \left( \frac{20b^2D}{F} \right)^{1/6}, \quad (6)$$

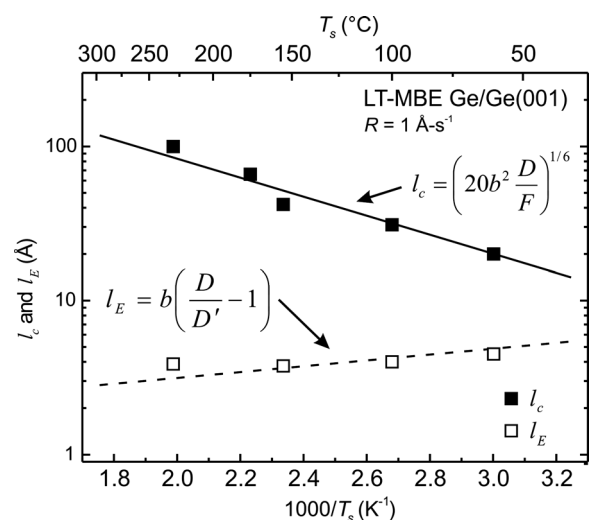


FIG. 2. Nucleation  $l_c$  and Ehrlich lengths  $l_E$  based upon STM data obtained during LT-MBE Ge(001) homoepitaxy over the temperature range  $T_s = 60$ – $230$  °C with  $R = 1$  Å s<sup>−1</sup> (data from Refs. 9 and 27).

in which  $b = 4.0 \text{ \AA}$  is the separation between individual dimers along  $\langle 110 \rangle$ ,  $F$  is the incident Ge flux in  $\text{ML s}^{-1}$ ,  $D = (b^2 v/4) \exp(-E_m/kT_s)$  is the surface diffusion constant,  $E_m = 0.65 \text{ eV}$  (Ref. 9) is the activation energy for diffusion, and  $v = 8.27 \times 10^{12} \text{ s}^{-1}$  is the Ge Debye frequency.<sup>28</sup> Values for the dimer separation  $b$  and diffusion barrier  $E_m$  correspond to the direction parallel to the underlying dimer rows on the Ge(001) $2 \times 1$  reconstructed surface. For simplicity, the incident flux is set at  $F = 1 \text{ ML s}^{-1}$  yielding a deposition rate of  $R = 1.4 \text{ \AA s}^{-1}$ . A fit to  $l_E$  is obtained using the expression

$$l_E = b \left( \frac{D}{D'} - 1 \right). \quad (7)$$

$D/D' = \exp(\Delta E_d/kT_s)$  with  $\Delta E_d = 0.024 \text{ eV}$  the asymmetry in attachment activation energies at ascending and descending steps.  $D'/b^2 = (v/4) \exp(-E_b/kT)$  is the adatom hopping rate over down steps.

### III. RESULTS AND DISCUSSION

Typical simulated surface profiles obtained from layers deposited at  $T_s = 155 \text{ }^\circ\text{C}$  to thicknesses  $h = 15, 500, 2000, 4000,$  and  $8100 \text{ \AA}$  are shown in Figs. 3(a)–3(e). The results show that the surface begins to roughen essentially immediately upon initiation of film growth. For small  $h$  values ( $\leq 500 \text{ \AA}$  at  $155 \text{ }^\circ\text{C}$ ), a high density of compact islands is obtained initially [e.g., Fig. 3(a) with  $h = 15 \text{ \AA}$ ]. The mounds broaden, become better defined, and are separated by deep trenches as  $h$  is increased to  $500$  and  $2000 \text{ \AA}$  [see Figs. 3(b) and 3(c)]. Continued island coalescence with increasing  $h$  results in a

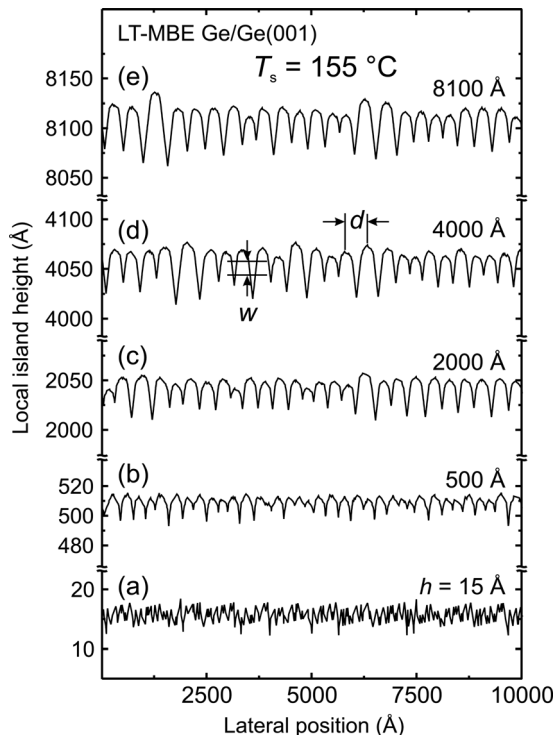


FIG. 3. Calculated surface height profiles for LT-MBE Ge/Ge(001) layers grown at  $T_s = 155 \text{ }^\circ\text{C}$  to thicknesses  $h$  of (a) 15, (b) 500, (c) 2000, (d) 4000, and (e) 8100  $\text{\AA}$ .

persistent increase in the mean interisland separation and a corresponding decrease in the island density. While  $w(h)$  and  $d(h)$  initially increase rapidly, they begin to saturate at  $h > 2000 \text{ \AA}$  [compare, for example, Fig. 3(d),  $h = 4000 \text{ \AA}$  with Fig. 3(e),  $h = 8000 \text{ \AA}$ ]. Simulation results in Fig. 3 correlate well with experimental observations of Ge(001) surface roughening at  $T_s = 155 \text{ }^\circ\text{C}$  shown in Fig. 4 of Ref. 10. The same general trends are observed at all  $T_s$  values, but roughening and island coarsening rates increase with increasing  $T_s$ .

Figure 4 contains plots of calculated  $w$  and  $d$  values, together with the aspect ratio  $w/d$ , as a function of  $h$  and  $T_s$ . For clarity, only a representative sample of all simulated values is provided in Fig. 4. With  $T_s \leq 100 \text{ }^\circ\text{C}$  and  $h \leq 1600 \text{ \AA}$ ,  $w$  and  $d$  both increase monotonically with  $h$ .  $w$  increases from  $1.4 \text{ \AA}$  at  $h = 10 \text{ \AA}$  to  $2.5 \text{ \AA}$  at  $h = 60 \text{ \AA}$  with  $T_s = 45 \text{ }^\circ\text{C}$  and from  $1.3 \text{ \AA}$  at  $h = 17$  to  $7 \text{ \AA}$  at  $h = 1600 \text{ \AA}$  for  $T_s = 85 \text{ }^\circ\text{C}$  as  $d$  increases from  $50$  to  $70 \text{ \AA}$  and from  $85$  to  $185 \text{ \AA}$  over the same film thickness and temperature ranges.  $w$  and  $d$  follow scaling relationships  $w \propto h^\beta$  and  $d \propto h^n$  with roughening and coarsening exponents in this growth temperature range of  $\beta \cong 0.4$  and  $n \cong 0.2$ . Thus, the mound roughening rate is larger than the coarsening rate. This leads, as shown in Fig. 4(c), to a slow increase in the aspect ratio  $w/d$  from  $0.028$  at  $h = 10 \text{ \AA}$  to  $0.036$  at  $h = 60 \text{ \AA}$  for  $T_s = 45 \text{ }^\circ\text{C}$  and

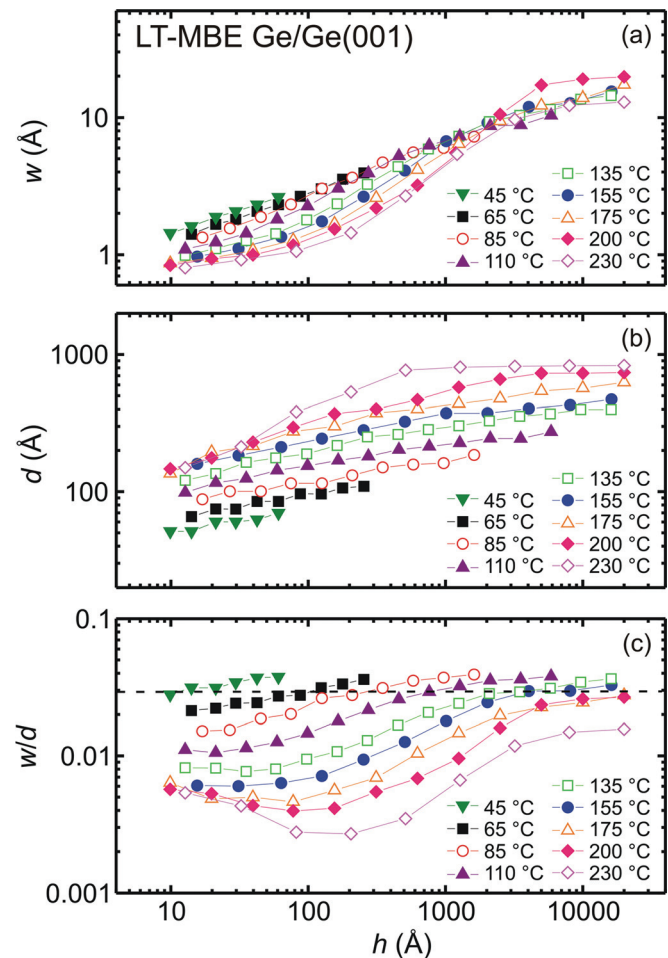


FIG. 4. (Color online) Calculated (a) surface widths  $w$ , (b) in-plane coherence lengths  $d$ , and (c) aspect ratios  $w/d$  as a function of film thickness  $h$  during Ge/Ge(001) LT-MBE at temperatures  $T_s = 45\text{--}230 \text{ }^\circ\text{C}$ .



from 0.015 at  $h = 17 \text{ \AA}$  to 0.038 at  $h = 1600 \text{ \AA}$  with  $T_s = 85 \text{ }^\circ\text{C}$ . The STM results of Van Nostrand and co-workers<sup>6,9</sup> for LT-MBE Ge(001) show that, with  $T_s = 60\text{--}100 \text{ }^\circ\text{C}$ , the experimentally determined roughening and coarsening exponents remain approximately constant at  $\beta \cong 0.45$  and  $n \cong 0.20$ , respectively, in agreement with our simulated values over the same temperature ranges.

At higher growth temperatures ( $T_s = 110\text{--}230 \text{ }^\circ\text{C}$ ), the simulated surfaces are initially flat with  $w$  of the order of  $0.8\text{--}1.0 \text{ \AA}$  for the first few ML; then  $w$  increases linearly with  $h$  at a  $T_s$ -dependent rate. For layer thicknesses exceeding  $3000 \text{ \AA}$ ,  $w$  begins to saturate at  $h$  values of  $10\text{--}20 \text{ \AA}$  with the saturation value being a function of temperature.  $d(h)$  increases continuously with  $h$ , but otherwise follows the general behavior observed for  $w(h)$ . The saturation value of  $d$  increases with  $T_s$  from  $400 \text{ \AA}$  at  $T_s = 135 \text{ }^\circ\text{C}$  to  $850 \text{ \AA}$  at  $230 \text{ }^\circ\text{C}$ , while the film thickness at which saturation begins to occur decreases from approximately  $1 \text{ }\mu\text{m}$  at  $T_s = 135 \text{ }^\circ\text{C}$  to  $500 \text{ \AA}$  at  $230 \text{ }^\circ\text{C}$ . The simulated roughening and coarsening exponents, as measured over the linear portion of the curves, increase from  $\beta \cong 0.5$  and  $n \cong 0.2$  at  $T_s = 110 \text{ }^\circ\text{C}$  to  $0.7$  and  $0.3$  at  $230 \text{ }^\circ\text{C}$ . Experimentally,  $\beta$  and  $n$  increase continuously from  $0.45$  and  $0.20$ , respectively, at  $T_s = 100 \text{ }^\circ\text{C}$  to  $0.70$  and  $0.35$  at  $T_s = 230 \text{ }^\circ\text{C}$ .<sup>6,9,10</sup>

A comparison of experimental and simulation results reveals that they exhibit good quantitative agreement. Figure 4(c) shows that over the temperature range  $110\text{--}230 \text{ }^\circ\text{C}$ , the aspect ratio  $w/d$  is  $0.006\text{--}0.010$  initially and then begins to decrease as the island coarsening rate exceeds the roughening rate, allowing the surface to smoothen. With further increase in  $h$ , the calculated profiles now begin to roughen as the mounds grow faster vertically than laterally. Eventually, at large film thicknesses ( $h > 3000 \text{ \AA}$ ),  $w/d$  saturates at values ranging from  $0.040$  at  $T_s = 110 \text{ }^\circ\text{C}$  to  $0.015$  at  $230 \text{ }^\circ\text{C}$ .

We have previously demonstrated that epitaxial breakdown during Ge(001) LT-MBE is initiated at a film thickness  $h = h_I(T_s)$  when the surface roughness reaches a critical  $T_s$ -independent aspect ratio.<sup>10</sup> These experimental results are captured in our simulation by defining  $h_I$  as the film thickness at which the mound aspect ratio reaches a critical value  $w/d = 0.03$ .  $h_I(w/d = 0.03)$  for each  $T_s$  in Fig. 4(c) is summarized in Fig. 5 as a phase map plotted as  $h_I$  vs  $T_s$  ( $45\text{--}230 \text{ }^\circ\text{C}$ ). The total set of simulation results is remarkably self-consistent over the entire temperature range and agree extremely well with  $h_I$  values determined experimentally by both XTEM and reflection high-energy electron diffraction (experimental results also plotted in Fig. 5).  $h_I$  increases exponentially with  $T_s$  and is well fit by the expression  $h_I \propto \exp(-E_I/kT_s)$  with  $E_I = 0.63 \pm 0.05 \text{ eV}$ .<sup>4,10</sup> The energy  $E_I$  is equal to the measured activation barrier for Ge adatom diffusion on Ge(001).<sup>9</sup>

Since the thickness at which epitaxial breakdown is initiated can be modeled by defining  $h_I(T_s)$  as the point at which the surface roughness reaches a critical aspect ratio, irrespective of  $T_s$ , there must be a direct relationship between the critical layer thicknesses plotted in Fig. 5 and adatom surface diffusivity. We have previously shown<sup>10</sup> that epitaxial breakdown is initiated when  $x > L$ , where  $x$  and  $L$  are the island peak-to-valley distance and adatom mean diffusion

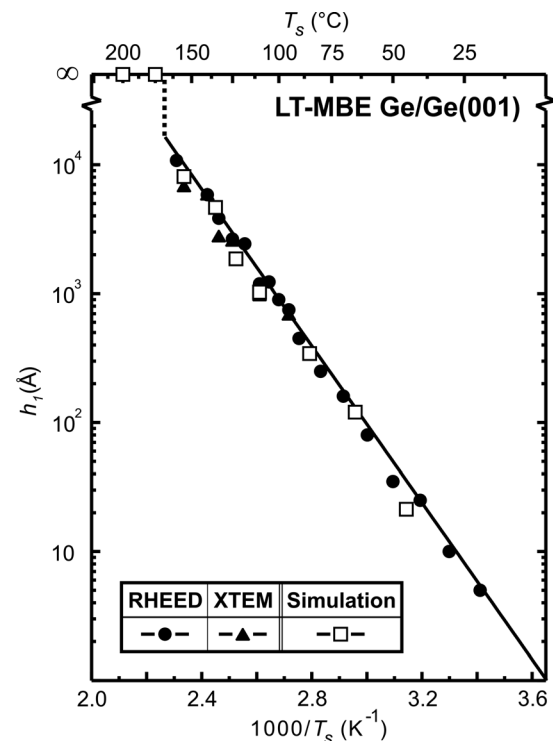


FIG. 5. Growth phase map obtained from simulations and LT-MBE experiments at  $T_s = 45\text{--}230 \text{ }^\circ\text{C}$ . The calculated data points correspond to the thicknesses  $h_I$  at which the aspect ratio reaches a critical value  $w/d = 0.03$ . Experimental data is from Refs. 4 and 10.

length, respectively. In this limit, adatoms can no longer fill the trenches during deposition. Epitaxial breakdown is initiated at  $h \geq h_I$  as limited adatom mobilities lead to a reduction in the deposition rate at interisland trenches.

Figure 4(c) shows that for  $T_s > 170 \text{ }^\circ\text{C}$ , the critical aspect ratio  $w/d = 0.03$  is never reached. This indicates that infinitely thick epitaxial Ge(001) layers can be grown, in agreement with experimental results.<sup>10</sup> Thus, growth at  $T_s > 170 \text{ }^\circ\text{C}$  leads to the formation of mounds with slopes which, while still dependent on  $T_s$ , are no longer a function of  $h$  at large film thicknesses and, most importantly,  $w/d$  remains below  $0.03$ .

In our simulation results, the values of the nucleation and Ehrlich lengths  $l_c$  and  $l_E$ , have been shown to play a crucial role in determining the average surface roughening rate and, hence, the epitaxial thickness.  $l_c$  and  $l_E$  are related to  $E_m$  and  $E_b$ , respectively, through Eqs. 6 and 7. Since  $l_c \propto \exp(-E_m/kT_s)$  [see Eq. (6)], either a higher growth temperature  $T_s$  or a lower diffusion activation energy  $E_m$  (via, for example, surfactant effects as noted below) will produce a corresponding increase in  $l_c$ . Stated differently, an increase in the adatom mobility produces a corresponding increase in the minimum terrace width necessary to nucleate a new island. The Ehrlich length  $l_E$  is defined as the terrace width below which all adatoms migrate to an up-step and is proportional to  $\exp(\Delta E_d/kT_s)$  [Eq. (7)]. An increase in  $T_s$  or a reduction in the adatom attachment asymmetry activation energy  $\Delta E_d$ , both of which result in enhanced down-step crossing probabilities, give rise to a decrease in  $l_E$ .

Thus, a decrease (increase) in  $l_c$  and/or an increase (decrease) in  $l_E$  lead to a corresponding increase (decrease)

in the average roughening rate since the critical aspect ratio  $w/d$  is attained at a smaller (larger) film thickness. This has been demonstrated experimentally during the LT growth of Sn-doped Ge(001) layers.<sup>16,17</sup> Dilute Sn concentrations,  $1 \times 10^{18} \text{ cm}^{-3}$  to  $< 2.0 \text{ at. } \%$  at  $T_s = 155 \text{ }^\circ\text{C}$ , act as a surfactant leading to a reduction in the ratio of the activation energies  $E_b/E_m$  and, hence, an increase in  $l_c/l_E$ . The net result is surface smoothening and a corresponding increase in the epitaxial thickness  $h_I(T_s)$ . As the Sn concentration is raised above  $2.0 \text{ at. } \%$ , strain-induced roughening overcomes surfactant surface smoothening effects.

#### IV. CONCLUSION

We quantitatively describe the surface morphological evolution of Ge(001) layers during LT-MBE homoepitaxial growth with a numerical simulation based upon continuum equations for the motion of step edges. Using measured and extrapolated nucleation length  $l_c$  and Ehrlich length  $l_E$  values, we calculate surface roughness profiles to obtain the surface width  $w$  and in-plane coherence length  $d$  as a function of film thickness  $h$  and deposition temperature  $T_s$ . Calculated  $w(h, T_s)$  and  $d(h, T_s)$  results exhibit quantitative agreement with experimental data. We show that by defining a critical  $T_s$ -independent aspect ratio,  $w/d = 0.03$ , the exponential dependence of the epitaxial thickness  $h_I$  on temperature follows the relationship  $h_I \propto \exp(-E_I/kT_s)$ , with  $E_I = 0.63 \pm 0.05 \text{ eV}$ , also in good agreement with experiment. Above a critical temperature  $T_s = 170 \text{ }^\circ\text{C}$ ,  $w/d$  saturates at large  $h$  values without having reached the critical aspect ratio, indicating that epitaxial breakdown no longer occurs, as observed experimentally. These results show that  $E_I$  and  $T_c$  depend directly on  $l_c$  and  $l_E$ , respectively, which are determined, in turn, by  $E_m$  and  $E_b$ . The latter surface activation barriers can be altered through the addition of dilute surfactants such as Sn during LT-MBE Ge(001) as was demonstrated experimentally in Refs. 16 and 17.

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