PHYSICAL REVIEW B **66**, 205307 (2002)

Monte Carlo studies of stress fields and intermixing in Ge/Si(100) quantum dots

Ph. Sonnet[1],* and P. C. Kelires[1,2]
[1]*Foundation for Research and Technology-Hellas (FORTH), P.O. Box 1527, 711 10 Heraclion, Crete, Greece*
[2]*Physics Department, University of Crete, P.O. Box 2208, 710 03, Heraclion, Crete, Greece*

(Received 18 June 2002; published 7 November 2002)

Intermixing in islands grown on semiconductor surfaces is an important effect, because it drastically alters the optoelectronic properties. Here, we demonstrate a direct simulational approach, based on the Monte Carlo method, which is able to extract with quantitative accuracy the composition profiles in quantum dots, and link them to the stress field. We apply this approach to Ge/Si pyramidal islands. We find that the profiles are not homogeneous, but show strong variations in both the lateral and vertical directions. Outstanding features, such as Si-rich rings in the island layers, are directly linked to the stress pattern. A limiting behavior of composition as a function of temperature and island size is predicted.

DOI: 10.1103/PhysRevB.66.205307 PACS number(s): 68.55.−a, 68.35.Bs, 68.35.Dv, 68.35.Fx

I. INTRODUCTION

Germanium islands formed during Ge/Si heteroepitaxy have been the subject of intense studies during the last decade. These Si-based quantum nanostructures, usually referred to as quantum dots (QDs), are of great fundamental and technological interest. Much of the latter stems from their property to localize and confine strongly the carriers spatially in three dimensions within a nanometer scale, which makes them promising candidates for optically active devices with strong photoemission signals.[1]

From a more fundamental point of view, the interest in Ge dots derives mainly from the remarkable and complex nature of their nucleation and self-organization. Thus, a great effort has been devoted to unravel the island nucleation process, and to elucidate the crucial factors that drive this effect. Both strain-driven mechanisms[2] and kinetic effects[3] have been explored to this end. Several other intriguing phenomena, such as self-assembling[4] and shape transitions,[5] have been extensively studied and they are rather well understood.

Despite this progress, some issues about Ge QDs remain unclear. Perhaps the most significant gap in our knowledge concerns the composition profiles within the islands. Simple arguments suggest that interdiffusion of species is favored, provided that kinetic barriers are overcome, because it lowers the effective lattice mismatch and thus reduces the elastic strain. Whether this phenomenon takes place during or after growth, or both, cannot be easily answered. Naturally, higher growth or annealing temperatures would provide the necessary energy to overcome the potential barriers. Also, what cannot be speculated beforehand is how compositions vary within the islands and as a function of temperature and size.

A number of experimental studies have recently addressed this issue,[6–14] suggesting that intermixing takes place, but its degree and the stage at which this happens remains controversial. Some of these studies[11–14] suggested that intermixing takes place already during growth, especially at high temperatures, albeit without quantifying its extent. Other studies[6–8] provided firm evidence that intermixing at medium growth temperatures is rather initiated after island nucleation, and showed that this is possible at even higher temperatures by controlling the deposition rate. But setting aside this issue for the moment, we could say that the most important missing information so far concerns the variations of compositions in the islands, especially the lateral ones, which are completely unknown. This ‘‘inhomogeneity question,’’ not just the average Si content in the dots, is expected to be important for the optoelectronic properties.

In a significant theoretical contribution to the problem, Tersoff[15] showed within continuum elasticity theory that when islands nucleate on a strained alloy, there is segregation of the larger-misfit component to the islands. This work, however, did not address the question of inhomogeneity. In a related work, Liu *et al.*[16] found experimentally a nonuniform composition profile in $In_{0.5}Ga_{0.5}As$ QDs. The theoretical analysis used to explain this particular profile treated the problem in two dimensions. It assumed that the composition is determined solely by the variation in strain across the growing island surface, and that there is negligible bulk diffusion within the island. Thus, when the equilibrium surface composition is buried by further growth, it becomes a composition of the interior. It is not clear whether this analysis is applicable to more general cases, and as far as we know it has not been applied to Ge QDs. On the other hand, direct simulational approaches to the intermixing problem are lacking.

We present here a detailed theoretical atomistic description of intermixing in Ge islands on Si(100). We use a ‘‘quasiequilibrium’’ approach, based on Monte Carlo (MC) simulations, which is consistent with several experimental observations. We extract with quantitative accuracy the inhomogeneous composition profiles within the islands and at the interfacial regions, and study their dependence on temperature and dot size. We show that interdiffusion is driven by significant stress relaxation, both in the islands and in the wetting layer (WL). We unravel strong variations of composition in both the lateral and vertical directions. In the following, we first describe our theoretical methods. We then analyze the stress fields site by site and show that they determine to a large degree the composition profile and the extent of intermixing. Finally, we give our conclusions and prospects for future work.

II. METHODOLOGY

The key element in any simulational approach to this problem is *compositional* equilibration of the system. Thermodynamically, islands are in a metastable phase, and so one can properly sample statistical averages over the local equilibrium states. The true thermodynamic equilibrium state of the Ge/Si system would be a dilute GeSi alloy, with Ge atoms dissolved deep in the Si bulk relaxing the epitaxial strain. In practice, the system never reaches this state due to the slow bulk diffusion. Instead, strain is relaxed through islanding and limited interdiffusion at the surface region. This is possible because diffusion in the surface region, including the island, the WL, and a few monolayers in the substrate is much faster and strain enhances this trend. As a result of the enhanced diffusion, local equilibrium is established. So, what is needed to model the situation is a ‘‘quasiequilibrium’’ approach, constrained to sample over the local equilibria of the various metastable phases of the Ge/Si system in the surface region, as defined above.

Due to high barriers of diffusion, molecular-dynamics methods cannot reach equilibrium in practical times. Therefore, they are not suitable to tackle this problem. Also, *ab initio* approaches are impractical, simply because of the immense number of configurations needed. At present, only MC methods can achieve this goal, since they can sample over millions of compositionally distinct equilibrium configurations without tracing the actual path of the diffusing species. In our MC algorithm used here, this is achieved through Ising-type identity flips: we choose randomly a pair of Si and Ge atoms, no matter how distant they are, and attempt to switch their identity (from Si to Ge and vice versa). The acceptance of such moves depends on temperature and on the local environment. The higher the temperature, the easier to accept the move. Identity flips near the surface are accepted more often than events in the interior, because the barriers are lower; the environment is more flexible to accommodate such changes. At the limit of many thousands of flips per site, compositional equilibration is achieved, and the average site occupancies can be estimated.[17–19] The overall process models intermixing between the originally pure Ge components (island and WL) and the Si substrate, while keeping the composition of the whole system constant. The identity flips are accompanied by the usual MC random atomic moves and volume changes. The method was used with success in the past to study equilibrium properties of strained SiGe(C) alloys.[17–19] Here, we extend its application to the more complex case of quantum nanostructures.

The simulational cells to start with consist of coherent Ge islands, having pyramidal shape with a square base and {105} facets, on top of a WL of Ge and a Si substrate in the (100) orientation. The top layer of the WL and the dot facets are reconstructed in the usual 2×1 dimer configuration. The base of the dots is oriented at an angle of 45° with respect to the dimer rows of the WL.[20] The width of the WL is fixed at 3 monolayers (ML).[20] We found a limiting Ge diffusion depth in the substrate down to 8–10 ML, and so in the following we report results for cells with 10 ML in the substrate (the bottom layer is fixed, and identity switches occur down to 8 ML). The cells are constrained to have laterally the Si lattice dimensions, with relaxation occurring vertically. Periodic boundary conditions are imposed in the lateral directions. The size of the dots varies, the largest one containing 1750 atoms arranged in 7 ML, with a base width of ~ 92 Å. The total number of atoms in the cells approaches 18 000. Although the size of the islands is smaller than observed in experiment, we made sure that the aspect ratio (height over base width, $h/a \sim 0.1$) and the contact angle ($\sim 11°$) are close to the experimental values.

We emphasize that this study models intermixing once Ge islands have been already nucleated. This approach is consistent with experimental evidence[6,7] that small pyramidal islands, such as those simulated here, *alloy only after they have existed for some time after nucleating* at medium growth temperatures ($450\,°\mathrm{C}$ to $600\,°\mathrm{C}$). More recent work by the same group[8] showed that even at elevated temperatures ($700\,°\mathrm{C}$) *pure* Ge islands can be grown, prior to Si interdiffusion, by raising the deposition rate. These authors also showed that SiGe alloyed pyramids form via Si interdiffusion into pure Ge pyramids. Our approach is also consistent with a wide class of postgrowth annealing experiments reporting siginificant, thermally activated intermixing. These kinds of experiments indicate a ‘‘quasiequilibrium’’ nature of the process. Based on this, several experimental findings have been interpreted, such as, for example the dome-to-pyramid shape transition reported by Henstrom *et al.*[10] who pointed out the thermodynamics of this transformation, and explained it in terms of strain reduction in domes following intermixing during annealing. Other situations that are relevant to our approach include intermixing after the embedding or capping of dots with the host material.

Contrary to the above picture, it is often argued by some researchers, although never shown explicitly, that significant intermixing occurs at the starting point of growth. This reasoning is counterintuitive: if the strains and the elastic energy in the wetting layer due to the mismatch were significantly reduced through extensive intermixing, the primary driving force for islanding would be dramatically weakened. In such a case, mainly kinetic factors would be responsible for islanding. This exaggerates the role of kinetic processes. We believe that kinetic barriers significantly limit interdiffusion until more or less islands of smaller size are formed, especially at medium growth temperatures. A quite possible scenario is that at first strain is mostly relieved by three-dimensional growth (islanding) and at a second stage by intermixing. This hypothesis has to be checked in the future. For the moment, we restrict our analysis within the quasiequilibrium approach described above. Intermixing during growth and its extensiveness will be the subject of further study (this requires the insertion of nonequilibrium growth modes into our algorithm).

To make the simulations tractable, we use the well-established interatomic potentials of Tersoff for multicomponent systems[21] to model the interactions. These have been used with success in similar contexts.[17–19] In particular, the energetics, bonding, and strain fields induced by the Si(100)-2×1 surface reconstruction are accurately described. This

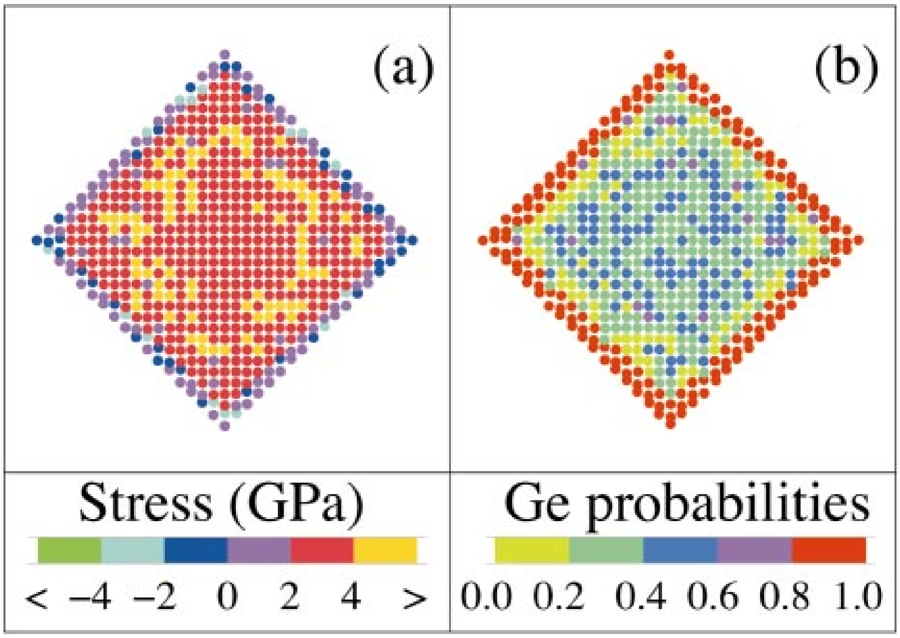

FIG. 1. (Color) (a) Atomic stresses before, and (b) Ge average site occupancies after intermixing, in the base layer of a pyramidal island with a side size of 92 Å.

gives confidence that the stress fields due to islanding will also be treated correctly, and that the reconstruction at the top of the WL and at the island facets will be properly modeled.

III. RESULTS AND DISCUSSION

A. Stress field

We begin with the analysis of the stress field in the islands. For this purpose, we use as a probe the concept of *atomic level stresses*. Their usefulness in unraveling the details of the stress field in inhomogeneous systems has been demonstrated in the past. A relevant example is the case of the SiGe(100)-2×1 reconstructed surface.[17] The local stress can be viewed as an atomic hydrostatic compression (tension), defined by $\sigma_i = -dE_i/d\ln V \sim p\Omega_i$, where E_i is the energy of atom *i* (as obtained by decomposition of the total energy into atomic contributions; this is readily done in the present empirical potential approach), and V is the volume. Dividing by the appropriate atomic volume, Ω_i converts into units of pressure p.[22] Summing up the σ_i's over a group of atoms in the system (such as over a ML or over the whole island) yields the average stress over the specific configuration.

The application of this site-by-site analysis is demonstrated in Fig. 1(a), which shows the atoms in the base layer of the largest island, colored according to their local stress at 800 K, *before* allowing atom flips (pure Ge dot). The stresses are overwhelmingly compressive, as expected. Only atoms near and around the periphery have neutral or slightly tensile stress. (In general, stresses at the boundaries are tensile due to the dimer reconstruction). A key finding is that the overall distribution of stress is inhomogeneous. An outstanding feature is revealed by the ring of highly compressed atoms, formed around the center of the layer and as we approach the edges. It indicates that atoms near the periphery and at the center are able to relax some excessive stress, leaving the atoms in the ring overcompressed. Similar patterns are seen in every layer in the island, but the stresses are becoming progressively less compressive and the ring features fade away close to the top. While earlier works[3,23,24] have pointed out the accumulation of stress and strain energy in the bottom of pyramidal islands, such subtle variations as the local overconcentration of stress within a ring, in the bottom layers, has not been proposed before. We emphasize that because the stress profile determines to a large degree the compositions, as we shall show below, such stress inhomogeneities might affect the optoelectronic properties in a different way than what a uniform profile would do.

A more quantitative picture of the stress conditions in the island at 800 K is given in Fig. 2(a). Each full symbol denotes the average stress in a given layer. The solid line portrays the variation as we move from the base of the island (layer numbered 1) to the top. A nonlinear decrease of compression takes place. Stress near the top varies more rapidly. The average stress over the whole island σ_{QD}^{bef} is 1.4 GPa/atom. This shows that despite the three-dimensional formation and the accompanying outward atomic relaxations, the compressive stress in the dot is still substantial.

A similar analysis is carried out for the WL. The results are given in Fig. 2(b). Interestingly, the middle layer comes out to be significantly more compressed than either the top reconstructed layer (numbered 1) or the layer just above the Si substrate. To explain this effect consider that in the first Ge layer at the interface the bonding is half Ge-Si, and so the mismatch with the Si-Si bonds in the substrate is smaller than the one between the second Ge layer (all Ge-Ge bonds) and the substrate. The third layer would have been even more compressed (its mismatch approaches that of strained *bulk* Ge) but, being the top reconstructed surface layer, it relieves part of the stress. Additionally, the 2×1 reconstruction induces large compressive stresses in the layer below,[17] which add to the already generated stresses due to the mismatch. The average stress in the WL σ_{WL}^{bef} is 2.2 GPa/atom.

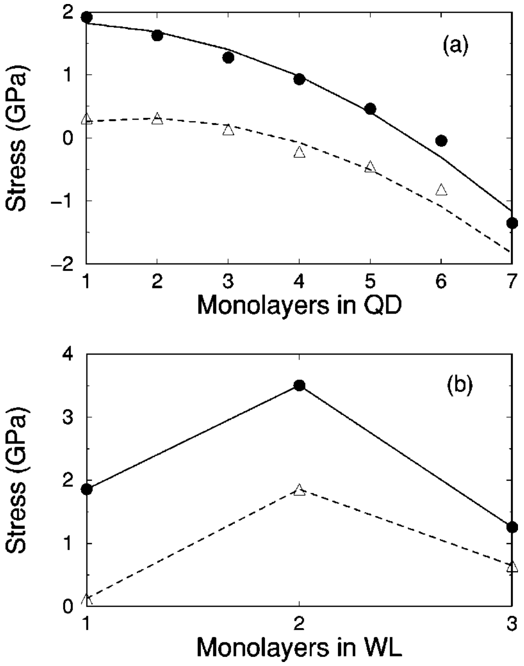

FIG. 2. Stresses per layer in (a) the QD and in (b) the WL, before (full symbols) and after (open symbols) intermixing.

Stress conditions change dramatically when we allow atom-identity flips, and thus permit interdiffusion of species between the three components of the system (QD, WL, and substrate). Let us analyze the layer-by-layer average stresses shown in Fig. 2 (open symbols, dashed lines). A remarkable reduction of compressive stress takes place in the QD, especially near its base. Now, the average stress in the island σ_{QD}^{aft} is 0.1 GPa/atom, nearly compensated. This shows clearly that the dominant factor driving segregation in the island is stress relaxation, much more powerful in this case than the intrinsic tendency of the Si-Ge system to randomly mix. Equally important is the relaxation of stress in the WL, where the average stress σ_{WL}^{aft} is now 0.9 GPa/atom. Much of the relaxation occurs in the top layer, which is practically stress free, and in the middle layer.

B. Composition profiles

We map the composition profiles in the islands by extracting the local compositions. These are indicated by the average site occupancies. Figure 1(b) illustrates the atomic sites in the base of the island, colored according to their average Ge occupancy. A highly nonuniform pattern arises. The periphery is clearly dominated by high Ge probabilities, while the interior sites have in general lower Ge occupancies. Remarkably, the lowest Ge composition is found in and around the overcompressed ring of sites, shown in the stress pattern of Fig. 1(a); this is because sites under compression tend to be occupied by the smaller species in the system.[17] Thus, local stress conditions determine to a large degree the inhomogeneous features of the composition profile. The other important factor, that competes with the stress factor in shaping up the profile, is the lower surface energy of Ge. This factor is particularly strong in the periphery and at the faceted edges. Similar patterns are found as we move up to the top of the island, but with progressively enhanced Ge population, especially at and near the faceted edges.

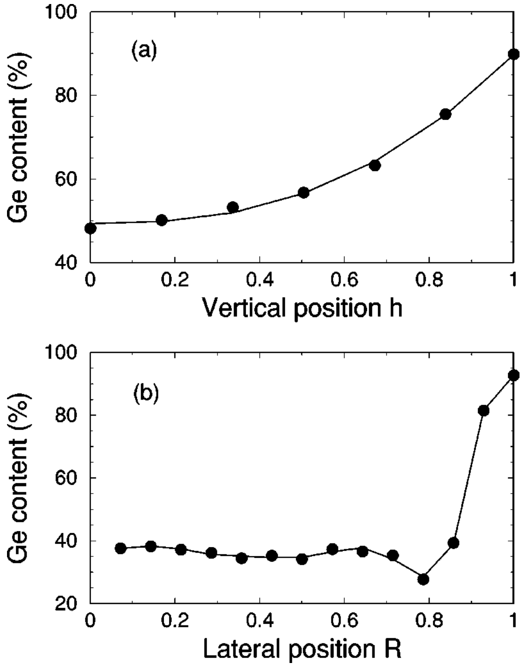

FIG. 3. Variations of Ge content in the intermixed island. (a) Vertical variation. (b) Lateral variation in the base layer. See text for details.

Our methodology gives with quantitative accuracy the overall composition profiles in the island, both vertically and laterally. These are shown in Fig. 3. (Only the base-layer lateral variation is drawn.) By calculating an average value within each layer, the vertical variation of Ge content as a function of the normalized island height h (measured from the base) can be extracted. It is near parabolic and is very well fitted with the power-law function, $x_{\mathrm{Ge}}=a_0+a_1\times h^{a_2}$, with $a_0=49.4$, $a_1=40.3$, and $a_2=2.5$. Thus, the Ge content is slowly varying in the bottom and rapidly varying when approaching the top of the island. We checked that this simple behavior is valid in all cases studied, with the exponent lying in the range of values 2.5 ± 0.2.

Liao *et al.*[13] used energy dispersive x-ray spectrometry to extract the vertical variation of the relative Si/Ge ratio in dislocated islands. They found this ratio to be higher closer to the substrate, in agreement with our results, but its variation is opposite to ours: the Ge fraction increases rapidly in the bottom and remains nearly constant at the top. Possible sources of this discrepancy might be the neglect in the experimental analysis of the lateral variations of composition, which by necessity affect the outcome for the vertical variations. In a subsequent work on coherent islands, the same group[14] performed image simulations and compared to transmission electron microscopy results, again assuming constant lateral composition, and found that the model with Ge at the top fits the experimental data better, but they did not extract the details of the vertical variation.

The lateral variation is constructed by drawing concentric shells of square shape, starting from the center of the layer and moving outwards to the edges. Within each shell an average Ge content is calculated from the site occupancies, and is plotted versus the normalized radius R (from the center). An accurate fit to the variation is done using higher-order polynomials. Although the polynomial coefficients vary from layer to layer, there is a unique and common composition behavior in all layers in the dot. The variation is characterized by slight oscillations of the Ge content up to a distance of ~ 0.6–0.7, where a deep minimum appears, and then by a steep increase in Ge content when approaching the edges. Thus, the Si content is indeed enhanced within the shells of overcompressed sites near the edges, as observed above from the visual inspection, but not at the boundary, as proposed by Chaparro *et al.*,[6] because of the lower surface energy of Ge.

An interesting comparison of our inhomogeneous composition profile can be made with the work of Liu *et al.*[16] on $In_{0.5}Ga_{0.5}As$ QDs. They found an inhomogeneous profile with an In-rich core having an inverted-triangle shape. The two profiles agree in that the top region of the island is enriched with the larger-misfit component (fully with In in one case, mostly with Ge in the other). A striking difference is that our profile shows Ge enriching the regions near the edges, even at the bottom of the dot, while they find the In fraction to decrease from center to edge and vanish at the bottom region of the island outside the In-rich core. This difference indicates that, beside the chemistry, the lateral variations of stress are dissimilar in the two classes of heteroepitaxial systems.

The average of site occupancies over the whole island yields a Si content of $\sim$47% at 800 K. In the WL we find 58%. It is useful to know how the Si content in the dot varies with simulational annealing temperature. This is shown in Fig. 4(a). A weak dependence is found, the difference between the lowest (300 K) and highest (1300 K) T's considered being only $\sim 7\%$. For the proper interpretation of this result and comparison with experiment, one should bear in mind that our MC simulations can equilibrate the system even at low (room) T's because they are designed to partially overcome the potential barriers for atom exchanges, and thermal activation only enhances this capability. On the other hand, thermal activation is necessary for experiment to initiate intermixing, because it lowers the diffusion barriers and thus enhances the interdiffusion rates. Therefore better comparison of our results with experiment can be made at higher temperatures.

At this high-T regime (~ 1150 K), Capellini *et al.*[11] found from photoemission measurements that the Si content in Ge/Si epilayers (QD plus WL) rises to 72%. Our result for the epilayer at this temperature is $\sim 55\%$. A possible reason for this difference might be again the neglect of lateral variations in the modeling used to extract the compositions from the measurements. Better agreement is reached with the work of Zhang *et al.*[8] who found a Si content of 56% in dome islands at ~ 1000 K. At this temperature our pyramids contain $\sim$49% of Si. Taking into account that domes probably have somewhat higher Si contents brings theory and experiment into very good agreement. Indeed, we have preliminary results from simulations of a dome structure, giving us 57% of Si, but we need further calculations to establish this trend.

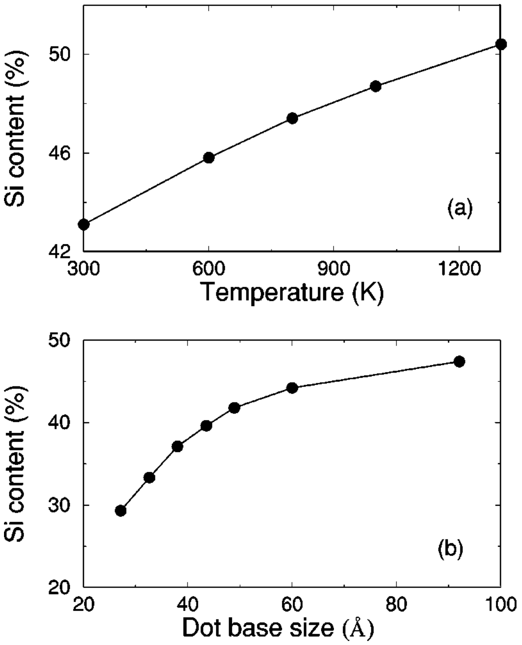

FIG. 4. (a) Annealing temperature and (b) size dependence (at 800 K) of the Si content in pyramidal islands.

It is also interesting to know how the Si content in the dot varies with size. We demonstrate this dependence in Fig. 4(b). We observe that the Si content (at 800 K) initially rises sharply with dot size, but it eventually reaches a limiting value that seems to stay close to 50% for larger islands. This means that beyond a critical size the composition remains nearly constant. This result is also in agreement with the recent work of Zhang *et al.*[8] who found that the composition appears to be independent of island size.

A comparison with the theoretical predictions of Tersoff[15] can be readily made if we assume that the WL is already alloyed before the nucleation of islands. According to Tersoff, at typical growth temperatures, and for the corresponding elastic and misfit strain parameters, a 58% Si content in the WL yields $\sim$55% of Si in the island. We find 47%. The small difference might be due both to any inaccuracy in the treatment of strain by the empirical potentials, and to the neglect in Tersoff's theory of island inhomogeneity. Another interesting comparison is made at the high-T limit where Tersoff proposes no decomposition of the alloyed film (the island composition equals the alloyed WL composition). We do not observe such behavior even at 1300 K, at which we find 59% of Si in the WL and 53% in the dot. This result shows that at this limit the stress factor operates still more efficiently in the WL.

IV. CONCLUSIONS

We reported in this paper a direct and quantitative simulational study of intermixing in Ge/Si(100) quantum dots. We make the reasonable assumption, supported by experimental evidence, that small pyramidal clusters are formed before interdiffusion takes place. Under these conditions, our MC simulations unravel inhomogeneous composition profiles in the islands and show that their nonuniformity is largely determined by the stress fields. We specified quantitatively the composition variations in both the vertical and lateral directions. The latter are completely unknown both theoretically and experimentally, and so this prediction could help experimental works to calibrate their measurements for a more accurate investigation of the composition profile. (Experimental attempts to address this issue assumed a constant lateral composition; this affects the outcome for the vertical variations, which have to be reexamined.)

The average composition in the pyramidal islands approaches 50%, and it appears to be independent of size, in good agreement with recent experimental work. We emphasize that the alloyed islands cannot be characterized as SiGe random solutions, because of the inhomogeneous distribution of species, and so the optoelectronic properties should deviate from those of the random mixture.

Finally, we mention that future applications of this simulational approach to intermixing include the nucleation process at the initial stages. For this, the appropriate MC algorithms are being developed to generalize the effect by taking into account intermixing while the island is growing. We are also currently working on the problem of stacked and buried dot layers, and we intend to study how intermixing affects the pyramid-dome transition.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge stimulating discussions with G. Bauer, and helpful comments of J. Tersoff. This work was supported by the EU RTN program under Grant No. HPRN-CT-1999-00123.

---

*Present address: CNRS, Laboratoire de Physique et de Spectroscopie Electronique, 68093 Mulhouse Cedex, France.

[1] K. Eberl, Phys. World **10**, 47 (1997); O. G. Schmidt, C. Lange, and K. Eberl, Appl. Phys. Lett. **75**, 1905 (1999).

[2] J. Tersoff and R. M. Tromp, Phys. Rev. Lett. **70**, 2782 (1993); J. Tersoff and F. K. LeGoues, *ibid.* **72**, 3570 (1994).

[3] A.-L. Barabási, Appl. Phys. Lett. **70**, 2565 (1997); M. Kästner and B. Voigtländer, Phys. Rev. Lett. **82**, 2745 (1999).

[4] J. Tersoff, C. Teichert, and M. G. Lagally, Phys. Rev. Lett. **76**, 1675 (1996).

[5] F. M. Ross, J. Tersoff, and R. M. Tromp, Phys. Rev. Lett. **80**, 984 (1998).

[6] S. A. Chaparro, J. Drucker, Y. Zhang, D. Chandrasekhar, M. R. McCartney, and D. J. Smith, Phys. Rev. Lett. **83**, 1199 (1999).

[7] S. A. Chaparro, Y. Zhang, J. Drucker, D. Chandrasekhar, and D. J. Smith, J. Appl. Phys. **87**, 2245 (2000).

[8] Y. Zhang, M. Floyd, K. P. Driver, J. Drucker, P. A. Crozier, and D. J. Smith, Appl. Phys. Lett. **80**, 3623 (2002).

[9] F. Boscherini, G. Capellini, L. Di Gaspare, F. Rosei, N. Motta, and S. Mobilio, Appl. Phys. Lett. **76**, 682 (2000).

[10] W. L. Henstrom, C. Liu, J. M. Gibson, T. I. Kamins, and R. S. Williams, Appl. Phys. Lett. **77**, 1623 (2000).

[11] G. Capellini, M. De Seta, and F. Evangelisti, Appl. Phys. Lett. **78**, 303 (2001).

[12] X. Z. Liao, J. Zou, D. J. H. Cockayne, J. Qin, Z. M. Jiang, X. Wang, and R. Leon, Phys. Rev. B **60**, 15 605 (1999).

[13] X. Z. Liao, J. Zou, D. J. H. Cockayne, Z. M. Jiang, X. Wang, and R. Leon, Appl. Phys. Lett. **77**, 1304 (2000).

[14] X. Z. Liao, J. Zou, D. J. H. Cockayne, Z. M. Jiang, and X. Wang, J. Appl. Phys. **90**, 2725 (2001).

[15] J. Tersoff, Phys. Rev. Lett. **81**, 3183 (1998).

[16] N. Liu, J. Tersoff, O. Baklenov, A. L. Holmes, Jr., and C. K. Shih, Phys. Rev. Lett. **84**, 334 (2000).

[17] P. C. Kelires and J. Tersoff, Phys. Rev. Lett. **63**, 1164 (1989).

[18] P. C. Kelires, Phys. Rev. Lett. **75**, 1114 (1995).

[19] P. C. Kelires and E. Kaxiras, Phys. Rev. Lett. **78**, 3479 (1997).

[20] Y.-W. Mo, D. E. Savage, B. S. Swartzentruber, and M. G. Lagally, Phys. Rev. Lett. **65**, 1020 (1990).

[21] J. Tersoff, Phys. Rev. B **39**, 5566 (1989).

[22] Due to our definition of local stresses, a positive (negative) sign indicates compressive (tensile) stress.

[23] N. Moll, M. Scheffler, and E. Pehlke, Phys. Rev. B **58**, 4566 (1998).

[24] D. E. Jesson, G. Chen, K. M. Chen, and S. J. Pennycook, Phys. Rev. Lett. **80**, 5156 (1998).