

## Dependence of Surface Strain on Island Geometry in Embedded Quantum-Dot Systems

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Strain fields induced by embedded islands of pyramidal shape are examined using the continuum theory of elasticity with Ge/Si systems as a specific example. We show that, upon increasing spacer thickness, the decay of the strain field on the spacer surface undergoes a crossover from a non-cubic inverse power law to a cubic inverse power law. The exponent for the non-cubic inverse power law depends on island slope with a smaller exponent corresponding to a smaller slope. Additionally, the strain is nearly proportional to the island volume when the slope is large but to the island area when the slope is small. These findings reconcile several diverse predictions derived from large-scale atomistic simulations for islands of different geometries.

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Quantum dots have many important potential technological applications. Strain-driven formation of nanoscale coherent islands on lattice-mismatched layers in heteroepitaxy offers an attractive way for effective fabrication of quantum dots of large density [1, 2]. Normally, these islands are not well organized in space and show large dispersion in size distribution. Recent experiments showed that the spatial ordering and size uniformity of islands can be greatly improved by growing multilayers of islands separated with spacer layers [3–9]. Vertical alignment of islands was found in semiconductor systems including InAs/GaAs [3, 6] and Ge/Si [4, 5], and also in magnetic systems including Co/Au [7]. Taking advantage of the anisotropic nature of strain fields in some semiconductor materials, anticorrelation of island positions and a fcc-like structure of islands was further observed in CdZnSe/ZnSe [8] and in PbSe/PbEuTe [9], respectively.

The self-organization of the stacked islands is believed to be the result of the strain field on the spacer surfaces induced by the embedded islands. This was demonstrated by analyzing the net atomic current to the locations of strain concentration due to strain-biased diffusion [3], by analyzing the strain modulation of nucleation centers [4], by considering the strain-induced interactions of islands [10], and by kinetic Monte-Carlo simulations [11, 12]. In these studies [3, 4, 11, 12], an embedded island is modeled as a force dipole of zero dimension within the continuum theory of elasticity that gives rise to strain and stress fields characterized by a cubic inverse power-law dependence on the spacer thickness and a linear dependence on the island volume. In reality, embedded islands have finite spatial extent and show no cubic or spherical symmetry. The accuracy of the force dipole model has not been fully justified as indicated in recent studies [13, 14].

Three different approaches have been used in calculating strain fields for embedded islands of finite dimensions. The first one is the Green function method within continuum theory [15, 16], using the solution for a force

dipole as the Green function. The second approach involves continuum finite element calculations, which was shown to give the same results as the Green function method [16]. The third approach [17, 18] emphasizes the discrete atomic nature and utilizes large scale atomistic simulations such as molecular dynamics, which can provide accurate results but at a large computational cost. An attractive advantage of the Green function method within continuum theory is its simplicity and efficiency in calculations. One expects that the continuum theory should be valid for heteroepitaxial quantum-dot systems with small lattice mismatch [19]. However, it is still an open question whether the continuum theory can give reliable results for embedded quantum-dot systems as there has been no evidence from the direct comparison between results obtained by the continuum theory and the atomistic simulations. Potentially complicating this comparison, diverse predictions from atomistic simulations were reported recently [17, 18] for the stress fields at the Si spacer surfaces induced by Ge islands of the pyramidal shape suggested by experiments [20]. One claimed that [17] the stress field can be well approximated by the force dipole model in continuum theory. The other found that [18] the stress field deviates significantly from the description of the force dipole, exhibiting a nearly linear inverse dependence on spacer thickness and a linear dependence on island surface area.

In this letter, we provide a clear understanding of the diverse predictions from atomistic simulations by examining the dependence of surface strain on island geometry using the Green function method within continuum theory. As a specific example, we analyze the strain fields on the Si spacer surfaces induced by embedded Ge islands of pyramidal shape. Our results obtained by the Green function method are in excellent agreement with the results obtained previously by atomistic simulations, confirming the validity of the continuum theory for embedded quantum-dot systems. Furthermore, we show that, upon increasing spacer thickness, the decay of the

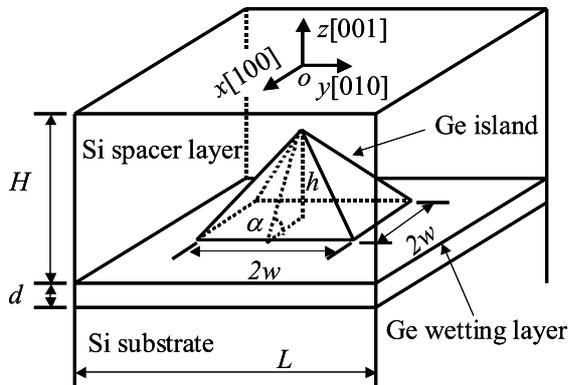


FIG. 1: Schematic illustration of the system. A germanium island of pyramidal shape with a germanium wetting layer above a silicon substrate is capped by a spacer layer of silicon.

strain field exhibits a crossover behavior from a non-cubic inverse power law to a cubic inverse power law. The exponents for the non-cubic inverse power laws depend on island slopes with smaller exponents corresponding to smaller slopes. In this regime, the strain dependence on island size also displays intriguing behaviors. It shows a nearly linear dependence on the island volume when the island slope is large but exhibits a nearly linear dependence on the island surface area when the slope is small. This complete view of the strain dependence on island geometry reconciles the diverse predictions derived from atomistic simulations for embedded islands of different slopes.

The unit cell of our system is schematically shown in Fig. 1. A pyramidal Ge island with an initially formed wetting layer of thickness  $d$  on a Si(001) substrate is capped by a Si spacer layer of thickness  $H$ . The base of the pyramid is a square of width  $2w$ , oriented in [100] and [010] directions. Island height is given by  $h = w \times \tan \alpha$ , where  $\alpha$  is the slope angle. The wetting layer is always very thin (about 3 monolayers for Ge/Si) and its contribution to the strain field at the spacer surface is only a small constant. We neglect it by choosing  $d = 0$ . The periodicity of the system is  $L$ , and  $L \rightarrow \infty$  gives a system which consists of only one embedded island.

We start our analysis for a single Ge island with volume  $V$  embedded in Si. In continuum theory, an embedded island can be modeled as an inclusion and can be further treated as a collection of individual force dipoles of infinitesimal size  $dV$  comprising the volume  $V$ . The strain field outside the island is then given by the superposition of the contribution from each force dipole. In other words, the strain field for a force dipole is the Green function for the strain field of the island. Suppose a force dipole with  $dV = dx'dy'dz'$  is located at position  $(x', y', z')$  in an isotropic material such as Si, one can show that [21] the trace of the strain tensor,

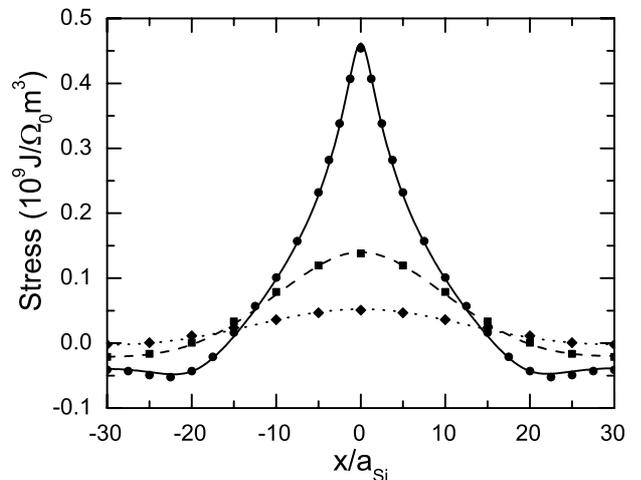


FIG. 2: Stress  $\sigma$  at  $y = z = 0$  as a function of  $x$  for islands with  $w = 20a_{\text{Si}}$ ,  $h = 17\text{ML}$ , and  $L = 60a_{\text{Si}}$ . Symbols are results from reference [18] obtained by atomistic simulations. Circles, squares, and diamonds correspond to  $H = 21\text{ML}$ ,  $49\text{ML}$ , and  $81\text{ML}$ , respectively. Lines are results obtained by the Green function method within continuum theory.

$G = G_{xx} + G_{yy} + G_{zz}$ , at the spacer surface is given by

$$G = -\frac{\epsilon_0(1+\nu)(1-2\nu)dV}{\pi(1-\nu)}\left(1 - \frac{3z'^2}{R^2}\right)/R^3, \quad (1)$$

where  $R = \sqrt{(x-x')^2 + (y-y')^2 + z'^2}$ ,  $\nu$  is Poisson's ratio of the spacer material, and  $\epsilon_0$  the lattice misfit with  $\epsilon_0 = (a_i - a_s)/a_i$ . Here,  $a_i$  and  $a_s$  are the lattice constants for the inclusion and spacer materials, respectively. The strain field  $\epsilon$  for the embedded island is then given by the integration of the Green function in Eq. (1) over the volume of the island [15, 16, 21], namely,  $\epsilon = \int_V G(x', y', z') dx' dy' dz'$ . The trace of the stress tensor reads  $\sigma = \frac{E}{1-2\nu}\epsilon$ , where  $E$  is the Young's modulus. The strain and stress fields for arrays of embedded islands can be obtained further by superposition of the contribution from each island. In our calculations for Ge/Si systems, we have  $a_i = a_{\text{Ge}} = 5.656\text{\AA}$  and  $a_s = a_{\text{Si}} = 5.431\text{\AA}$ . We choose  $\nu = 0.218$  as used in reference [17].

In Fig. 2, we compare our calculations of the stress fields for a periodic lattice of embedded Ge islands ( $L = 60a_{\text{Si}}$ ) with the results from atomistic simulations. The Ge islands have pyramidal shape of  $\{105\}$  facets with  $w = 20a_{\text{Si}}$  and  $h = 17\text{ML}$ . Symbols in Fig. 2 are from the atomistic simulations [18] after removal of the contribution coming from the spacer surface reconstruction by subtraction of a constant term  $p_d$  [18]. Lines are our results using  $E = 8.404 \times 10^9 \text{J}/\Omega_0 m^3$ ,  $10.152 \times 10^9 \text{J}/\Omega_0 m^3$ , and  $10.152 \times 10^9 \text{J}/\Omega_0 m^3$  for  $H = 21\text{ML}$ ,  $49\text{ML}$ , and  $81\text{ML}$ , respectively, which gives an excellent fit to the results of atomistic simulations. Here,  $\Omega_0 = \Omega/a_{\text{Si}}^3$  is the dimensionless average atomic volume [18]. The constant term  $p_d$  is the stress associated with the surface dimerization. The fit shown in Fig. 2 leads to  $p_d =$

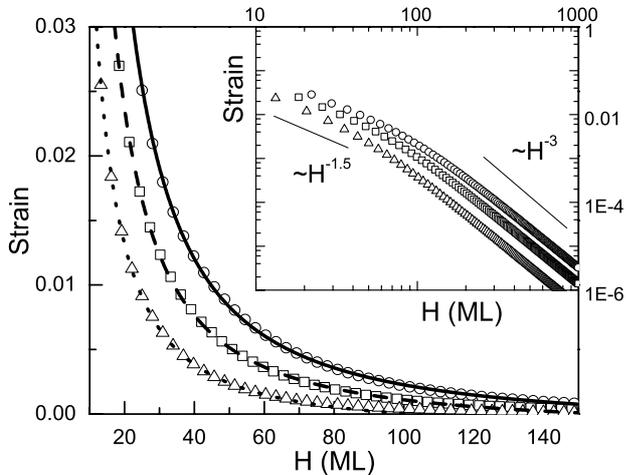


FIG. 3: Strain  $\epsilon$  at  $x = y = 0$  as a function of spacer thickness  $H$ . Circles, squares, and triangles correspond to islands with  $(w, h) = (20a_{\text{Si}}, 17\text{ML})$ ,  $(15a_{\text{Si}}, 13\text{ML})$ , and  $(10a_{\text{Si}}, 9\text{ML})$ , respectively. Thick lines are corresponding fitting results in the regime of small  $H$  that give  $\epsilon = a_0 + a_1/H^{1.50}$  with  $(a_0, a_1) = (-1.26 \times 10^{-3}, 1.29)$ ,  $(-9.20 \times 10^{-4}, 2.06)$ , and  $(-1.04 \times 10^{-3}, 3.30)$ , respectively. Inset shows the crossover behavior upon increasing  $H$ .

$0.754(10^9\text{J}/\Omega_0 m^3)$ , which is very close to the approximate value  $0.747(10^9\text{J}/\Omega_0 m^3)$  obtained in atomistic simulations [18]. We note that the Young's modulus takes a different value when the Si spacer layer is thin such as 21ML. This may be attributed to the slight change of the mechanical properties of the Si material when the spacer surface is so close to the island. We also performed calculations for a single embedded Ge island ( $L \rightarrow \infty$ ) and found that the local surface stress fields at the location directly above the island in these two systems with  $L = 60a_{\text{Si}}$  and  $L \rightarrow \infty$  differ by a small amount, indicating that the strain and stress fields decay sufficiently fast that the contribution from the nearest-neighbor islands are negligible. In the following, we focus on analyzing the surface strain for individual embedded Ge islands.

Fig. 3 illustrates the strain at  $x = y = 0$  as a function of spacer thickness. Symbols are our results from Green function method for pyramidal Ge islands with  $\{105\}$  facets of three different sizes. Inset of Fig. 3 is the log-log plot of the strain versus spacer thickness. Circles, squares, and triangles correspond to islands described by  $(w, h) = (20a_{\text{Si}}, 17\text{ML})$ ,  $(15a_{\text{Si}}, 13\text{ML})$ , and  $(10a_{\text{Si}}, 9\text{ML})$ , respectively. Thick lines are the fitting results in the regime of small spacer thickness that give  $\epsilon = a_0 + a_1/H^\gamma$  with  $\gamma = 1.50$  and corresponding parameters  $(a_0, a_1) = (-1.26 \times 10^{-3}, 1.29)$ ,  $(-9.20 \times 10^{-4}, 2.06)$ , and  $(-1.04 \times 10^{-3}, 3.30)$ . Another exponent  $\gamma \approx 1$  was found for the same islands in atomistic simulations [18], where less data points were used for fitting. Our results based on large number of data points show that the best fit gives  $\gamma = 1.50$ . Moreover, the Green function method allows us to deal with the regime of large spacer thickness where

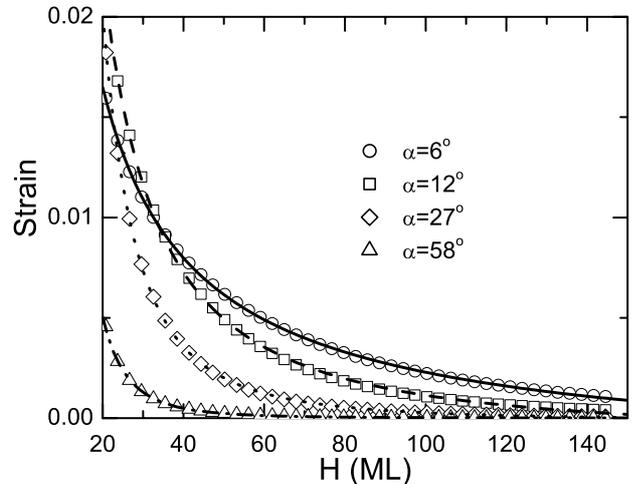


FIG. 4: Strain  $\epsilon$  at  $x = y = 0$  as a function of spacer thickness  $H$ . Circles, squares, diamonds, and triangles correspond to systems with slope angles  $\alpha = 6^\circ$ ,  $12^\circ$ ,  $27^\circ$ , and  $58^\circ$ , respectively. Lines show fitting results that give  $\epsilon = a_0 + a_1/H^\gamma$  with  $(a_0, a_1, \gamma) = (-2.48 \times 10^{-3}, 0.25, 0.86)$ ,  $(-9.20 \times 10^{-4}, 2.06, 1.50)$ ,  $(-1.10 \times 10^{-4}, 33.02, 2.47)$ , and  $(2.78 \times 10^{-6}, 116.78, 3.36)$ , respectively.

the application of atomistic simulations is not possible so far. The inset of Fig. 3 shows that, upon increasing the spacer thickness, the decay of the strain field exhibits a crossover behavior from  $\gamma = 1.5$  to  $\gamma = 3$ .

We find that the exponent  $\gamma$  is a function of island slope with a larger exponent corresponding to a larger slope. We show in Fig. 4 the decay behavior of the strain fields for four pyramidal islands of different slopes, where circles, squares, diamonds, and triangles are results for islands with  $(w, h) = (30a_{\text{Si}}, 13\text{ML})$ ,  $(15a_{\text{Si}}, 13\text{ML})$ ,  $(6.5a_{\text{Si}}, 13\text{ML})$ , and  $(2a_{\text{Si}}, 13\text{ML})$ , respectively, corresponding to slope angles  $\alpha = 6^\circ$ ,  $12^\circ$ ,  $27^\circ$ , and  $58^\circ$ . The decay can be well fitted to  $\epsilon = a_0 + a_1/H^\gamma$  with  $(a_0, a_1, \gamma) = (-2.48 \times 10^{-3}, 0.25, 0.86)$ ,  $(-9.20 \times 10^{-4}, 2.06, 1.50)$ ,  $(-1.10 \times 10^{-4}, 33.02, 2.47)$ , and  $(2.78 \times 10^{-6}, 116.78, 3.36)$ , respectively. Atomistic simulations found that [17] the strain for a pyramidal island with  $w = 5.6\text{nm}$  and  $h = 2.8\text{nm}$  ( $\alpha = 27^\circ$ ) can be approximated by the force dipole model with  $\gamma = 3$ . Our calculations give  $\gamma = 2.47$  close to  $\gamma = 3$ .

The strain dependence on island size also displays interesting behaviors. Fig. 5 illustrates the strain fields at position  $x = y = z = 0$  as a function of island width for pyramidal islands of different slopes embedded at  $H = 81\text{ML}$ . The strain is normalized by the island surface area  $s = 4w \times h / \sin(\alpha)$ . It is clear that when the island width is small compared with the spacer thickness, the normalized strain is always proportional to the island width, showing a linear dependence of the strain on island volume consistent with the force dipole model. However, for islands of large sizes compared with the spacer thickness, the strain dependence on island size

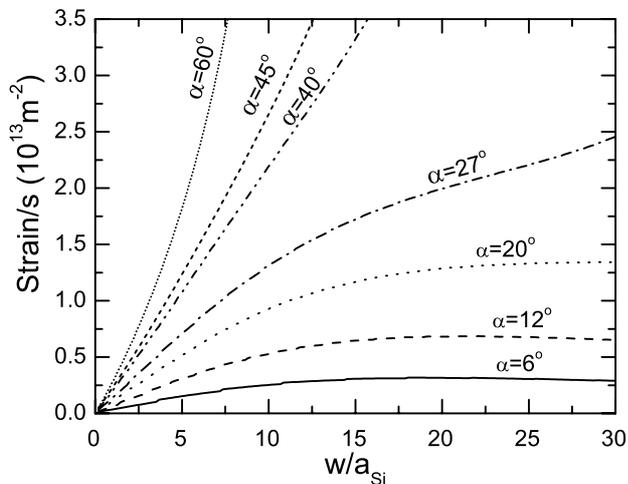


FIG. 5: Normalized strain  $\epsilon/s$  at  $x = y = z = 0$  as a function of island width for islands of different slopes at  $H = 81\text{ML}$ .

critically depends on island slope. For islands with small slope angles  $\alpha < 20^\circ$ , the normalized strain changes very slowly with the island width, indicating that the strain is nearly proportional to the island surface area. Differently, for  $20^\circ < \alpha < 45^\circ$ , the normalized strain is proportional to the width, giving a volume dependence similar to the case for small islands. For islands with  $\alpha > 45^\circ$ , a super linear dependence of strain on island volume exists. For pyramidal Ge islands of sizes  $(w, h) = (20a_{\text{Si}}, 17\text{ML})$ ,  $(15a_{\text{Si}}, 13\text{ML})$ , and  $(10a_{\text{Si}}, 9\text{ML})$ , all have slope angles  $\alpha = 12^\circ$ . For these islands, Fig. 5 predicts that the strain is nearly proportional to the island surface area, consistent with the observation in atomistic simulations [18]. For Ge island with  $w = 2h = 5.6\text{nm}$  and  $\alpha = 27^\circ$ , the prediction from Fig. 5 of a nearly linear strain de-

pendence on island volume is again consistent with the atomistic simulations [17].

In summary, we have examined the strain fields on spacer layer surfaces induced by embedded islands of pyramidal shape in the framework of continuum theory with Ge/Si systems as a specific example. We found that the diverse properties of the strain fields for these systems obtained previously by atomistic simulations can be well described by the continuum theory after integrating the contribution of island geometry using the Green function method, confirming the validity of the continuum theory for these systems. Our results show that, in the regime of small spacer thickness, the strain fields depend critically on island geometry, with smaller island slopes corresponding to larger deviations from the description of the force dipole model. We emphasize that, in the large separation regime, the force dipole approximation is consistent with our results, as one would expect when the island size is negligible compared to the spacer thickness. However, it is the small separation regime that is interesting and important for applications, and it is within this regime that the effects of finite dimensions and island geometry must be considered. We believe that the established complete view of the strain dependence on island geometry have significant importance in fully understanding the growth process of these systems.

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