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HTML ABSTRACT + LINKS

Local self-organization of islands in embedded nanodot systems

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We show that strain distribution on the surface of an isotropic spacer layer induced by an embedded island of large base-to-height aspect ratio deviates significantly from the description of the point force dipole model in the regime of small spacer layer thickness. In this regime, the strain profile displays several local maxima above the embedded island. The regions with local strain maxima serve as nucleation centers for growth of surface islands under appropriate growth conditions, resulting in locally well-organized surface islands above the embedded island. Our theoretical results are in excellent agreement with recent experiments for Ge islands embedded in Si. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1669079]

Nanodots have many important potential technological applications. Strain-driven formation of nanoscale islands on lattice-mismatched layers in heteroepitaxy offers an attractive way for effective fabrication of coherent nanodots of large density. Moreover, recent experiments showed that both the spatial ordering and size uniformity of islands are significantly improved by growing multilayers of islands separated with spacer layers.[1–8]

The self-organization of stacked islands is a result of the strain fields on spacer layer surfaces induced by embedded islands.[1,2,4] This was first demonstrated in isotropic systems such as Ge/Si and InAs/GaAs by modeling three-dimensional embedded islands as point force dipoles of zero dimension in the regime of large spacer layer thickness compared to island width.[1,2] Considering its large base-to-height aspect ratio, an embedded island was later modeled as a two-dimensional inclusion in the regime where the spacer layer thickness is close to the island width but much larger than island height.[4] In these models, the strain profile on the spacer surface induced by an embedded island is characterized by a single maximum above the center of the embedded island. As a consequence, surface islands nucleate above the embedded islands, forming vertical alignment of stacked islands as observed in many experiments.[1–5] A remarkably different result was recently observed, showing that decrease of growth temperatures results in growth of a cluster of highly ordered surface Ge islands above an embedded Ge island in the regime of small spacer layer thickness very close to island height.[6] Because of the weak anisotropy in the Ge/Si system, the deviation from the vertical alignment is not due to the anisotropy effect as observed in strongly anisotropic systems such as CdZnSe/ZnSe[7] and PbSe/PbEuTe.[8] The observed local self-organization of surface islands was attributed[6] to the dipole repulsive interactions between adjacent surface islands. Although such interactions lead to a certain degree of ordering of islands,[9] it cannot explain why surface islands inside a cluster perfectly show the same symmetry and orientation as the base of the embedded island. Further progress in controlling growth of ordered arrays of islands requires a clear understanding of the underlying mechanism for the local self-organization. Moreover, growth of clusters of locally well-organized islands may find important applications in synthesis of nanodot molecules for quantum information processing.[10]

In this letter, we show that the local self-organization of islands is a result of local strain modulation of island nucleation centers induced by an embedded island of finite dimension. For an embedded island of rectangular-prism shape with a large base-to-height aspect ratio, the surface strain field has four symmetrically distributed maximums above the embedded island as the spacer layer thickness is close to the island height. Positions of the strain maximums exhibit the same symmetry and orientation as the base of the embedded island. As the spacer layer thickness increases, the four strain maximums disappear and a nearly constant strain distribution occurs above the embedded island in a wide range of small spacer layer thickness compared to island width. Different from the point force dipole model, the finite size effect of embedded islands on strain distribution predicts growth of a cluster of islands on top of an embedded island with or without symmetrical distributions of the islands depending on the spacer layer thickness and growth temperatures. Our theoretical results are in excellent agreement with the recent experimental observations in the Ge/Si system.

We calculate the surface strain using the Green's function method in the framework of continuum theory of elasticity, which was shown to give the same results as large-scale atomic-level simulations.[11] Compared with atomic-level simulations, the continuum theory significantly facilitates calculations of the strain fields induced by embedded islands. Nevertheless, one should note that the continuum theory cannot give accurate results for the strain fields at the interfaces between the embedded island and the spacer-layer. In our case, we are interested in the strain fields on the spacer-layer surface, where continuum theory applies. In continuum theory, an embedded island is treated as a col-

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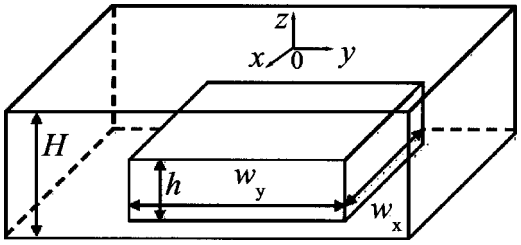

FIG. 1. Schematic illustration of the system.

lection of individual force dipoles of infinitesimal size dV comprising the volume. The strain field outside of the island is then given by the superposition of the contribution from each force dipole. For a force dipole with dV located at (x',y',z'), the trace of the strain tensor at the spacer layer surface $(x,y,0)$ is given by[12]

$$G=\frac{\varepsilon_0(1+\upsilon)(2\upsilon-1)dV}{\pi(1-\upsilon)R^3}\left(1-\frac{3z'^2}{R^2}\right),$$

where $R=\sqrt{(x-x')^2+(y-y')^2+z'^2}$, υ is Poisson's ratio of the spacer material, and $\varepsilon_0=(a_e-a_s)/a_s$ is the lattice mismatch constant with a_e and a_s being the lattice constants for the embedded and spacer materials, respectively. Considering the square-shaped bases and large base-to-height aspect ratios of embedded Ge islands, we model the embedded island as a rectangular prism as illustrated in Fig. 1. Taking the integral of G over the volume of the embedded island, we derive the following exact formula for the strain on the spacer-layer surface:

$$\varepsilon=\frac{\varepsilon_0(1+\upsilon)(1-2\upsilon)}{\pi(1-\upsilon)}\sum_{i,j,k=1}^{2}(-1)^{i+j+k}\times\tan^{-1}\frac{x_i y_j}{z_k\sqrt{x_i^2+y_j^2+z_k^2}},$$

where $x_i=x\pm w_x/2$, $y_i=y\pm w_y/2$, $z_1=H$, and $z_2=H-h$. For the Ge/Si system, we have $a_e=a_{\mathrm{Ge}}=0.5656$ nm, $a_s=a_{\mathrm{Si}}=0.5431$ nm, and $\upsilon=0.218$. We consider $w_x\equiv w_y=w$ in order compare our results to experiments.

Figure 2 shows the strain profiles on the Si spacer-layer surface induced by an embedded Ge island of $w=200$ nm and $h=34.9$ nm with different H. Parameters of w and H are taken directly from experiments and the island height is chosen to be slightly smaller than 35 nm based on experimental observations.[6] It is easy to see from Figs. 2(a)–2(c) that the strain in a limited region above the embedded island for $H\leqslant 65$ nm is significantly larger than the strain at other places on the surface. Moreover, the strain field decreases as increasing H and displays different behaviors in different regimes of H. For $H\sim h$, the strain has four maximums at the positions exhibiting the same symmetry and orientation as the base of the embedded island [see Figs. 2(a) and 2(b)]. We find that the value of the strain maximums is approximately 2.5 times larger than the strain above the center of the embedded island as H approaches h. In the regime $H\sim w/4+h/2$, the strain shows a nearly constant distribution above the embedded island as shown in Fig. 2(c). Finally, a large H corresponds to a very weak strain distribution as shown in Fig. 2(d). The strain distributions for small H (compared to w) shown in Figs. 2(a)–2(c) remarkably differ from the description by a point force dipole model, where one only finds a single strain maximum above the center of an embedded island. Our detailed analysis shows that the strain approximates to the description of the point force dipole model as $H>2w$.

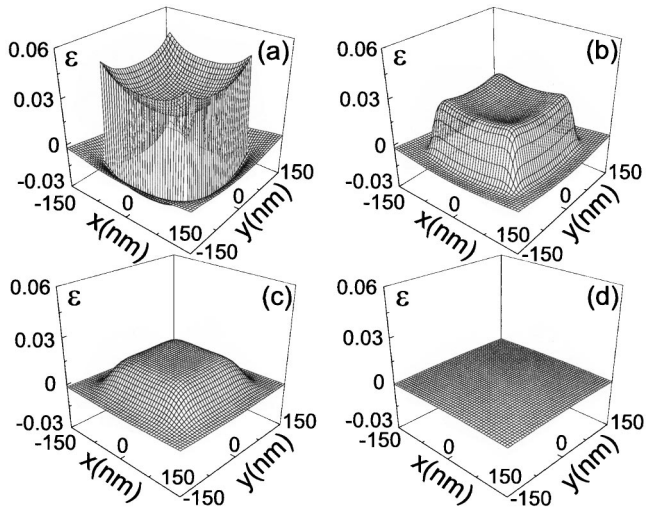

FIG. 2. Strain fields on the Si spacer layer surfaces induced by an embedded Ge island of $w=200$ nm and $h=34.9$ nm with different spacer-layer thicknesses H. (a) $H=35$ nm, (b) $H=45$ nm, (c) $H=65$ nm, and (d) $H=200$ nm.

We further show that the surface strain induced by a template consisting of a column of embedded islands displays the same behaviors as described above. In the experiments, clusters of islands were grown on a template with ten stacked islands.[6] The significance of growing stacked islands as a template is to refine the structure of the embedded islands for uniform size distribution.[4] Our calculations show that only few upper layers of the embedded islands in a template have noticeable contribution to the strain field on the surface. Figure 3 illustrates the strain profiles on the final Si spacer surface of a template of five stacked Ge islands. The Si spacer thickness in the template is 60 nm as used in the experiments[6] and the embedded islands have the same size as

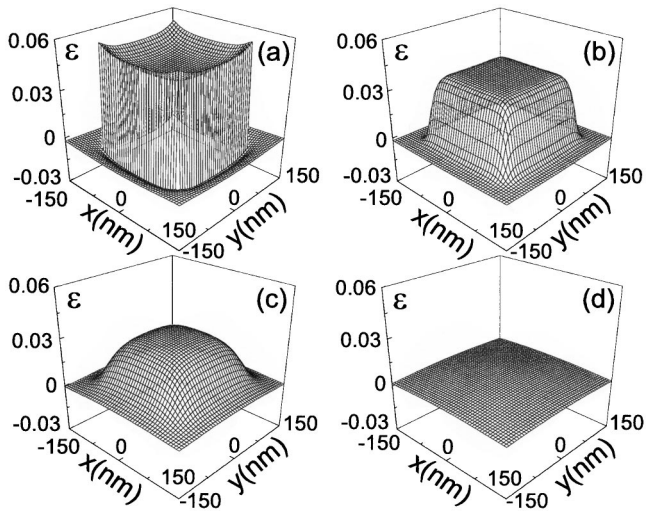

FIG. 3. Strain fields on templates of five embedded Ge islands of $w=200$ nm and $h=34.9$ nm with different thicknesses H of the final spacer layer. (a) $H=35$ nm, (b) $H=45$ nm, (c) $H=65$ nm, and (d) $H=200$ nm.

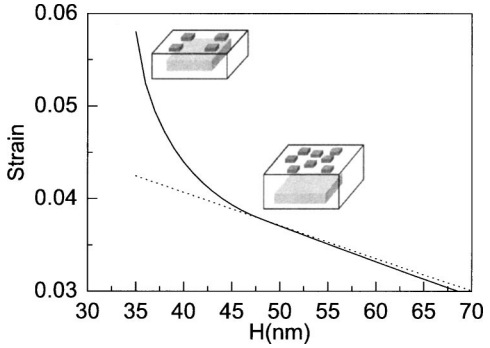

FIG. 4. Strain fields at different positions on a template of five embedded Ge islands of $w=200$ nm and $h=34.9$ nm as a function of thickness H of the final spacer layer. Solid line corresponds to the strain maximums for $H<49$ nm and to the strain at the corner sites of a square of size 46 nm $\times 46$ nm for $H\geqslant 49$ nm. The dotted line corresponds to the strain above the center of embedded islands. Insets illustrate the two different types of clusters of surface islands in different regimes of H.

in Fig. 2. Comparing Fig. 3 to Fig. 2, we can see that the surface strain induced by a template of stacked islands displays the same behaviors as that induced by a single embedded island. The transition separating the regime with four strain maximums from a nearly constant strain distribution occurs at $H=49$ nm as shown in Fig. 4. In a wide range of H above the transition point (from 49 to 70 nm), we find a constant strain distribution within an area of 46 nm$\times$46 nm above the embedded islands.

We apply our findings to elucidating the experimental observations. Our analysis is based on a widely accepted concept, namely, the preferential nucleation of islands in tensile-strained regions on the spacer layer surface.[2,4] From Figs. 3 and 4, we can see that the four strain maximums are much larger than the strain fields at other places when H is very close h. In this case, we expect that four islands nucleate in the regions with maximum strain distribution, as illustrated in Fig. 4. We note that in order to perfectly locate the surface islands, dedicated control of growth conditions is needed. At elevated temperatures or a relatively large spacer layer thickness, the energy difference at different places on the surface may not be large enough to confine adatoms in the regions with local strain maximums due to the large kinetic energy of adatoms. Experiments showed that decrease of growth temperature from 750 to 600 °C in the regime $H\sim h$ results in a cluster of islands above a column of embedded islands.[6] For $H=35$ nm, four surface islands occur on top of the embedded island at the positions which exhibit the same symmetry and orientation as the base of the embedded island.[6] This observation is in excellent agreement with our results. From Figs. 3 and 4, we can see that the strain fields in the regime from 45 to 70 nm are nearly constant above the embedded islands. As a consequence, we expect that surface islands preferentially nucleate into clusters above the embedded islands but the islands inside each cluster nucleate at random positions due to the lack of remarkable strain differences at different positions as illustrated in Fig. 4. Again, this result agrees very well with the experiments, where one finds that surface islands form clusters without well-defined symmetric distribution inside each cluster for $H=45$ nm and $H=65$ nm.[6] Finally, experiments[6] showed that surface islands grow randomly on the entire surface at $H=200$ nm, as expected due to the weak strain field.

In conclusion, we have shown that the finite size effect of embedded islands on strain distribution allows growth of a cluster of islands on top of an embedded island with or without symmetrical distributions by choosing appropriate spacer layer thickness and growth temperatures. Our theoretical results are in excellent agreement with recent experiments, indicating that the underlying mechanism for the local self-organization of islands above embedded islands is due to the strain-induced modulation of nucleation centers instead of the dipole repulsive interaction between adjacent islands. This finding opens a new avenue to growth of well-organized nanodot molecules as well as to control of spatial ordering of nanodot arrays.

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