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The effect of plastic strain relaxation on the morphology of Ge quantum dot superlattices

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Abstract

A series of Ge quantum dot superlattices were prepared to study the relationship of the dot morphology evolution with the number of layers. Strain relaxation was observed in thicker films and the dots transited from broad size distribution to size equalization and eventually to broad size distribution again as a result of the generation of threading dislocations in the quantum dot superlattice films.

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Physical self-assembly growth of semiconductor quantum dots has been studied intensively in the last several years. Strain accommodation and relaxation are the basic phenomena in physical self-assembly process as the formation of any semiconductor quantum dots is a heteroepitaxial process between materials with different lattice constants. As a matter of fact, the strain accommodation and relaxation have direct impact on the morphology of the self-assembled quantum dots. By properly tailoring the strain distribution on the substrate, one can have desired quantum dot arrays for different potential applications. In the multi-layered Ge dot structures, the dots are normally vertically correlated [1–6]. Previously, it was also believed that dots transit from a broad size distribution in the first layer to intraplanar size equalization at the upper layers [7]. Nevertheless, it

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was recently shown that following the nature of heteroepitaxy, thick self-assembled quantum dot superlattices also have critical thickness issues [8]. The propagation of misfit dislocations in the multilayered system had the influence on the vertical ordering and size distribution of stacked dots [9]. In this work, we present systematic studies of the strain relaxation effect on the morphology of multi-layered Ge quantum dots. The strain of Ge quantum dot superlattice can be relaxed by the formation of quantum dot itself, Si/Ge interdiffusion and misfit dislocations in self-assembled heteroepitaxy. Threading dislocations are generally generated in thick Ge quantum dot superlattice films and terminated on the surface of the film when the in-plane biaxial misfit strain is relaxed. We show that the uniformity of dots at the upper layers of dot superlattice films worsens after the introduction of threading dislocations.

A total of seven samples were grown by solid source molecular beam epitaxy on Si (1 0 0) substrates at 540 °C and consisted of 100 nm Si buffers, followed by Ge/Si bilayers having a thickness of 1.5 and 20 nm for the Ge layer and Si layer, respectively. The growth sequence in each period is Si layer first and then Ge layer, which allows us to check the dot morphology using atomic force microscope (AFM). The only variable parameter for these samples was the period, i.e., 1, 2, 5, 10, 20, 35 and 50, respectively.

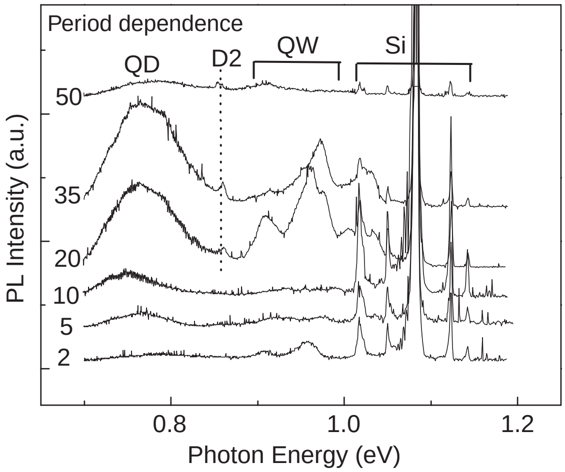

Fig. 1. PL spectra of quantum dot superlattices with different periods.

Fig. 1 shows the Photoluminescence (PL) results of a series of samples with different periods of 2, 5, 10, 20, 35, and 50, respectively. Peaks at 1.153, 1.132, 1.095, 1.061, and 1.027 eV observed for all samples originate from Si and correspond to non-phonon (NP) replica, transverse acoustic (TA), transverse optical (TO), 2TA + TO, and TO + OΓ peaks, respectively. Peaks ranging from 0.9 to 1.0 eV are associated with quantum wells (wetting layers). The effect of the period on the quantum dot peak is obvious. As the period increases to about 10, the peak energy decreases after which the peak energy begins to increase again. At fewer than 10 periods, dot-coarsening effects [6] play an important role and the average dot size increases and therefore the dot peak shows a red shift. After 10 periods, the increase of the peak energy with increasing periods (blue shift) is due to the strain relaxation of the dots. Strain relaxation in multilayered Ge dots have been discussed previously [8,9]. Plastic strain relaxes in thick quantum dot superlattices by forming misfit and threading dislocations, and therefore critical thickness can be defined [8], the same as that in two-dimensional heteroepitaxial films, such as quantum well superlattices and alloys. Evidence of this strain relaxation is observed in the spectra. In the samples having 20, 35 and 50 periods of Si/Ge, a D2 dislocation related peak around 0.86 eV is observed. The integrated PL intensity of the quantum dot peak increases with increasing number of periods up to 35 periods, after which the intensity suddenly decreases for 50-period sample. This may be due to a much greater threading dislocation density as a result of more strain relaxation in this thick sample.

To verify the formation of dislocations, transmission electron microscope (TEM) measurements were performed. Fig. 2 shows cross-sectional TEM images of the four samples, with a period of 10, 20, 35, and 50, respectively. Vertically correlated Ge dots were observed for the 10, 20, and 35-period samples. For the 50-period sample, however, dislocations were nucleated at the surface of the nth layer of Ge dots and subsequently extended to the surface.

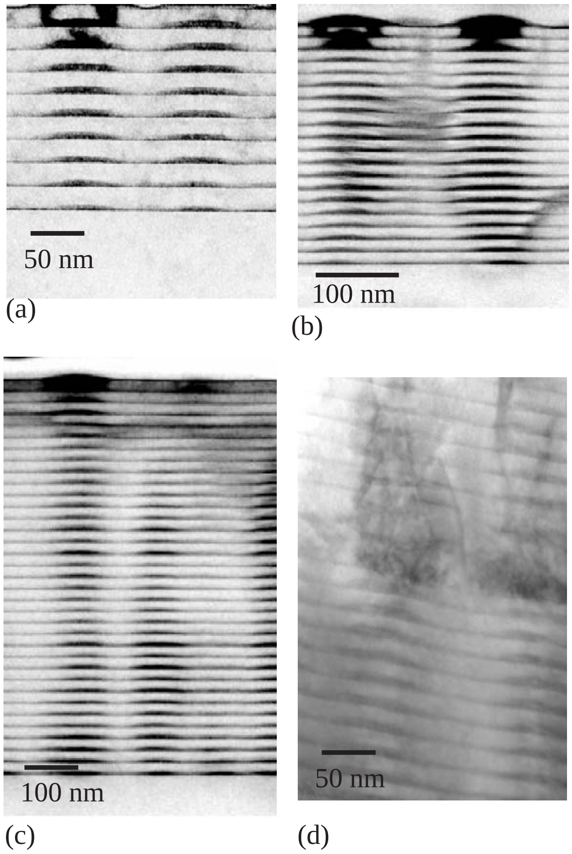

Fig. 2. Cross-sectional TEM images of (a) 10 (b) 20 (c) 35 and (d) 50-period Si(20 nm)/Ge(1.5 nm) superlattice samples. Vertically correlated dots are observed for 10, 20, and 35-period samples. For the 50-period sample, dots are still vertically correlated but the high-density dislocations are evident.

It should be noted that no threading dislocations were observed in the cross-sectional TEM image for the 20- and 35-period sample, even though the PL spectrum showed evidence of dislocations via the D2 dislocation peak. TEM is an excellent tool to examine the structure of the dot superlattice at a high resolution, but is not the preferred tool to characterize samples with low threading dislocation density ($<10^7\,\mathrm{cm}^{-2}$) due to the small field of view and so if the Si/Ge quantum dot superlattice structures were partially relaxed with only a few dislocations, it most likely would not be captured by TEM. Nevertheless, the partial strain relaxation in 20, and 35-period superlattices can be extracted in these TEM images. As a matter of fact, in the fully strain-driven multilayered quantum dots, a continuous increase of the island size at the upper layers (dot coarsening) is anticipated due to more uniform misfit strain distribution as widely observed previously (for example, Refs. [1–6]) and evident in the 10-period sample as shown in Fig. 2a. In 20- and 35-period samples, however, the dot sizes in each vertical correlated dot column fluctuate from layer to layer. This phenomenon is an indicative of strain relaxation [9].

The strain relaxation effect on the evolution of the dot morphology was also characterized by AFM. Fig. 3 shows the AFM images of the top surfaces of the Ge quantum dot superlattice

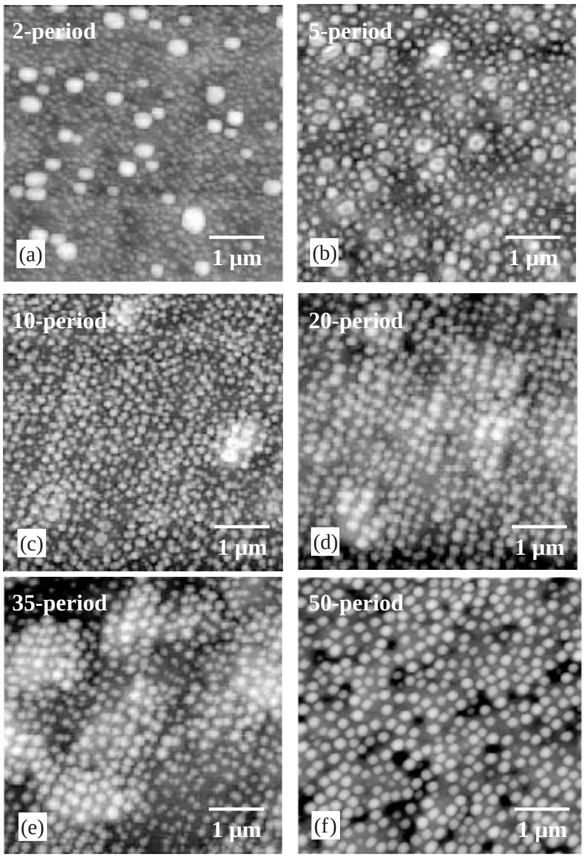

Fig. 3. AFM images of Si (20 nm)/Ge (1.5 nm) superlattices of (a) 2 (b) 5 (c) 10 (d) 20 (e) 35, and, (f) 50 periods. The dot morphology is different among the samples.

samples with different periods of 2, 5, 10, 20, 35, and 50. The different morphology such as dot uniformity and dot density are observed among samples. Moreover, the surface under the dot layer for samples with less than 35 periods is reasonably flat while for the 50-period sample, the surface under the dot layer shows holes, a result from the threading dislocations.

Fig. 4 shows 2D and its corresponding 3D AFM images of magnified local area near some dislocation-induced pits on the surface of the 50-period sample, respectively. A circular hole with Ge dots arranged at its edge is clearly observed in the center of the images. It should be noted that there are also elongated holes on the surface due to the piles-up effect from more than one threading dislocation. By counting the pits on the surface, the density is around $10^8\,\mathrm{cm}^{-2}$, which is similar to threading dislocation density characterized in previous TEM measurements. The Ge atoms deposited near to these holes preferably diffuse to form dots at their edges as shown in these images. This phenomenon is similar to the formation of SiGe islands at the edge of the rectangular-shaped pits induced by embedded carbon [10]. At the edge of each of dislocation-induced holes, the convex curvature of the Si lattice results in a larger local Si lattice constant, therefore, reducing the mismatch between Si and Ge and providing an energetically favorable site for Ge nucleation [11]. The dots near to these holes tend to nucleate at the edge. Different dot morphology is anticipated.

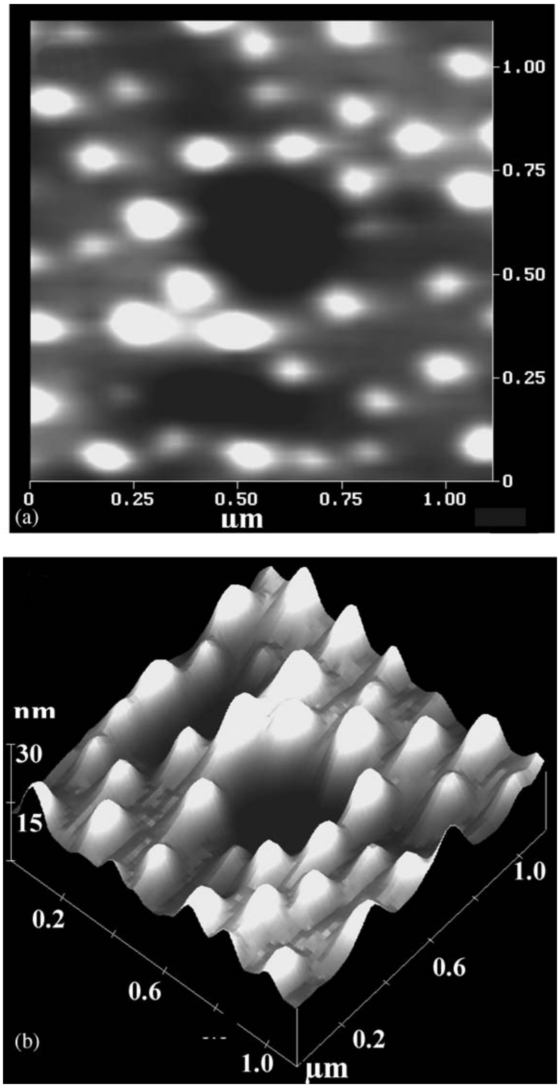

Fig. 4. (a) 2D and 3D AFM images of magnified area of the 50-period sample, respectively. A circular hole in the center and an elongated hole due to the effect from more than one dislocation were observed with dots nucleated at their edges.

Fig. 5 shows the quantum dot density and root-mean-square dot height relative to average dot height (non-uniformity) as a function of the number of bilayers. The density of the sample with only one Ge layer is estimated to be $8\times10^9\,\mathrm{cm}^{-2}$. The density decreases dramatically as the period increases and saturates to about $2\times10^9\,\mathrm{cm}^{-2}$ when the number of periods reaches 20. After 35 periods, the density increases slightly, indicating a change in the growth mode or the generation of threading dislocations, which provide additional sites for nucleation of the Ge dots. The solid circle symbols are experimental root-mean-square variation of dot height relative to average height $\Delta H/\langle H\rangle$ for different samples. The selection of height rather than base or volume of the dots to represent the size uniformity of the dots is due to the non-trivial determination of real base value of a dot associated with the AFM tip effect. The increasing uniformity with the superlattice period less than 35 is evident, which is a result of the increasing uniformity of misfit strain distribution at the upper layers predicted by elastic continuum model, where no defects and

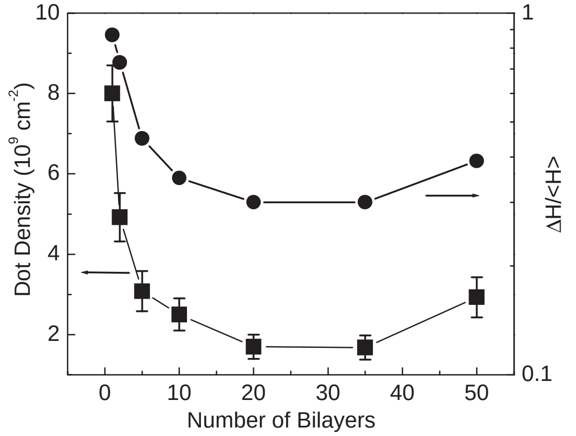

Fig. 5. Ge quantum dot density and root-mean-square height relative to average height as a function of the period for Si(20 nm)/Ge(1.5 nm) superlattices. The density decreases dramatically as the period increases and saturates to about $2\times10^{9}\,\mathrm{cm}^{-2}$ when the period reaches 20. After 35 periods, the density increases slightly. For the dot height characterization, the increasing uniformity with the superlattice period less than 35 is observed. After 35 periods, the uniformity becomes worse. The trend of the data for both density and height of the dots suggests the change of the growth mode or the generation of threading dislocations in the thick samples.

dislocations were assumed [7]. It should be noted that in the 20- and 35-period samples, there are already a few dislocations due to partial strain relaxation, but the effect of the small amount of dislocations is not enough to degrade the uniformity until after 35 periods, the uniformity becomes worse, indicative of the generation of very high-density threading dislocations, as observed in our PL, AFM and TEM measurements.

In summary, we studied the effect of plastic strain relaxation on the morphology of Ge quantum dot superlattices. It was found that strain in thick dot superlattice films is relaxed by forming misfit/threading dislocations. The dot morphology of slightly increased dot density and non-uniformity was observed for thick superlattice samples with high-density threading dislocations.

Acknowledgments

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