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Strain effects in and crystal structures of self-assembled InAs/GaAs quantum dots

H. S. Lee[a)] and J. Y. Lee
Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea

T. W. Kim[b)]
Advanced Semiconductor Research Center, Division of Electrical and Computer Engineering, Hanyang University, 17 Haengdang-dong, Seongdong-gu, Seoul 133-791, Korea

M. D. Kim
Quantum Dot Technology Laboratory, Division of Chemical Metrology and Material Evaluation, Korea Research Institute Standards and Science, P.O. Box 102, Yuseong-Gu, Daejeon 305-600, Korea

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The strain effects in and the crystal structures of self-assembled InAs/GaAs quantum dots (QDs) were investigated by using transmission electron microscopy (TEM). The in-plane lattice constant of the InAs QDs was larger than that of the GaAs substrate, and the vertical lattice constant of the InAs QDs was smaller than that of the InAs bulk. The variation of the lattice constant for the InAs QD originated from the strain effect. A schematic diagram of a strained InAs QD based on the TEM results, indicative of the strain distribution around the QD, is presented. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1612894]

The formation of self-assembled InAs quantum dots (QDs) on GaAs substrates has attracted much interest due to their use in promising nanoscale devices such as QD lasers,[1] optical memories,[2] and QD infrared photodetectors.[3] Nanoscale devices utilizing QDs can be fabricated without an additional lithography process because QDs already maintain discrete atom-like energy levels with good optical properties.[4] Self-assembled QDs in lattice-mismatched systems, such as InAs/GaAs and SiGe/Si QDs, can be achieved by using the Stranski–Krastanow (SK) growth mode.[5] In the SK growth mode, the mismatched layer grows on the substrate two-dimensionally during the initial stage; then, above a critical thickness, strain-induced and dislocation-free QDs with a three-dimensional shape are formed on a residual two-dimensional wetting layer.[6] An appropriate regulation of the optimized growth conditions may provide the possibility for controlling precisely the size and the density of the QDs.[7]

The shapes and the sizes of QDs are important parameters in determining their electrical and optical properties.[8] The microstructural parameters of QDs are generally investigated by using transmission electron microscopy (TEM),[9] atomic force microscopy (AFM),[10] scanning tunneling microscopy (STM),[11] and x-ray diffraction (XRD).[12] AFM and STM measurements have been generally performed to measure the surface morphologies of QDs. XRD measurements have been carried out to measure the average strain relaxation of QDs in dots-in-a-well. TEM measurements are the only powerful tool for investigations of buried QDs. Also, under the usual on-zone axis or two-beam imaging condition, a diffraction contrast image is formed mainly by the strain field around the QDs. By using high-resolution TEM (HRTEM), we can study the shapes and the sizes of the QDs and measure the lattice constant of the QDs directly. Therefore, among the various measurement methods, HRTEM measurements are a particularly powerful tool for investigating the strain distribution around an island.[13]

This letter reports data for the strain distribution around islands in lattice-mismatched InAs QDs on (100) GaAs substrates. In particular, the lattice relaxation of the self-assembled InAs QDs on (100) GaAs substrates was investigated by using HRTEM measurements. A possible crystal structure for the InAs QDs is presented on the basis of the HRTEM results.

The samples used in this work were grown on semi-insulating (100)-oriented GaAs substrates by using molecular beam epitaxy, and the surface coverage due to molecular adsorption was studied by using a reflection high-energy electron diffraction (RHEED) system. The substrate temperature was monitored with an infrared pyrometer. The native oxide layer on the substrate surface was thermally removed at 530 °C under an As_4 pressure of approximately 10^{-5} Torr. The InAs and the GaAs growth rates were set to 0.077 and 1.42 monolayers (ML)/s, respectively. The whole growth process was controlled by using *in situ* RHEED. Two kinds of the samples were grown. Sample S1 was a single layer consisting of QDs, and sample S2 was a five-stacked layer of QDs. Both samples were grown without capping layers. The QD samples in this study consisted of the following structures: First, a 100-nm-thick GaAs buffer layer was grown on a GaAs substrate at 530 °C. Then, the substrate temperature was lowered to 410 °C for the growth of a single layer and five periods of the InAs/GaAs QD array. Finally, a 1.5 ML InAs wetting layer was deposited, followed by a 4 nm GaAs spacer layer after a 20 s growth interruption.

The TEM observations were performed in a JEM 3010 transmission electron microscope operating at 300 kV. The

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[a)] Electronic mail: hslee0409@kaist.ac.kr

[b)] Author to whom correspondence should be addressed; electronic mail: twk@hanyang.ac.kr

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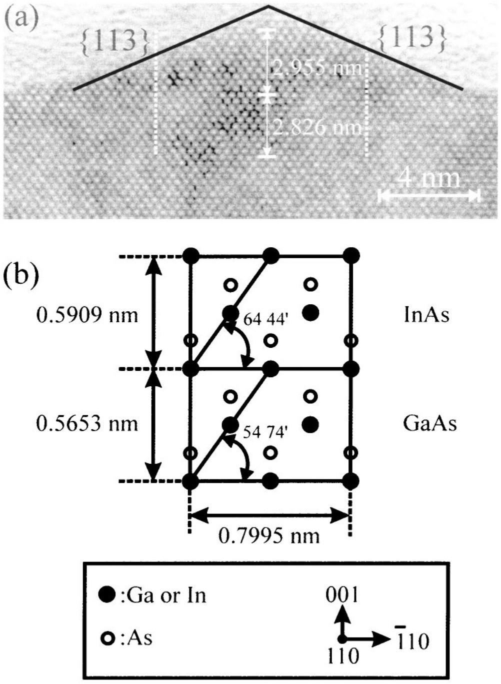

FIG. 1. (a) A cross-sectional high-resolution TEM image along the [110] zone axis of a single layer of the InAs/GaAs QD without a capping layer. (b) A possible schematic diagram of the (110) projection of the crystal structure for an InAs/GaAs QD, taking into account strain effects.

samples for the cross-sectional TEM measurements were prepared by cutting and polishing with a diamond paper to a thickness of approximately 30 μm and then argon-ion milling at liquid-nitrogen temperature to electron transparency.

Figure 1(a) is a HRTEM image of sample S1 showing an InAs QD formed on a GaAs substrate. The side facets of the island consist of {113} planes, which is in reasonable agreement with the RHEED results.[14] The lattice constants of the vertical components of the GaAs substrate and the InAs QD determined from Fig. 1(a) are 0.5653 and 0.5909 nm, respectively. The lattice constants of the horizontal components of the GaAs substrate and the InAs QD determined from Fig. 1(a) are similar to those of the GaAs bulk. This result indicates that InAs QDs receive a compressive strain. To investigate the magnitude of the strain and the stress of the InAs QDs, we assumed that during the initial stage, the InAs QDs were pseudomorphically grown on GaAs substrates. The crystal structure of the InAs layer can be simplified by using the atomic structure due to only the strains in the biaxial direction. A possible schematic diagram of the (110) projection of the crystal structure for an InAs/GaAs QD, taking into account strain effects, is shown in Fig. 1(b). The relationship between the biaxial stress (σ_i) and the strain (ε_i) components is given by

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} \\ C_{12} & C_{11} & C_{12} \\ C_{12} & C_{12} & C_{11} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \end{bmatrix}, \tag{1}$$

where C_{ij} is the elastic modulus of the ij component. When the InAs layers are grown on GaAs substrates, they receive a compressive strain. When the InAs wetting layer is pseudomorphically grown on GaAs substrates, since the value of σ_3 is zero, the other components of the strain are given by

$$\varepsilon_3 = -\frac{2C_{12}}{C_{11}}\varepsilon_1 . \tag{2}$$

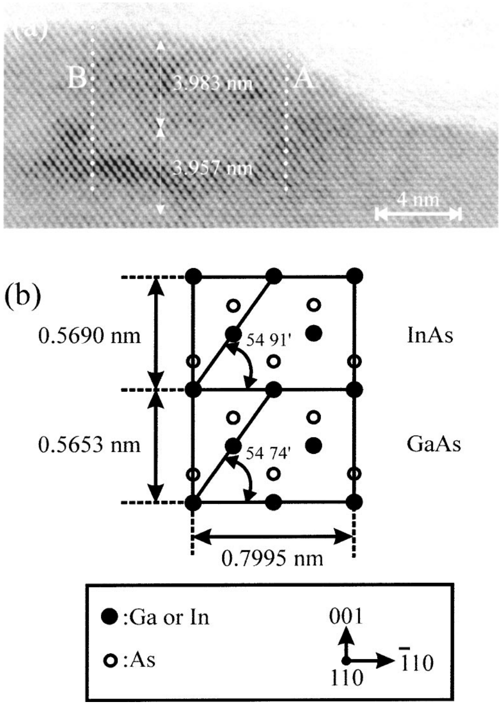

FIG. 2. (a) A cross-sectional high-resolution TEM image along the [110] zone axis of a five-stacked layer of the InAs/GaAs QD without a capping layer. (b) A possible schematic diagram of the (110) projection of the crystal structure for an InAs/GaAs QD, taking into account strain effects.

If the elastic modulus of the InAs layer and Eq. (2) are used, the magnitude of the strain in the vertical direction, the strain component in the horizontal direction, the lattice constant of the InAs layer, and the stress component in the vertical direction can be obtained. The calculated c-axis lattice constant of the InAs layer is 0.6431 nm. This value is different from the measured value of 0.5909 nm. This result indicates that the formation process for InAs QDs is not only pseudomorphic. The angle between the ⟨110⟩ and the ⟨111⟩ directions for the InAs layers is 64.44°.

Figure 2(a) is a HRTEM image of sample S2 corresponding to the top region of five vertically stacked QD layers without a capping layer. The vertical components of the lattice constants of the GaAs substrate and the InAs QD determined from Fig. 2(a) are approximately 0.5653 and 0.5690 nm, respectively. However, the parallel component (0.5741 nm) of the lattice constant of the InAs QD is slightly larger than that (0.5653 nm) of the GaAs substrate. This means that the InAs QD receives a compressive strain. However, the lattice constant of an edge side of a QD denoted by "A" region in Fig. 2 is larger than that of the core side of a QD denoted by "B" region. The angle between the ⟨110⟩ and the ⟨111⟩ directions for the InAs layers is 54.91°. A possible schematic diagram of the (110) projection of the crystal structure for an InAs/GaAs QD, taking into account strain effects, is shown in Fig. 2(b).

Figure 3 shows schematic diagrams of a strain-relaxation process of an InAs/GaAs QD, indicative of the strain distri-

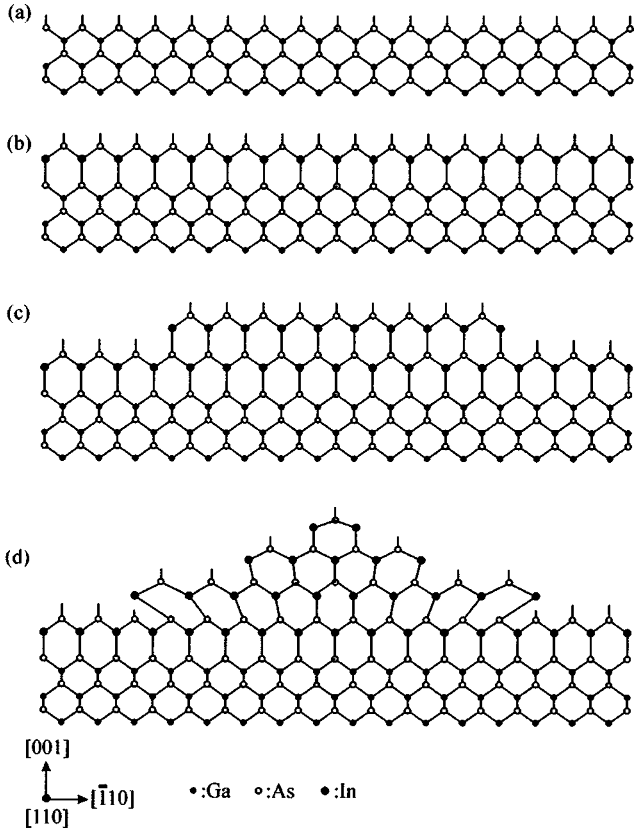

FIG. 3. Schematic diagrams of a strain-relaxation process of an InAs/GaAs QD: (a) the surface of GaAs substrate before deposition of an InAs layer, (b) the surface after depositing one monolayer deposition of an InAs layer, (c) the surface after attachment of a partial InAs layer, and (d) the preferential arrangement of In atoms and As atoms due to strain effect between the InAs island and the GaAs substrate. The in-plane lattice constant of the island is higher than that of the two-dimensional region due to partial strain relaxation.

bution around the island; (a) the surface of GaAs substrate before deposition of an InAs layer, (b) the surface after depositing one monolayer deposition of an InAs layer, (c) the surface after attachment of a partial InAs layer, and (d) the preferential arrangement of In atoms and As atoms due to strain effect between the InAs island and the GaAs substrate. It is reasonable to assume that the lattice constant of the island approaches that of unstrained InAs; thus, the islands become less strained regions. Since the island has a finite lateral dimension, a relaxation of the lattice strain existing in the island can occur, and the island can expand laterally. As a result, the value of the lattice strain in three-dimensional islands is smaller than that in two-dimensional regions, where the strain of the wetting layer is thought to be uniformly distributed. Since a cubic unit cell in the InAs wetting layer is initially distorted into a tetragonal cell, the lateral relaxation of the lattice strain in the InAs QD occurs. The in-plane lattice constant of the QD is higher than that of the two-dimensional region because of a partial relaxation of the strain, as shown in Fig. 2. Therefore, the effective parameter of the lattice mismatch of the island decreases when going from the bottom atomic layer to the top layer.

In summary, the strain distribution around a QD island was observed by using HRTEM. The in-plane surface lattice parameter of the InAs layer was determined to investigate the strain relaxation behavior of the InAs QDs. A schematic diagram of a strained InAs/GaAs QD was presented on the basis of the HRTEM results. These results provide important information on the growth process for and the strain-relaxation behavior of InAs/GaAs QDs.

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