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TEM Investigations of the Compositions in Ge(Si)/Si(001) Quantum Dots

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Semiconductor quantum dots (QDs) have potential applications in key areas of modern technology. Knowledge on the composition of hetero-epitaxial grown QDs is very important for revealing the growth mechanisms and the structure-property relationships of the QDs. However, composition determination in QDs is not an easy task because of the small QD sizes especially in the vertical dimension. In this study, we used two techniques -- [001] zone-axis bright-field diffraction contrast imaging combined with image simulations and electron energy filtering imaging (EFI) – to investigate the composition distributions in Ge(Si)/Si(001) QDs.

Pure Ge was deposited on the surface of Si(001) using molecular beam epitaxy (MBE). Sample A was grown using solid-source MBE at 700°C with a deposition thickness of 0.8 nm and a growth rate of 0.12 nm/min. Sample B was grown using gas-source MBE at a lower temperature of 575°C with a deposition thickness of 1.6 nm and a growth rate of 0.4 nm/min. The resulting QDs in both samples A and B are GeSi alloys. Plan-view TEM observations were carried out using a Philips EM430 operating at 300 kV, and cross-section TEM investigations were carried out using a Philips CM120 operating at 120kV.

Experimental plan-view [001] bright-field diffraction contrast images of the QDs in sample A show strong periodicity with the change of the sample substrate thickness and the period is equal to the effective extinction distance of the transmitted beam. Typical images are shown in Fig. 1 (a_E) – (d_E). Since the contrast arises from strain field in the QDs and the strain field is related to the size, shape and composition in the QDs, it is possible to extract the composition information from the diffraction contrast images through image simulations.

Image simulations were carried out using multi-beam diffraction theory with strain fields obtained from finite element (FE) analysis. The QD shape and size used in the FE model was determined from cross-section investigation. FE models with various composition distributions have been tested for the image simulations. The model that has the highest Ge content at the top of the QD and the lowest Ge content at the QD/substrate interface presents simulated images best fitting the experimental ones. The simulated results are demonstrated in Fig. 1 (a_S) – (d_S) which correspond to Fig. 1 (a_E) – (d_E), respectively.

Sample B was investigated using EFI from cross-section. Elemental mapping was performed with the GIF using the three-window technique. The Si $L_{2,3}$ edge at 99.2 eV was used for Si mapping. Ge maps were obtained using the Ge $L_{2,3}$ edge at 1217 eV. To cancel the intensity change in EFI images possibly induced by thickness variations, the atomic ratio map technique is used, in which the atomic ratio of two elements is related to the ratio of their elemental map intensities by a k-factor (ratio of partial ionization cross-sections of the two elements). However, because the parameters (recording time, beam convergence, and slit width, etc.) for acquiring the Ge and Si maps are different, determining a k-factor is very difficult. As a result, only a relative composition distribution was obtained. Figures 2 (a) and (b) show Ge and Si maps, respectively. Figure 2 (c) shows the relative atomic ratio of Ge and Si obtained from the Ge map divided by the Si map and Fig. 2 (d) is a pseudo-color (spectrum) image of Fig. 2 (c) to see more clearly the intensity distribution and the interfacial structure in Fig. 2 (c). It is clear that, different from the elemental distribution in sample A, the highest Ge content in sample B is located at the QD center.

Detailed investigation of the interfacial structures and the compositions in QDs and wetting layers leads to the conclusion that alloying, elemental enrichment, elemental interdiffusion and redistribution happen subsequently during the Ge deposition processes.

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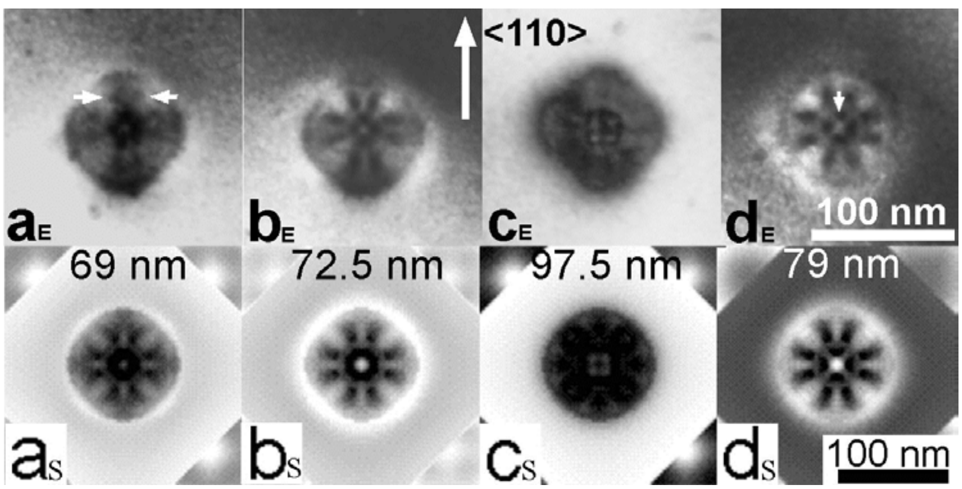

Figure 1. (a_E) – (d_E) Experimental [001] bright-field diffraction contrast images of QDs in sample A taken from areas with different substrate thickness; (a_S) – (d_S) Simulated images based on a model with the Ge content increases up to the QD top. The substrate thickness used in each simulation is shown on the top of the simulated image.

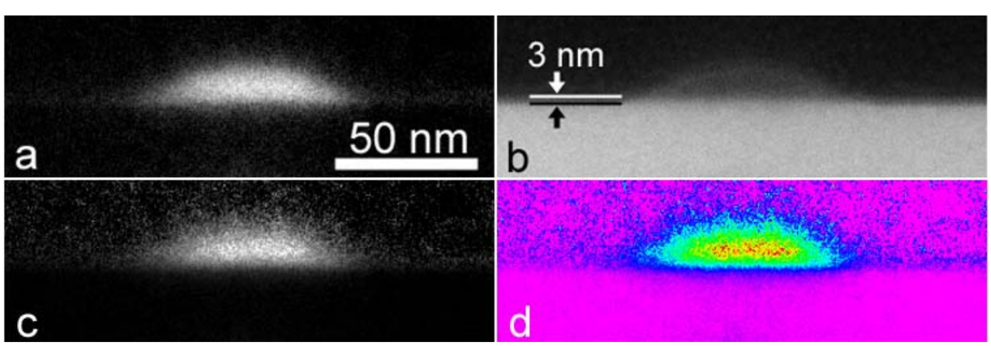

Figure 2. (a) A Ge map; (b) a Si map; (c) the result of the Ge map divided by the Si map; and (d) the pseudo-color image of (c) showing the highest Ge content at the QD center.

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