Grazing-Incidence X-ray Diffraction Analysis of Si/Ge/Si(001) Heterostructures

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Introduction

The ability to grow high-quality heteroepitaxial Si/Ge/Si on Si(001) with abrupt interfaces is limited by both the lattice mismatch (4.2%) between Ge and Si and by the propensity for Ge to segregate in Si during growth. Initial reflected high-energy electron diffraction (RHEED)[1] and transmission electron microscopy[2] studies indicate that the introduction of Te as a surfactant, prior to Ge deposition, can enhance epitaxial quality. From these studies, it is speculated that Te passivates the Si(001) surface and that Te restricts the surface mobility of Ge. We use grazing-incidence x-ray diffraction (GIXD) to measure the in-plane structure of Si/Ge/Si(001) heteroepitaxial structures grown with and without Te as the surfactant.

Methods and Materials

The Si/Ge/Si(001) samples were grown using molecular beam epitaxy. Approximately one monolayer (ML) of Te was predeposited onto a clean 2 × 1 reconstructed Si(001) surface. Ge was then deposited at 410°C; the Ge thickness varied from 1 to 11 MLs. Finally, a Si cap of 60 to 70 Å was deposited at the same temperature. The absolute Ge coverage was determined with x-ray fluorescence combined with a Rutherford backscattering spectroscopy (RBS) calibration. The Si cap thickness was verified with x-ray reflectivity. Grazing-incidence x-ray diffraction measurements were performed at the DND CAT 5-BM-D station at an incident energy of 10.5 keV. In this experiment, the angle of incidence was kept near the critical angle (0.17°) for total external reflection from Si. By varying this angle slightly we were able to selectively probe different depths within the heterolayer.

Results and Discussion

Figure 1 shows in-plane H-H (r.l.u.) scans at L = 0.03 for two different samples. (Each had a 65-Å-thick Si cap.) At this grazing-incidence condition, the scattering depth is ca. 75 Å, and thus the in-plane scattering is sensitive to the structure of the Si cap and Ge buried layer. For the 10 ML sample grown without a surfactant, a peak is present at H = 1.93. This is close to the expected H = 1.92 position for a pure Ge bulk lattice constant, implying that relaxed Ge is present in the heterostructure. The 11.3 ML sample that was grown with Te as a surfactant shows no feature at this H value, a result indicating that the Ge epilayer is strained with an in-plane lattice constant constrained to that of Si(001). Figure 2 displays two scans at different depth sensitivities for the 10 ML sample that was grown without surfactant. At L = 0.01, the peak at H = 1.93 still appears, but not at L = 0.005, where the penetration depth is 35 Å. This may indicate that the relaxed Ge is buried.

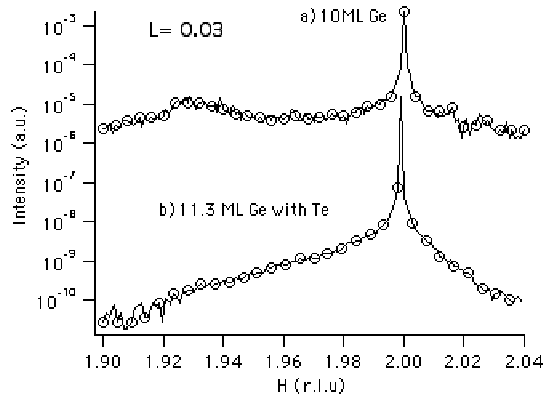

FIG. 1. GIXD measurement of two different Si/Ge/Si(001) heterolayer structures around the Si (2 2 L = 0.3) Bragg peak: (a) 10 ML Ge with no surfactant; (b) 11.3 ML Ge with Te as a surfactant.

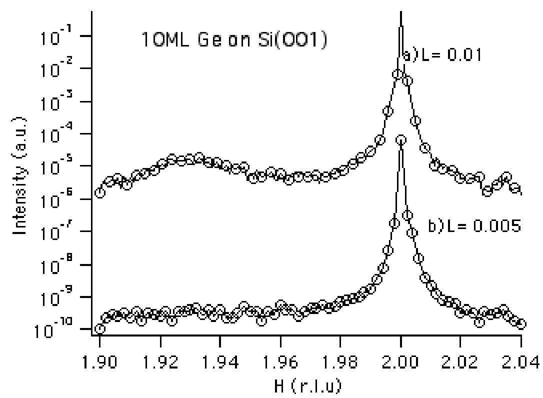

FIG. 2. GIXD measurement of sample with 10 ML Ge and no surfactant: (a) for L = 0.01; (b) for L = 0.005.

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