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Monolayer Heterostructures Studied by Surface-Sensitive EXAFS

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Surface-sensitive EXAFS (extended X-ray absorption fine structure) technique which can probe the local structure of epitaxially grown monolayer heterostructures has been developed. The Si/$(Ge)_m$/Si heterostructures and $(Ge/Si)_m$ superlattices (m=1,4) grown by molecular beam epitaxy (MBE) have been studied. The Fourier transform analysis indicates that the ordered Si-Ge heterointerface is formed. The determined bond distance suggests that the dislocation-free growth of lattice-matched Si-Ge is stabilized not only by bond-bending but also by bondlength relaxation which partly compensates the strains confined at the interface.

1. Introduction

The recent advances in epitaxial-growth technique provided means to prepare ordered layered heterostructures by the alternating deposition of monolayers[1] of lattice-matched semiconductors. To control electronic properties of the heterostructures of III-V and IV semiconductors, the local structure information in relation with growth conditions are important. Surface-sensitive EXAFS[2] (extended X-ray absorption fine structure) technique has been developed, which can probe the local structure of epitaxially grown heterostructures within several tens of Å below the surface. In this paper, we demonstrate the capability of this technique and present the results of structural studies on Si/$(Ge)_m$/Si heterostructures and $(Ge/Si)_m$ superlattices (m=1,4) grown on Si(100) by MBE.

2. Results and Discussion

2.1 Sample Preparation

Si/$(Ge)_m$/Si and $(Ge/Si)_m$ samples with m=1,4 were grown on Si(100) at 400 °C by MBE technique after depositing 5000 Å thick Si buffer layers. Atomic layer growth was controlled by monitoring the reflection high energy electron diffraction (RHEED) intensity oscillation following procedures of Sakamoto et al[3]. One monolayer (ML)

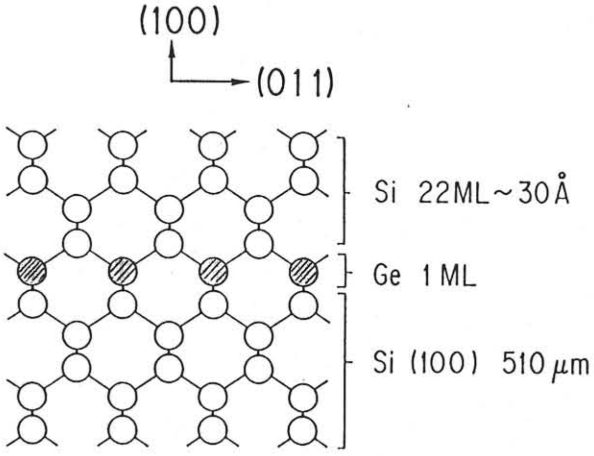

Fig. 1 Si/Ge/Si heterostructure

growth or full coverage corresponds to the maximum RHEED intensity. After depositing $(Ge)_m$ or $(Ge/Si)_m$ layers, 22 ML Si top layers were grown as indicated in Fig. 1.

2.2 Experimental Procedure

Surface-sensitive EXAFS technique is based on the fluorescence detection method[4] and total reflection geometry[5] to achieve surface-sensitivity or surface-selectivity. In this paper, we report a new fluorescence detection technique[6] using a high energy resolution detector. This detector eliminates distortions in spectra due to diffraction inherent to single crystalline materials, which made it possible to study the epitaxially-grown hetero-structures.

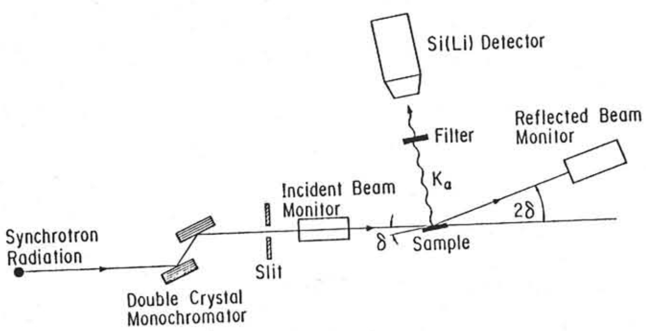

Fig. 2 Schematic of experimental setup.

In Fig. 2, a schematic drawing of experimental setup[7] is shown. To selectively excite the near-surface region, samples were irradiated with intense X-rays from synchrotron radiation in a total reflection geometry[5]. Using a sagittally bent Si (111) crystal monochromator[8], a typical photon flux of 3 x 10^{10} photons/sec with an energy resolution of 2 eV (9 keV) was obtained. A Si(Li) solid state detector (SSD) was used to record the fluorescence intensity variation as a function of excitation energy. With decreasing the glancing angle of incident X-ray beam, the surface sensitivity increases. Below the critical angle, X-rays are totally reflected and cannot penetrate into the region beyond ca. 50 Å. This can reduce the background scattering or fluorescence from bulk. X-ray filter is used to reduce scattering radiation.

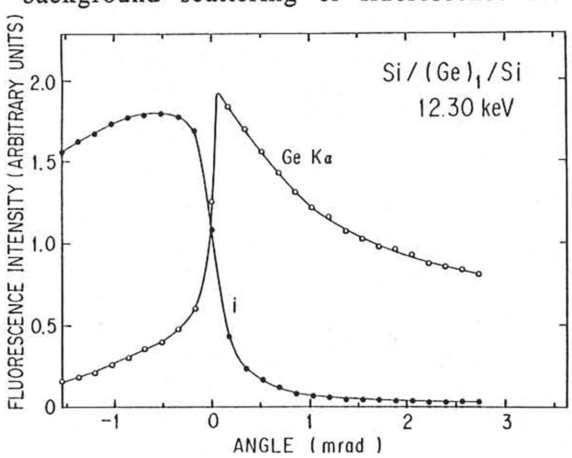

Fig. 3 Reflected beam and fluorescence signal intensity

2.3 $Si/(Ge)_m/Si$ heterostructure

Figure 3 shows the reflected beam (closed circle) and Ge K_α fluorescence (open circle) intensities as a function of glancing angle for Si/Ge/Si heterostructure. In Fi. 4, the K_α fluorescence yield spectrum[6] measued in a total reflection regime is plotted as a function of photon energy. Below the critical angle θ_c (ca. 3 mrad), X-ray evanescent waves decay exponentially, which enhances the surface sensitivity by roughly three orders of magnitude. A high signal-to-background ratio (ca. 30) and absence of artifacts due to diffractions are achieved by the improved surface-sensitivity and energy discriminating capability of a SSD.

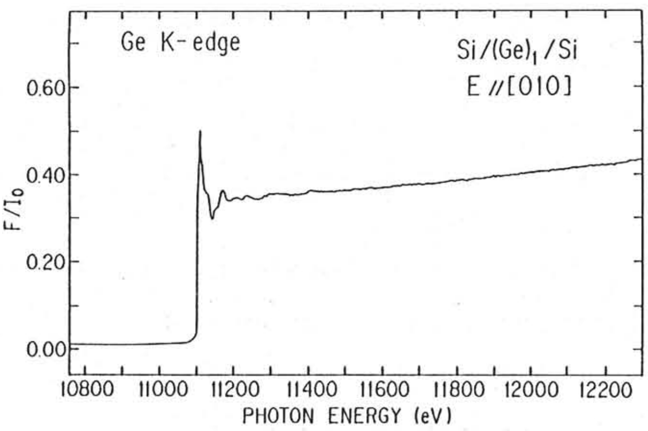

Fig. 4 Ge K-fluorescence yield spectrum for Si/Ge/Si heterostructure.

The results of a standard Fourier transform[2] performed for the Ge K-EXAFS oscillations (Fig. 4) are shown in Fig. 5. Peaks in the upper curve in Fig. 5 indicate the positions of near-neighbors around Ge atom. The lower curve shows the results for crystalline (c-) Ge powder measured in a transmission mode. The

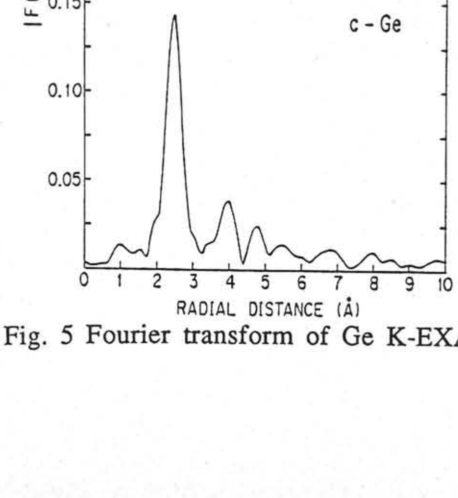

Fig. 5 Fourier transform of Ge K-EXAFS

presence of second (3.8 Å) and third nearest (4.8 Å) neighbor peaks indicates that Si/Ge/Si heterostructure is an ordered phase.

The k-dependence of EXAFS amplitude of Si/Ge/Si heterostructure shown in Fig. 6 suggests that the nearest neighbors are low-z element, i.e. Si. The number of like-atom (Ge-Ge) bonds is small. This rules out a possible three-dimensional (3-D) growth of Ge clusters.

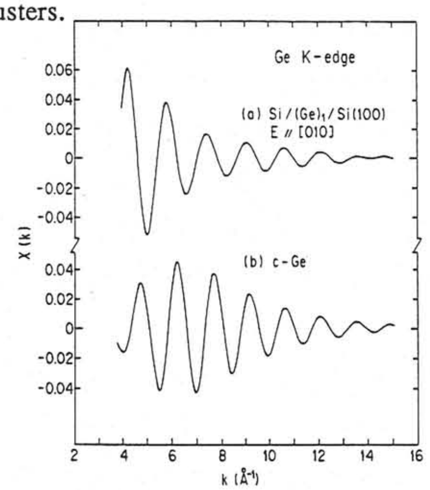

Fig. 6 Filtered Ge K-EXAFS oscillations.

To determine the Ge-Si distance, the filtered single-shell Ge-Si EXAFS oscillations were analyzed using theoretical phase shift and backscattering amplitude by Teo and Lee[9]. The absorption threshold was chosen, which gives k-independent Ge-Si distance. The observed Ge-Si distance (2.37 Å) is fairly shorter than the Ge-Ge length (2.45 Å) in c-Ge but close to the Si-Si distance (2.35 Å) in c-Si. These results suggest that the bond-bending strains at the heterointerface are partly compensated by bondlength relaxation. The strains caused by the elongation of Ge layers along the [100] direction is partly compensated by the bondlength relaxation (compression), which stabilizes the strained heterostructure. Therefore Ge layers are rather compressed from local structural viewpoints, which may modify band structure resulting in new optical transitions as reported by Pearsall et al[10].

The results for Si/$(Ge)_m$/Si (m=2,4) and $(Si/Ge)_m$ (m=4) show that the ordered heterointerface is stable up to at least four Ge layers.

3. Summary

We show that the local structure of monolayer heterostructures can be studied by surface-sensitive EXAFS technique using a high energy resolution fluorescence detector. This technique has been applied to Si/$(Ge)_m$/Si heterostructure and $(Ge/Si)_m$ superlattices. The results show that the ordered heterointerfaces are formed. We found that bond-bending strains confined within Ge layers are partly compensated by bondlength relaxation.

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