# X-ray standing wave and diffraction studies of Si /Ge/ Si(001) heterostructures

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## Introduction

As demonstrated earlier, surfactants can be used to influence the growth mode in strained-layer heteroepitaxy [1]. Due to a lower surface free energy, Ge segregates in Si resulting in poor interfacial quality in Si/Ge/Si heterostructures [2]. Surfactant-mediated epitaxy (SME) has been shown to improve the interface abruptness between Ge and Si [3]. Although Bi has been reported to act as a surfactant in other systems [4–6], little is known of its efficacy in growing Si/Ge/Si(001). We studied the SME of Si/Ge/Si(001) heterostructures with Bi as a surfactant using x-ray standing waves (XSW) and grazing incidence x-ray diffraction (GIXD).

## Methods and Materials

The samples were prepared by molecular beam epitaxy (MBE) in an ultrahigh vacuum (UHV) chamber. Ge and Bi were evaporated from Knudsen cells while Si was evaporated from an e-beam evaporator. Samples were grown at 400°C with and without Bi. For SME-grown samples, approximately one monolayer (ML) of Bi was deposited prior to deposition of Ge and Si. Samples were prepared with Ge coverage varying from 1 to 10 MLs. The nominal thickness of the deposited Si was 100 Å. The absolute Ge coverage of each sample was measured by comparing Kα fluorescence to a standard sample that was calibrated by Rutherford backscattering.

Referring to Figure 1, in these XSW measurements the XSW field shifts inward by one-half d-spacing when scanning in angle through a strong Bragg reflection from the substrate. By analyzing the Ge fluorescence modulation, the Si lattice positions of the Ge atoms can be determined from the coherent fraction ($f_H$) and coherent position ($P_H$). The XSW measurements were performed at the DND-CAT 5-ID-C station.

In GIXD, the incident and reflected beams make small angles with the surface and therefore the depth of scattered x-rays is very shallow. GIXD can therefore be used to study the in-plane structure of very thin films of a few monolayers thickness. The GIXD measurements were performed at the 5-ID-C and 2-BM-B stations.

## Results and Discussion

Figure 1 shows the (004) XSW results for two samples with a low (1–2 ML) coverage of Ge. The reflectivity at the Si(004) Bragg peak is also shown. The angular dependence of Ge Kα fluorescence for 1.1 ML of Ge buried in Si(001) without Bi and 1.5 ML of Ge with Bi as a surfactant show a significant difference. The solid lines are the best fits to dynamical diffraction theory. When Bi was used, the coherent fraction increased as the Ge atoms took the expected lattice positions predicted by continuum elasticity theory. When Bi was absent, a significant amount of Ge atoms segregated into the Si layer resulting in a lowered coherent fraction.

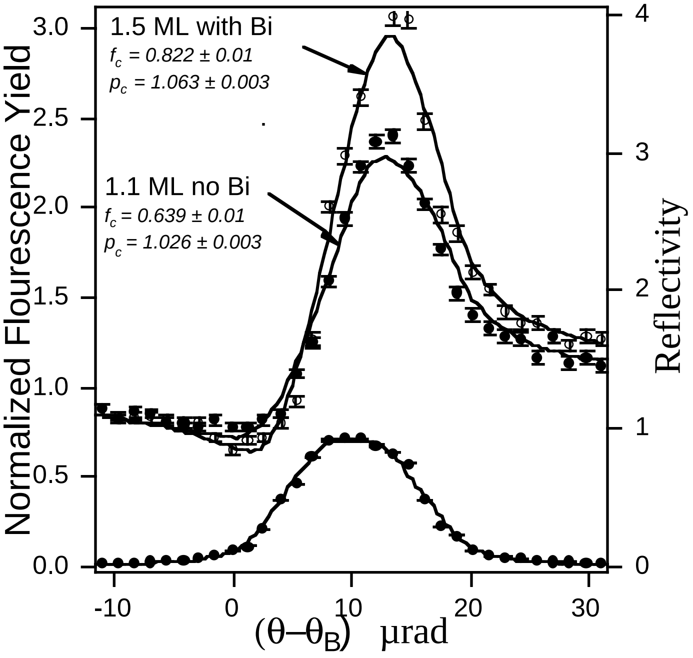

Figure 1: Ge XSW measurements for Si(004) reflection.

Figure 2 shows the GIXD measurements along the direction perpendicular to the (2 2 L) reflection at L = 0.01. At this grazing angle condition, the scattering depth is much less than the 100 Å thickness of the Si cap layer. The sharp peak in both curves is from Si. For the 10 ML sample grown with Bi, the Ge layer is very sharp as Bi prevented intermixing of Ge and Si layers. As the Ge layer is very well buried under the 100 Å thick Si layer, no peak is seen at the Ge position at H = K = 1.92.

For the sample without Bi (in addition to the Si peak), two more peaks are seen: a weak peak at the Ge position and another one between Si and Ge. These two peaks are from relaxed Ge and Ge-Si alloy, respectively. The Ge-Si alloy is formed by diffusion of Ge into the Si layer

Bi is therefore found to be effective in preventing segregation of Ge in Si. Our other XSW measurements for higher Ge coverage also showed that Bi decreased the disorder in Si/Ge/Si(001) heterostructures.

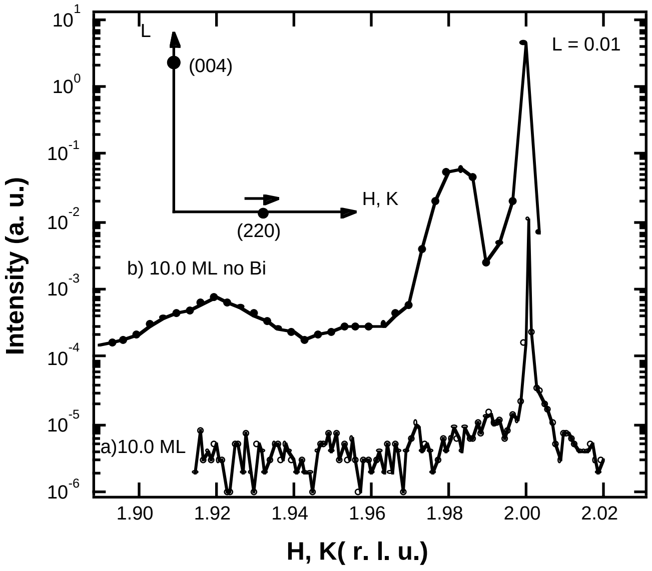

Figure 2: GIXD measurements around the Si(2 2 L) reflection.

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