Determination of Ge Vibrational Amplitude in Si/Ge/Si(001)

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Introduction

In the high-resolution analysis of surfaces and interface structures, it is important to know the vibrational amplitude of the atoms under investigation. In many circumstances, the vibrational amplitude is assumed to be "bulklike." This is often a good approximation; however, by performing multiple-order x-ray standing wave (XSW) experiments on the same sample, it is possible to experimentally solve for the vibrational amplitude of nonhost atoms [1, 2]. This study applied this technique to determine the vibrational amplitude of a buried ultrathin Ge layer grown on Si(001).

Methods and Materials

The Si/Ge/Si(001) sample was grown by using surfactant-mediated molecular beam epitaxy. As the surfactant species, one monolayer (ML) of Te was predeposited onto a clean 2×1 reconstructed Si(001) surface before Ge was deposited at 410°C. The thickness of the Ge for this particular sample was 1.3 ML. Finally, a Si cap of 50-70 Å was deposited at the same temperature. Te was used as a surfactant in order to prevent intermixing between the Ge layer and the Si cap layer. The absolute coverage of the Ge was determined with x-ray fluorescence, and the Si cap thickness and interface roughness were verified with x-ray reflectivity.

The XSW measurements were made at the 5-ID-C beamline of the APS. The sample used for the measurement was 1.3 ML of Ge grown with Te overpressure on Si(001) and buried in 60 Å of Si. The selection of 12.5-keV x-rays was made by using two symmetric Si(111) monochromator crystals. X-rays then passed through two post-monochromator Si "channel cut" crystals that were tuned to either the Si(004) or Si(008) reflection to minimize dispersion. The same sample was rocked through both the Si(004) and Si(008) reflections, and reflectivity and fluorescence were collected simultaneously.

Results and Discussion

Figures 1(a) and 1(b), respectively, show the (004) and (008) XSW measurement on the same sample. The important output parameter for this measurement is the coherent fraction (F). The (004) and (008) probe the structure of the Ge atoms in the [001] direction. The coherent position (P) of the Ge for the 004 should be twice that of the 008 by symmetry. The difference in the coherent fractions for the two reflections results from their different Debye-Waller factors. The Debye-Waller factor is directly related to the vibrational amplitude of the Ge. By combining these two measurements, we determined that the rms vibrational amplitude ($\langle u_{hkl}^2 \rangle^{1/2}$) of the Ge atoms were 0.08 ± 0.015 Å, which is close to the value for bulk Ge (0.068 Å)

Acknowledgments

Use of the APS was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-ENG-38. This work was supported by the National Science Foundation under Contract Nos. DMR-9973436 and DMR-0076097.

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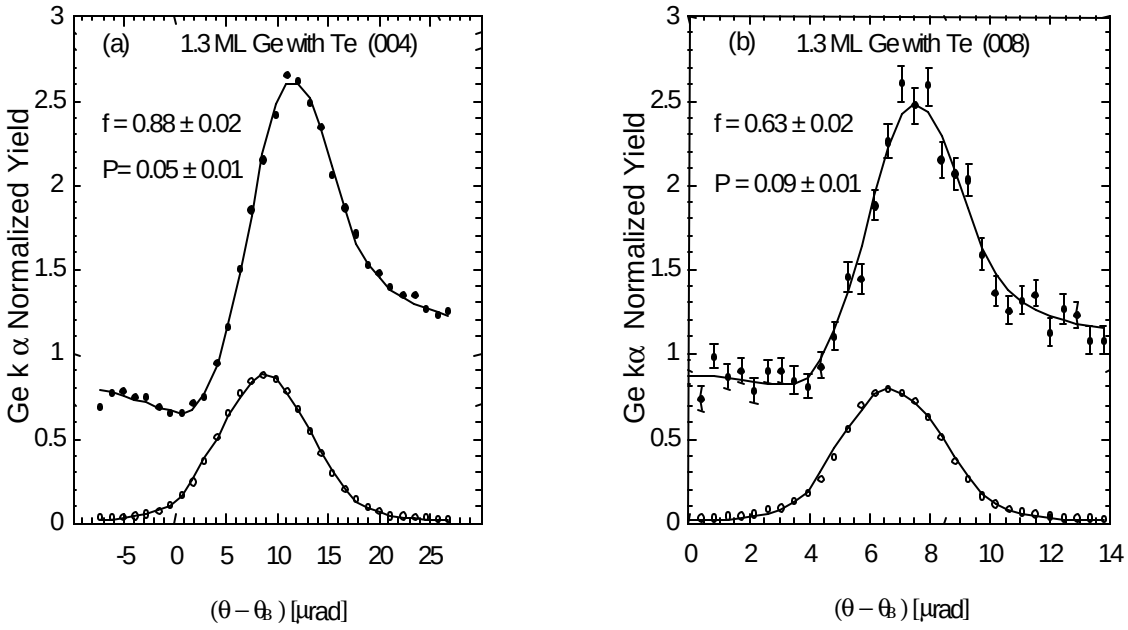

FIG. 1. The experimental and theoretical angular dependency of the Ge Kα fluorescence yield and reflectivity collected while scanning in angle through the (a) Si(004) and (b) Si(008) reflection. The sample is 1.3 ML Ge/Si(001) with Te as a surfactant.