Si(100) and Ge(100) core-level shifts: A reevaluation

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High resolution core level photoemission was used to study the Si 2*p* core levels of the clean Si(100) surface and other related surfaces, and the Ge 3*d* core level of the clean Ge(100) surface and other related surfaces. Two surface components *S* and *S'* for the Si 2*p* core level from the clean Si(100) surface have been resolved. The *S* and *S'* components were resolved for the Ge 3*d* core level from clean Ge(100) surface for the first time. On both surfaces, *S* and *S'* components are identified to be the contribution from surface dimer atoms and the subsurface layer, respectively.

I. INTRODUCTION

The Si(100) and Ge(100) surfaces have been subjected to extensive theoretical and experimental studies. Although their atomic structures are fairly well understood, a number of questions related to their electronic structures remain unanswered. For example, the number of surface core-level shifts and the origin of these shifts are still not clear. Two surface components (*S*, *S'*) have been reported in the Si 2*p* core level spectrum for Si(100) surface. However, the explanation for the origin of the surface components remains controversial. One explanation is that the *S* component is from the upward buckled Si dimer atoms and the *S'* component from the downward buckled dimer atoms.[1] Another explanation is that *S* is the contribution of all the dimer atoms and that *S'* is the contribution of the subsurface atoms.[2] Theoretical calculations have shown that the subsurface atoms relax from their ideal bulk positions,[3,4] but charge transfer to or from the subsurface atoms has not been clearly observed experimentally. Another puzzling fact is that only one surface component was observed in the Ge 3*d* core level for Ge(100) surface[5] even though the Ge(100) surface is very similar to the Si(100) surface. In order to understand the above problems, we have performed a high-resolution core-level photoemission study on these surfaces.

Core-level photoemission is an excellent tool to study the shifts induced by charge transfer.[6,7] However, before photoemission can give quantitative information, accurate knowledge of the natural line shape must be known. In the now conventional method, the line shape is obtained by analyzing the spectrum in bulk sensitive mode using photoelectrons of low kinetic energy. This line shape is later used to fit a spectrum taken in a surface sensitive mode using photons of appropriate energy. The problem with this conventional method is that the Gaussian line shapes are different for different photon energies. Another method to determine the natural line shape has been suggested,[8,9] in which a nonreactive epitaxial overlayer was used to eliminate the surface components in the substrate core-level spectrum without introducing a chemically shifted component. To accurately use this method, it is critical to choose an appropriate overlayer. Such a method has been used to obtain the Si surface core-level shifts using a Ge overlayer.[2,9] However, the Ge 3*d* core-level bulk line shape cannot be obtained with only a Si overlayer, because Si does not grow uniformly on Ge(100). An ordered Sb overlayer has been used to eliminate the surface components in the Ge core-level spectrum.[10] But the problem with an Sb overlayer is that only 1 monolayer (ML) of ordered Sb can be grown on Ge (100) surface, which may not be sufficient to eliminate the subsurface contribution to the surface.[2] In our experiment, the surfactant assisted growth method[11-13] was used to grow a Si(Ge) overlayer on the a Ge(Si) substrate with Sb as the surfactant. Epitaxial growth of Ge on Si and Si on Ge was achieved using this method.[14]

We have performed high-resolution core-level photoemission on clean Si(100), Sb/Si(100), Sb/Ge/Si(100), Ge(100), Sb/Ge(100), and Sb/Si/Ge(100) surfaces. The results are presented in the following sections.

II. EXPERIMENTAL DETAIL

The photoemission experiments were performed with a Vacuum Generators (VG) ADES-400 angle-resolved spectrometer using a toroidal grating monochromator (beam line 1-2) at the Stanford Synchrotron Radiation Laboratory. The overall instrumental resolution (monochromator and spectrometer) is between 0.2 and 0.25 eV. The chamber had a base pressure of less than 1×10^{-10} Torr.

A clean Si(100) surface was prepared as follows. *N*-type Si wafers were chemically precleaned and etched with HF before being introduced into the ultrahigh vacuum (UHV) chamber. Cleaning was achieved by pre-baking the sample at 600 °C for 1 h and then heating to 950 °C. The temperature was ramped up slowly in order to keep the chamber pressure in the 10^{-10} Torr range during the heating process to minimize contamination. After cleaning, the Si(100) wafer shows a sharp two-domain (2×1) low-energy electron diffraction (LEED) pattern and strong emission from surface states. No contamination is observed in the core-level spectra.

Sb/Si surfaces were prepared by depositing several monolayers of Sb on the clean Si(100) surface and then annealing at 500 °C. LEED showed a 1×1 pattern with diffuse 2×1 spots. This pattern indicates the presence of an ordered monolayer of Sb on the Si(100) surface. The Sb atoms form a dimer structure on the Sb/Si surface similar to the Si dimer on a clean Si(100) surface.[15]

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