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Core-level shifts of the Ge(100)-(2 × 1) surface and their origins

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The surface shifts of the Ge $3d$ core level from the clean Ge(100)-(2×1) surface have been investigated using Si epitaxial layers grown with Sb as a surfactant. We are able to obtain a line shape close to that of the natural line shape of the Ge $3d$ and, in turn, we have resolved two surface-related components in the core-level spectrum of the clean surface, in contrast to previously observed single component. The origin of these shifts is addressed: one comes from the top layer and the other from the layer below the surface. A comparison with the Si(100)-(2×1) surface is also presented.

The Si(100)-(2×1) and Ge(100)-(2×1) surfaces have been extensively studied for decades due to their practical importance and fundamental interest. Despite much progress, a number of questions regarding these reconstructed surfaces remain unanswered. For instance, there is no concensus about how many surface-related components are present in the core-level photoemission spectra. For Si(100)-(2×1), some studies have shown only one surface component but others reported two surface components.[1-5] For Ge(100)-(2×1), only one surface component has been observed.[6-8] The nature of these surface components also remains controversial. A number of theoretical calculations and experimental studies have attributed the observed surface core-level components to the contribution from the top-layer surface atoms, which then favors strong charge transfer between the two atoms within the dimer.[1-4,9,10] On the contrary, other suggest that the observed surface components may arise from different layers, implying that the charge transfer between the two dimer atoms may not be significant.[5,11] Much of the controversy stems from the lack of direct experimental determination of the surface shifts and the lack of convincing evidence of the origination of these surfaces.

The key to accurately resolve the surface shift in the core-level spectrum is to employ a core-level line shape that is close to the nature line shape to fit the experimental spectrum. In order to achieve such a goal, adsorbates that occupy the epitaxial sites of the surface are used to relax the surface and to make the substrate better approximate the bulk environment. In this case, one hopes to get rid of the surface shift(s) from the spectrum and take the remaining as the bulk component. Moreover, it is desired to have neither adsorbate-induced core-level shifts nor interference in the spectrum from the adsorbates themselves. The epitaxially grown adsorbate, Sb, has been successfully applied to the III-V(110) surfaces to resolve surface core-level shifts.[12] For some semiconductors, thick epitaxial layers were required to turn the substrate into a true bulk environment.[13] This has also been experimentally demonstrated in the case of Si(100).[5] For Ge(100), an epitaxial Si overlayer is probably the best candidate because Si and Ge are similar in many aspects, including electronic and chemical properties. Furthermore, with the help of the recently emerging surfactant-assisted growth technique one is able to achieve uniform and epitaxial growth of multilayer SI on the Ge(100) substrate, which has not been realized by other growth techniques.[14,15] In this work, we used Sb as a surfactant in Si, Ge epitaxial growth, and our results show that uniform layers can indeed be grown with good epitaxy.[16] We demonstrate that more than two epitaxial layers are required to yield the narrowest line shape in the core-level photoemission spectrum. With the obtained line shape, we are able to directly determine the core-level shifts, their positions, and amplitude. These data as well as their changes with epitaxial growth provide unambiguous evidence about the origin of these shifts.

The experiment was carried out at the Stanford Synchrotron Radiation Laboratory (SSRL) on beam line I-2 with a 6-m toroidal grating monochromator. A VG ADES400 angle-resolved system equipped with a hemispherical analyzer was used. The combined resolution was about 0.2 eV, including contributions from both the analyzer and the monochromator. In this particular study, photon energy was fixed. Thus, we eliminate potential complication in data analysis due to variation in monochromator resolution at different photon energies and in probing depth at different photoelectron kinetic energies. The n-type Ge(100) wafers with less than 1° miscut were cleaned by thermal annealing at $\sim 800\,^{\circ}\mathrm{C}$. A sharp (2×1) diffraction pattern with two domains from these surfaces was observed from the low-energy electron-diffraction (LEED) optics. Sb was evaporated from a tungsten filament evaporator, and Si was evaporated with an electron-beam evaporator. Thorough outgassing was performed prior to deposition, and no trace of contamination was found within the sensitivity of photoemission. The pressure was kept in the 10^{-10} torr range during evaporation with a base pressure around 1×10^{-10} torr.

After the Ge(100) surface was thermally cleaned, a couple of monolayers (ML) of Sb (1 ML$=6.27\times10^{-14}$ atom/cm^2) were deposited on this surface. After deposition thermal annealing up to $\sim 500\,^{\circ}\mathrm{C}$ leads to the formation of 1 ML of Sb on the surface.[17] This layer is ordered, as indicated by an observed (2×1) LEED pattern with weak and diffuse half-order spots. Further evidence for a single-ordered Sb monolayer is found in the observed dispersive features in angle-resolved photoemission (ARPES) valence-band spectra (not shown here). It is