Si(100) dimers on clean and acetylene covered surfaces

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The properties of acetylene adsorption on Si(100) are an example of the behavior of small hydrocarbons on silicon surfaces. There is considerable interest in bonding units that can be used for attaching functional groups to silicon surfaces, which would have a wide spectrum of applications[1]. The surface science understanding of Si surfaces has made key contributions for "wet" chemistry adsorption applications. Since near-flat (100) surfaces have two domains we use the property that a miscut of 3.5° or large gives a single-domain 2×1 surface, which reduces the complexities of surface-structure analysis. The 2×1 net is the result of Si surface atoms forming dimer pairs.

The Si(100) surfaces were cleaned by widely used methods which primarily consists of desorbing an oxide layer by heating in the ultrahigh vacuum condition. The well known surface components for the Si 2p level and the valence bands (VB) are obtained. A high energy-resolution energy distribution curve (EDC) is shown in Fig. 1, where the Si 2p peak is fitted with component lines. During the fitting, a Lorentzian width of 0.085 eV, a spin-orbit splitting of 0.602 eV and a branching ratio of 0.5 is used for all components. There are five of them, which could give concern for over interpretation of the data, but careful analysis and examination of the residual between the data and the fit demonstrates the appropriateness of the results. The line fitting is very close to that reported by others and we agree with their component assignments[2, 3, 4].

The surface is saturated with acetylene which is 0.5 monolayer (ML) film. The spectrum and its component lines are shown in Fig. 2, where only three components are found. Note, that the "minimum" between the spin-orbit pairs in the EDC is gone in the latter case because of the change in the environment of the Si atoms. Figure 3 shows the associated C 1s EDC. The valence band spectra that accompany the above spectra are shown in Fig. 4. It is again found that the surface state is extinguished by 0.5 ML of C_2H_2. The adsorption shifts the spectral features by about 200 meV due to the change in surface-Fermi-level position.

After C_2H_2 adsorption there remains only two of the component lines found in the clean surface EDC; B is for bulk Si atoms, S′ is for Si atoms in a site in the surface region, and is attributed to atoms in the second layer.. The small line C could be Si atoms in the third layer or at defect locations. The components S and SS are attributed to the up and down

Si atoms in the asymmetric surface dimers and are the lines are extinguished by the adsorption process.

What is the origin of the new component line A in the covered spectrum? It is attributed to first-layer Si dimer atoms which are no longer in an asymmetric configuration. The line has about the combined areas of the lines S and SS. The "singleness" of the line indicates that all the first-surface-layer Si atoms are in chemically-equivalent sites but not geometrically-equivalent sites. The symmetry and lack of the obvious components in C 1s spectra (Fig. 3) supports this assignment. As we have reported elsewhere the acetylene molecule is bonded to <u>four</u> surface Si atoms which supports the chemical-equivalency assignment for all the Si surface atoms.

The conclusion is that surface Si atoms still have dimers-like bonds and they are symmetric.

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References

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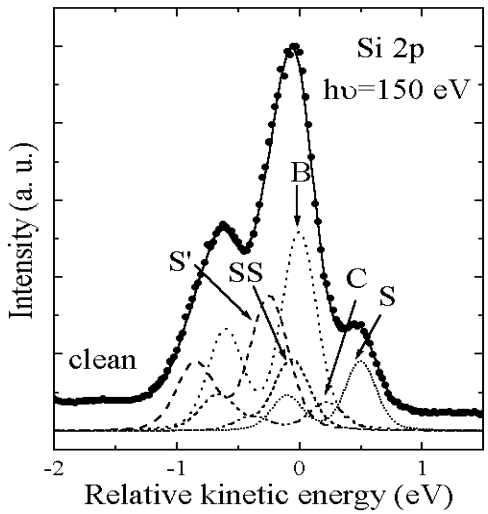

Fig. 1. Curve-fitting of Si 2p EDC for clean Si(100)-2×1 surface. The solid line is the fit line and the solid circles are experimental data. Component are assigned to Si atoms: B for bulk atoms; S for up atoms in dimers; SS for down atoms in dimers; S′ for second-layer atoms; C for atoms at defects or in the third layer.

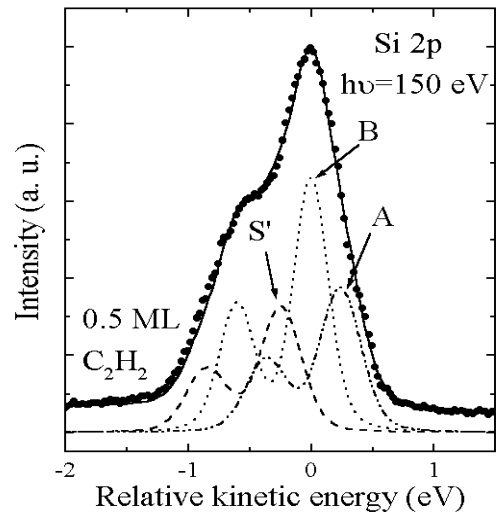

Fig. 2. Curve-fitting of Si 2p EDC for a saturated C_2H_2/Si(100)-2×1 surface. The solid line is the fit line and the solid circles are experimental data. Component A is due to Si atoms in dimers which bond to acetylene. Components B and S′ are found in the clean EDC andare due to bulk and second layer atoms, respectively.

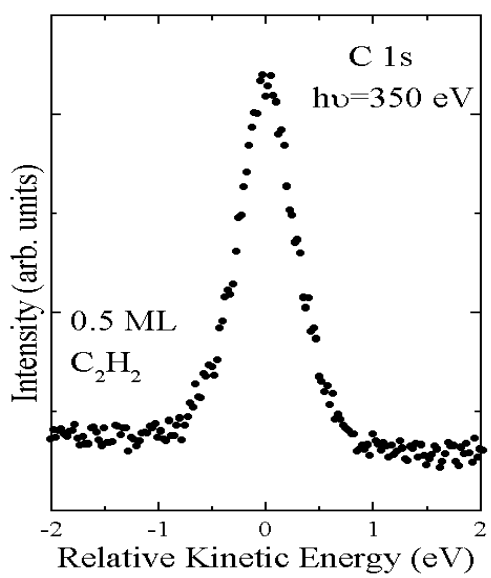

Fig. 3. High-energy-resolution C 1s core-level spectrum for 0.5 ML of acetylene at room temperature (RT).

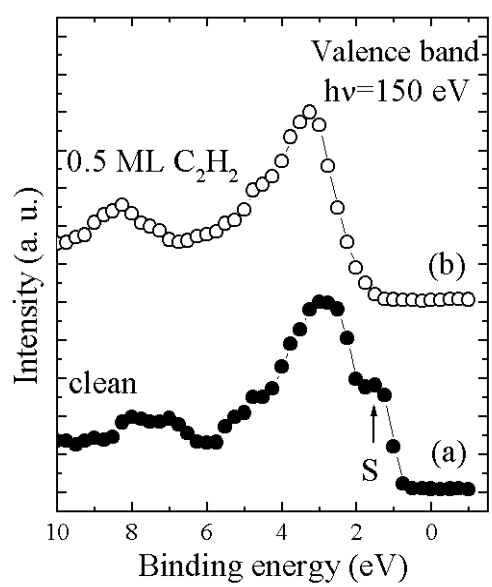

Fig. 4. The valence band spectra of (a) the clean surface; (b) the surface exposed 0.5 ML acetylene at RT. The surface state (S) is totally extinguished.