

Calculation of the optical properties for the Si(111)-das model: 3×3 reconstruction

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ABSTRACT – To understand the origin of the Si(111)-7×7 surface optical response, we have carried out microscopical calculations for a model 3×3 adatom-dimerstacking fault (DAS) structure. Based on these results, the optical properties of the Si(111)-7×7 surface are extrapolated and the main optical peaks are interpreted in terms of the surface band structures. A fair agreement with the experimental data for the Si(111)-7×7 reconstruction is obtained.

1. Introduction

Although Si(111)-7×7 is one of the most studied surfaces */1/*, the large size of its unit cell has hampered establishing a conclusive theory of its electronic structure. Among the several structural models which have been proposed */1/*, the most famous and generally believed to be correct is the DAS model of Takayanagi *et al. /2/*. The DAS model well describes almost all the important features of this surface. However some questions concerning its spectroscopy are still open, since the complexity of the 7×7 reconstruction has hampered the calculation of transition probabilities between electron states. Although optical techniques are a powerful tool to characterize semiconductor */3, 4/* and metallic surfaces */5/*, only a few results have been reported for Si(111)-7×7 */6, 7, 8/*. Moreover, a microscopic calculation of its optical properties, which is needed in order to interpret the spectra, is still lacking.

We have studied theoretically the optical properties of the Si(111)-2×2 and Si(111)-3×3 models, which together contain all the elements of the Si(111)-7×7 DAS reconstruction */9/*, and then have extrapolated the results to the Si(111)-7×7 surface. Since the Si(111)-3×3 structure mimics better the 7×7 reconstruction as compared with the 2×2 one */10/*, we will focus here on the optical response of the 3×3 DAS model.

2. Models and method of calculation

The Si(111)-3×3 model (Fig. 1) contains almost all DAS elements, namely 2 adatoms (AD's) at T₄ sites, 1 corner hole (CH), 3 dimers and the stacking fault (SF). Since the AD's saturate all the dangling bonds (DB's) of the atoms in the first layer, there are no restatoms (RA's) */9/*. (The next layer to the outermost adatom layer is called the first layer, the next to it the second layer, *etc.*.)

The electronic structure and the optical properties have been calculated using a semi-empirical tight binding approach with a *sp*³ *s*^{*} orbital basis */11/*. (For details see Ref. */12/*. We consider a slab of 14 layers, with a total of 104 atoms. X and Y axes are in the surface plane, while the

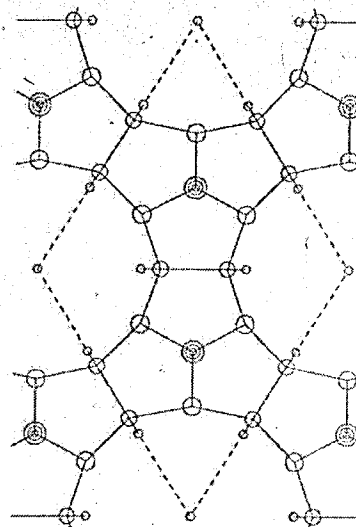


Fig. 1 – Sketch of Si(111)-3×3 structural model, top view. The sizes of the atoms are decreasing with the distance from surface. Unit cell is shown by a dashed line.

Z-axis is normal to the surface.

The atomic positions of the 3×3 have been extrapolated from a recent *ab-initio* molecular dynamics simulation */13/* for the Si(111)-7×7 surface. The correction to the Fresnel formula for the reflectivity, due to the presence of a surface, for normally incident light, is given by */14/*

$$\frac{\Delta R}{R} = \frac{8\pi\omega}{c} \text{Im} \left(\frac{\alpha^{hs}(\omega)}{\epsilon_b(\omega) - 1} \right), \quad (1)$$

where $\epsilon(\omega)$ is the bulk dielectric function, and $\alpha^{hs}(\omega)$ is the polarizability of the half of the slab. Transitions up to 13 eV were taken into account in calculating the imaginary part of the polarizability; therefore, the real part, obtained by the Kramers-Kronig transform, is accurate up to about 6 eV */12/*.

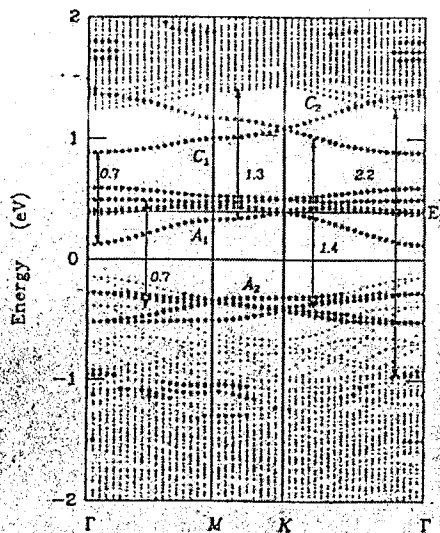


Fig. 2 - Si(111)-3x3 surface band structure. Dots and stars denote bulk and surface states respectively. E_F is the calculated Fermi level. Arrows denote the main optical transitions.

The 3x3 model considered here has the same point group symmetry as the 7x7 DAS model; in particular, both reconstructions are optically isotropic for light polarized in the surface plane.

3. Results and discussion

In Fig. 2, we present the calculated surface band structure for Si(111)-3x3. (In the text, energies are referred to the Fermi level, while in the figures they are referred to the top of the valence band.)

The Fermi level is ~ 0.39 eV above the top of the valence band. Close to E_F , we found several surface states. The upper two bands (they are actually split by the interaction of the two surfaces of the slab; only one band would appear in a semiinfinite crystal) at about 0.15 eV, and the lowest band A_1 , extending from -0.2 eV to about 0, mainly arise from AD DB's, while the central half-filled nearly flat band (again slightly split by the interaction of the surfaces) is due to CH DB's. This band yields a metallic behaviour for Si(111)-3x3, as it has been seen experimentally /15/ at Si(111)-7x7. Further below E_F there is a bunch of surface states, indicated altogether as A_2 , at about -0.8 eV, mostly due to AD backbands, with some mixing with dimer states. Resonance states due to AD backbands and to dimers in the second layer show up at ~ -1.7 eV. Above E_F there are two surface states C_1 and C_2 within the bulk gap, both between 0.5 eV and 1.0 eV. The lower-energy state, C_1 , is predominantly due to adatom DB's, while C_2 is due to AD back-antibonds. These states are degenerated at the K point. Within the conduction band, there are resonances at ~ 1.3 eV, that originate from the dimers on the second layer, and at ~ 3.4 eV (not shown in the figure) due to AD back-antibonds.

Several experiments /2, 15-22/ for the Si(111)-7x7 have

reported three occupied surface states, S_1 , S_2 and S_3 , at -0.25 eV, -0.85 eV and -1.8 eV, and two unoccupied surface states U_1 and U_2 , at 0.55 eV and $1.3-1.5$ eV, respectively. S_1 has been identified as an AD dangling bond, while S_3 has been attributed to AD and CH backbands, and S_2 has been attributed to RA dangling bonds /16/. In /17/ U_1 has been attributed to the AD p_z orbitals, and U_2 to AD back-antibonds. A metallic-like behaviour of the surface has been observed /15/, with the Fermi level crossing a very narrow band.

Within the 3x3 model, it is possible to identify the unoccupied surface state C_1 with U_1 , and the dimer resonance at 1.3 eV with U_2 ; moreover, A_1 and A_2 correspond to S_1 and S_2 respectively, and the CH DB band pins the Fermi level. The resonance at ~ -1.7 eV can be matched with the surface state S_3 . The only serious discrepancy concerns S_2 , which is here described in terms of AD backbands, while it is ascribed to RA DB's in Ref. /22/. This kind of discrepancy is however unavoidable, since the 3x3 model considered here does not have RA's. On the other hand, the 7x7 surface has twice as many DB's from the AD's than from the RA's. Then, as it has been pointed out by Carlisle *et al.* /21/, no predominant contribution from RA dangling bonds is expected.

We present in Fig. 3 the calculated surface contribution to reflectance at normal incidence, for the Si(111)-3x3 model, according to equation (1). In the same figure we also plot $\Delta R/R$ calculated according to equation (1) for Z-polarization (which has no experimental meaning, since s-light cannot be Z-polarized), to get a qualitative insight into transitions induced by Z-polarized light. We found three peaks due to transitions among surface states, at 0.2, 0.7 and 1.4 eV, stronger for light localized parallel to the surface. The first peak is of course due to transitions between AD-DB states near the Fermi level: the peak at 0.7 eV is due to transitions among A_1 and C_1 states, or among A_2 and the states near E_F . The third peak, at 1.4 eV, allowed only for X polarization, is due to s-s transitions between A_2 and C_1 , namely from the backbands to back-antibonds of the AD's.

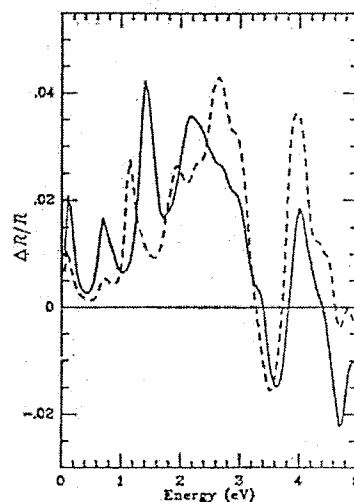


Fig. 3. - Surface contribution to reflectance of the Si(111)-3x3 surface for X- (full line) and Z- (dashed line) polarizations.

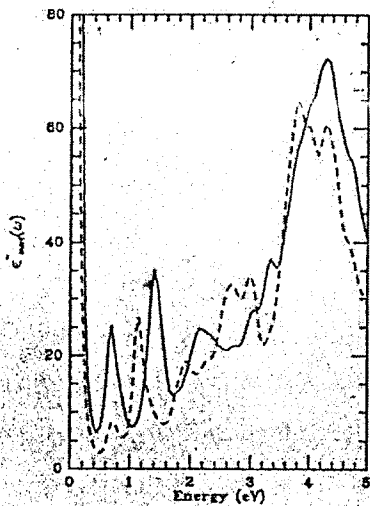


Fig. 4 - Imaginary part of the surface dielectric function ϵ''_{surf} versus frequency for X- (full line) and Z- (dashed line) polarizations.

A broad structure is present between 1.7 and 3 eV, due to mixed (i.e. s-b and b-s) transitions.

Chiarotti *et al.* /7/ have reported the surface absorption constant for the Si(111)-7×7 surface, using unpolarized, normally incident light in the near infrared. A weak structure was observed at 0.7 eV, with an intensity of ~0.8%. It well agrees, for position and intensity, with our calculations. Wierenga *et al.* /6/ measured the differential reflectance (DR) in the energy range from 1.0 to 3.0 eV, using unpolarized, normally incident light. They found, for two temperatures, 80 and 300K, two peaks at 1.76 eV and 2.9 eV. The second peak was observed later on also by Alameh and Borensztein /8/. In this last work, both s- and p-polarized light were used in a wider energy range, from 1.2 to 5.0 eV, at an angle of incidence of 60 degrees. The small signal-to-noise ratio at low frequencies has hampered the observation of the first peak. Both experiments /6, 8/ measured the difference of reflectance between the clean Si(111)-7×7 surface and the oxidized one. However, we can compare our results with the experimental data in the energy range below 3 eV, where the non absorbing oxide layer does not modify the reflectance (see eq. (1)). The first peak of Ref. /6/ can be associated with the s-s transition at 1.4 eV in Fig. 3, while the second peak might correspond to the calculated s-b and b-s structure between 1.7 and 3 eV, although the peak position and lineshape are quite different.

Our results can be better understood in terms of the surface dielectric function (ϵ_{surf}), since it is not affected by the properties of the oxidized surface. We have determined it by subtracting the bulk dielectric constant from that of the slab, having assumed a reasonable surface layer thickness (5 Å). In Fig. 4, we show the imaginary part of ϵ_{surf} (ϵ''_{surf}), of the Si(111)-3×3 model. The three lower-energy peaks are present: that at 0.2 eV is much stronger than it appears in reflectance, because of the ω factor in equation (1). In addition to these peaks, a further peak appears at 3.9 eV, in agreement with that of Ref. /8/. However, we interpret this peak as due to b-b transitions modified by the surface, and

not as involving surface states, as it was suggested by Alameh *et al.* /8/.

In conclusion, we have found good agreement of our theory with the available experimental results concerning the main optical-peak positions. The calculated intensities of these peaks in some cases, however, do not fit very well the experimental ones. This discrepancy might be due to the fact that the corresponding weight of the main structural units at the 7×7 surface is different as compared with the 3×3 structures.

4. Conclusions

We have calculated the electronic structure and optical properties of the Si(111)-3×3 surface. The reflectance spectrum has been interpreted in terms of transitions between surface and/or bulk states. We have found good agreement with the experimental data for the 7×7 surface. The most important drawback of the 3×3 model, namely the lack of RA's, may not be very important, in view of the limited RA contribution to 2×2 optical spectra /10/, and since only about 1/3 of DB's belong to RA's in the 7×7 DAS model. The states close to E_F give a metallic-like behaviour, as it has been observed experimentally for the 7×7 surface.

Acknowledgments

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