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BREMSSTRAHLUNG ISOCHROMAT STUDY OF Si(111) BY 6.2 eV PHOTONS

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We present the first experimental bremsstrahlung isochromats at an extremal low photon energy of 6.2 eV measured by using a grating spectrometer placed in the air outside the ultra-high-vacuum chamber. Isochromats of the Si(111) cleaved surface have been measured for normal incidence of electrons. We have found that a free electron approximation for the initial electron state is quite good for the interpretation of bulk interband transitions occurring in the 6.2 eV isochromat of Si(111). A strong sensitivity for surface roughness of the 6.2 eV isochromat is observed.

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The bremsstrahlung isochromat spectroscopy (BIS) has been applied for studies of the electronic structure of solids firstly for X-ray photons in the early fourties, and then in the late seventies for the vacuum ultraviolet (VUV) photons. For example, the X-ray BIS of Si was measured by Auleytner and Lidén [1], Kieser [2], Jackson et al. [3], and recently by Chelikowsky et al. [4]. The VUV BIS of Si at the photon energy of 9.5 eV was studied by Perfetti and Reihl [5]. Some bremsstrahlung spectra of Si were measured by Straub et al. [6] and Himpsel et al. [7] in a spectral mode using a grating spectrometer in the photon energy range 8–20 eV. A new technique of scanning tunneling microscopy can be also used for BIS studies, however the interpretation of its BIS spectra is nowadays rather complicated due to the field-emission resonances [8, 9].

A small mean-free-path for inelastic scattering of primary electrons in the UV BIS makes this method more sensitive for surface studies than the X-ray BIS spectroscopy. Opposite to the X-ray BIS which integrates the electronic structure all over the Brillouin zone, the ultraviolet BIS gives the opportunity to study electronic bands as a function of momentum k. To get the band structure as

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complete as possible one should apply spectrometers with tunable photon energy e.g. a grating spectrometer [10, 11].

The idea of our experiment was to measure BIS at the photon energy as low as possible by using a normal-incidence grating spectrograph placed in the air outside a small UHV chamber. A concave, holographic, $AlMgF_2$ coated grating had a radius 998.8 mm, a focusing angle $D = 25.48°$, and a groove density 2400 lines/mm. The grating was designed for the photon wavelength range 1000–3000 Å, or the photon energy range 4.1–12.4 eV. To gain the intensity, a focusing system of a concave mirror and MgF_2 lens were placed inside the chamber. The lens was mounted as a window in the UHV chamber. In our experimental setup the photons with energy higher than 6.5 eV were strongly absorbed by air. A photo-multiplier was used as a detector.

A low-energy electron gun with a BaO cathode was designed by Brenac [12] specially for angle resolved studies of bremsstrahlung spectra. The work function of the cathode was 2.3 eV and the FWHM of the energy distribution amounted 0.3 eV. The work function of Si was 4.8 eV, which was much greater than the work function of the BaO cathode. Therefore the electron current in the sample appeared if the voltage between cathode and the Si sample was greater than the limit value $U_{\min}$.

$$U_{\min} = (\varphi_{Si} - \varphi_{BaO})/e = 2.5 \text{ [V]}, \tag{1}$$

where φ_{Si} and φ_{BaO} is the work function of Si and BaO, respectively, and e is the electron charge. Our electron gun could focus the electron beam for voltage greater than about 3 V. In our experiment the focusing voltage of the electron gun was controlled in such a way as to ensure the optimal focusing of electrons on the sample for various electron energies.

The total electron current emitted from the BaO cathode was nearly constant during the experiment and equal to about 5 μA. The electron current incoming to the sample varied from 2.7 to 3.6 μA with the increasing electron energy. We have found that the grating spectrometer could register only photons from a small surface area of about 0.7 mm diameter, where the electron current was about 1 μA.

The Si crystal was cleaved parallelly to the (111) plane in the vacuum of 3×10^{-10} Torr. It is well known that the Si(111) cleaved surface is reconstructed showing the (2×1) LEED patern. There are possible three types of Si(111)2×1 domains, each of them can be rotated by $+60°$ or $-60°$ relatively to any other. Here we have studied only the case of normal electron incidence, therefore all three domains are equivalent. In Fig. 1 the two-dimensional reciprocal lattice of the Si(111)2×1 reconstructed surface is marked by filled circles, while the Si(111) unreconstructed surface by bigger open circles. The plane $(1\bar{1}0)$ is, but the plane $(\bar{1}\bar{1}2)$ is not a mirror plane in the Si crystal.

The BIS spectra were measured immediately after cleavage. A typical BIS spectrum of Si(111) measured at the photon energy of 6.2 eV is shown in Fig. 2. The experimental points are smoothed by a convolution with a 0.3 eV gaussian. We have tested the BIS measurements at two different photon energies 5.2 and 6.2 eV and found that the main maximum in Fig. 2 is actually due to the electronic structure of Si(111) and not to the electron current distribution, because the main

maximum had been shifted by 1 V down the voltage in the 5.2 eV BIS in comparison to the 6.2 eV BIS. We have done one more test, where the 6.2 eV BIS was measured for the crystal turned by an angle of 10° out of the normal incidence. In this spectrum the big maximum completly disappeared and the shape was more or less similar to the BIS spectrum shown in Fig. 3.

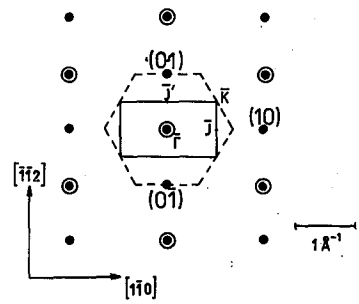

Fig. 1. Example of a Si(111)2 × 1 surface domain in the reciprocal space. The surface Brillouin zone is drawn for the Si(111)2 × 1 reconstructed surface (solid line) and Si(111) unreconstructed surface (dashed line).

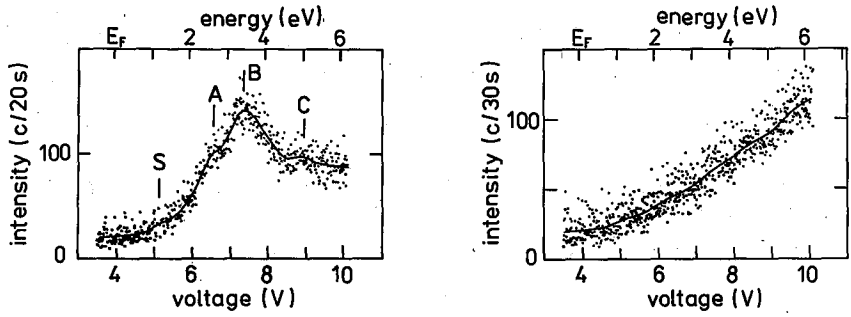

Fig. 2. The 6.2 eV normal incidence BIS of the Si(111) cleaved surface (points) and the same spectrum convoluted with a 0.3 eV gaussian (solid line).
Fig. 3. The 6.2 eV normal incidence BIS of the Si(111) badly cleaved surface (points) and the same spectrum convoluted with a 0.7 eV gaussian (solid line).

We assumed the initial states as free-electron parabolas

$$E_i(k_i) = h^2(k_i + G)^2/8\pi^2 m + V_0, \tag{2}$$

where V_0 was the inner potential equalled −17.6 eV and G was a bulk reciprocal lattice vector. The final states were taken from the electron band structure of Si calculated recently by Chelikowsky et al. [4]. Assuming the Fermi level at 0.4 eV

above the top of the valence band we have interpreted the peaks A and B as interband transitions to the two unoccupied electron bands on the ΓL line of the Si band structure. The primary cone transitions with $G = 0$ are shown by bold arrows in the left panel in Fig. 4. The secondary cone transitions involving the bulk umklapp by the G_{002} and $G_{00\bar{2}}$ vectors are shown in the left panel of Fig. 4 by thin arrows. They can contribute to the A, B, and C peaks. We expect, by analogy to

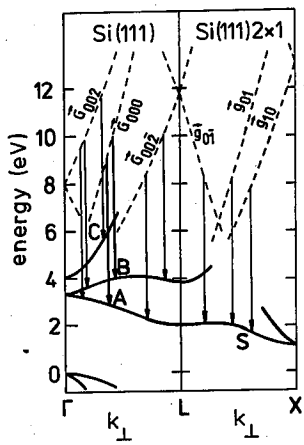

Fig. 4. Electron interband transitions A, B, and C (left panel) and surface resonance transitions S (right panel) by using a free electron approximation of the initial electron state. The Si band structure is taken from [4].

the photoemission, that the secondary cone transitions with $G \neq 0$ should be equal to about 10% of the primary cone transitions. It can explain the high intensity of the A and B peaks in comparison with the C peak.

The weak peak S in Fig. 2 is the surface state peak, which has been already observed in other works [5–7]. Its intensity is very low in our experiment due to surface contaminations growing up during the few hours of measurements. It is worth to discuss the origin of this surface peak. It is already known that the surface state in Si(111)2 × 1 is not located in the band gap. Its hybridization with bulk states creates surface resonances. They can be viewed as surface umklapp processes [7], where the momentum transfer parallel to the reconstructed (2 × 1) surface lattice

$$k_{\parallel}^{i} = k_{\parallel}^{f} = k_{\parallel} + g_{\parallel} \tag{3}$$

brings the incident electron to k-points on the LX line, which are not accessible for an unreconstructed surface. The initial electron states involving the surface umklapp by the g_{01}, g_{10}, and $g_{0\bar{1}}$ surface reciprocal vectors are separated from the bulk states and give three bands on the LX line shown by dashed lines in the right panel in Fig. 4. The electron transitions from these three bands to the lowest unoccupied bulk band in the LX line contribute to the S peak. The initial electron

states due to surface umklapp by the g_{02} and $g_{02\bar{}}$ vectors are not separated from the bulk states involving the umklapp by the G_{002} and $G_{00\bar{2}}$ vectors.

In a case of a bad cleavage with many steps on the surface the BIS spectrum had no pronounced maximum and the photon intensity was low. Such an example of the BIS spectrum is shown in Fig. 3. In the area of a surface step the electron beam is not normal to the surface and electrons entering the crystal are refracted with conservation of the parallel momentum $k_{\|}$. We have illustrated this effect in the momentum space in Fig. 5, where four electrons with the kinetic energy in vacuum equal to 0.5, 5, 10, and 20 eV enter the Si surface inclined by 20° to the (111) plane. It is seen that the smaller electron energy the stronger electron

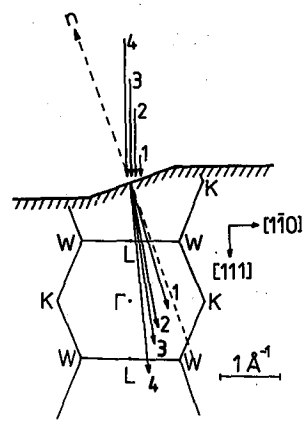

Fig. 5. Electron refraction on the Si(111) surface step for the kinetic energy in vacuum equal to: (1) 0.5 eV, (2) 5 eV, (3) 10 eV and (4) 20 eV.

refraction. In the presence of many various surface steps the 6.2 eV BIS spectrum of an crystal is not k-resolved any more. It is seen also in Fig. 5 that the influence of the surface roughness should be less dramatic in the case of bremsstrahlung spectra measured for the photon energy 20 eV. The low-energy BIS is however less dispersed with the angle θ between the electron beam and normal to the surface, because the parallel momentum $k_{\|} = k \sin\theta$ is small for small k.

Results of our work lead to the following conclusions:

1. The main maxima of the BIS spectrum of Si(111) at the photon energy 6.2 eV are related to interband transitions, which can be interpreted by using a free electron approximation for the initial electron state.

2. The surface state peak at the bottom of the conduction band can be interpreted as a surface resonance peak.

3. The 6.2 eV BIS spectrum at normal incidence is more sensitive for the surface roughness and less sensitive for the angle divergence of electrons than the 9.5 eV and higher energy BIS.

Acknowledgments

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