TEMPERATURE DEPENDENCE OF SURFACE PHOTOVOLTAGE EFFECT ON Si(111)-7x7

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1. Introduction

It is important to capture transient electronic states during phase transition of a material for understanding its dynamics. While numbers of the phase transitions have been reported on the solid crystal surfaces, the transition from Si(111)-7x7 surface to -1x1 surface has been one of the well-studied subjects. When a clean Si(111) surface is heated up above 830°C, the 7x7 superstructure changes into the 1x1 structure. The phase transition was reported to be the first order one that is associated with a hysteresis [1]. However, its ultrafast dynamics have remained uncertain. Thus, it is of interest to reveal the temporal change of its electronic structure by time-resolved photoelectron spectroscopy (PES).

2. Experimental

The time-resolved PES experiments were carried out at SPring-8 BL07LSU using a pump (laser) and probe (synchrotron radiation, SR) method [2]. Photon energy of the pump laser was set at 1.51eV and its second harmonics. The temporal durations of the laser and SR pulses were about 35 fs and 50 ps, respectively. The repetition rate of the pump laser was 1 kHz. A clean Si(111)7×7 surface was prepared by a cycle of *in situ* resistive heating of a heavily doped n-type (ρ = 0.02 Ω cm) Si(111) wafer. In order to induce the transition from 7x7 to 1x1, the pump laser was irradiated on the heated substrate just below the phase transition temperature of 830°C. Since the sample was resistively heated by electric current, electrical potential, applied to the sample, prevented precise measurements of the photoelectron kinetic energy. Therefore, we used a pulse heating system which cut off the heating current during the photoelectron spectroscopy measurement. Within the 1000 μs duration (the 1 kHz repetition), the heating current was switched "on" for 800 μs and "off" for 200 μs, alternately. The pulse heating system was synchronized with the pump laser and the SR. The SR light of hν=253 eV was used to measure Si 2*p* core level spectra and valence band spectra of the Si(111) surface.

3. Results and discussion

We have successfully measured the Si 2*p* spectra at high temperature by using the pulse heating system. Figure 1 shows binding energy of the Si 2*p* core level as a function of the sample temperature. The binding energy stayed almost constant from RT to 700°C and, then, decreased linearly with temperature above 700°C. It indicated that the surface pinning position of the Fermi level was kept up to 700°C. It is noted that the pinning level was previously reported to be 0.63 eV above the valence band maximum for a Si(111)-7x7 surface at RT [3]. The spectral variation above 700°C likely indicates electronic change of the 7x7 surface. Since the temperature is far below the critical temperature, it seems to be not related to the 7x7 to 1x1 transition.

Figure 2 shows the energy shift of Si 2*p* by the pulse laser irradiation as a function of the sample temperature. The Si 2*p* PES spectra were measured by the probe SR pulse with delay time of 1.0 ns after the pump laser (1.51 eV, 24.7 μJ/cm^2). As expected for the upward band bending of the Si(111)7x7 on the *n*-type Si substrate, the binding energy of the Si 2*p* at RT shifted to the higher binding energy due to surface photovoltage (SPV) effect. The SPV shift decreases with temperature up to ~600°C. The electronic behavior is understood by the change of the bulk Fermi level position due to the thermally activated carriers, i.e. electrons and holes. The intrinsic carrier density overcomes the extrinsic density by dopants at such high temperature and the Fermi level shifts to the center of the band gap. For the present sample surface, the band bending is expected to be slightly downward if the Fermi level is just at the gap center. This is consistent with the slight negative shift of the Si 2*p* above 600°C as shown in Figure 2. However, we could not observe any apparent changes in the binding energy and, thus, the SPV effect during the phase transition from 7x7 to 1x1, which should be occurred around the critical temperature at ~830°C. More detail and extensive studies would be required to understand the dynamics of the electronic structures during the phase transition, for example, surface component of Si 2*p* and valence band structures.

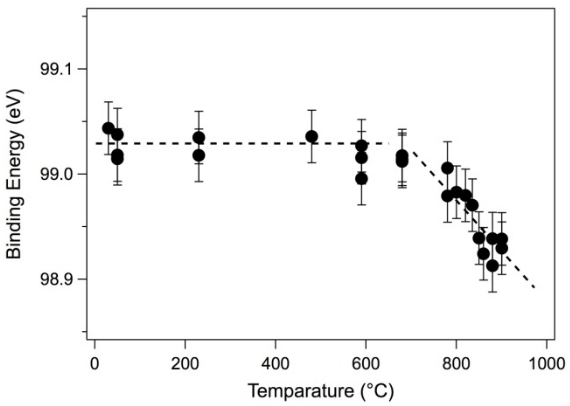

Figure 1: Binding energy of Si 2*p* core level peak as a function of sample temperature.

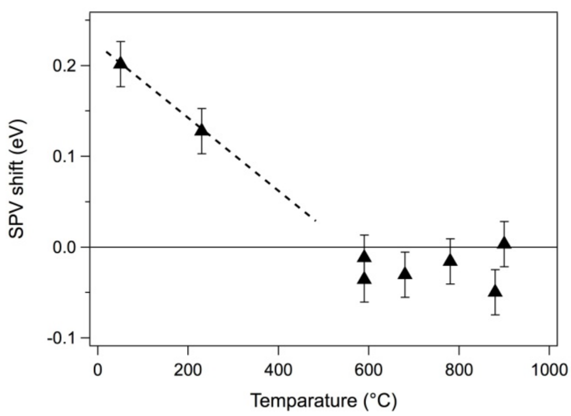

Figure 2: Energy shift of Si 2*p* by the pulse laser irradiation due to SPV effect.

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