PECULIARITIES OF SLOW ELECTRON SCATTERING BY Si-p (100) SURFACE

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Using the developed hypocycloidal electron spectrometer and elaborated techniques the studies of elastic electron reflection at 180° and energy-loss spectra for slow (0–5 eV) monoenergetic electrons by Si-p(100) surface were carried out. A distinct correlation in the energy positions of features in the elastic scattering and energy-loss spectra due to both possible interband transitions and excitation of surface electron states in Si was found.

Amongst the surface studies techniques in the recent years electron spectroscopy is being extensively used. Probing matter with slow electrons is widely applied in various electron spectroscopy techniques providing information of various sense and value. These techniques are slow electron diffraction, electron energy characteristic loss spectroscopy, integrated secondary electron spectroscopy, electron Auger spectroscopy, photoelectron and X-ray emission spectroscopy, reverse photoemission spectroscopy etc. providing information on surface structure, chemical composition, chemical binding character, surface lattice vibration etc. on pure and covered with adsorbate molecules solid surfaces [1].

Application of slow electrons for solid surface probing is related to certain problems in obtaining intense enough and well collimated electron beams with high uniformity of their energy distribution. Since primary electrons with energy ≤5 eV can penetrate into the solid by ≥50 Å [2 (Fig. 3.2)], they, similarly to ultraviolet electron spectroscopy, can be expected to probe the energy bands in the bulk, not only the surface energy states. When electron, incident on the surface, excites interband electron transitions in the bulk, energy and momentum conservation laws should be obeyed. While in the case of photoemission the photon momentum can be neglected in comparison with the emitted electron momentum, in the case under consideration the incident electron momentum should also be taken into account (at E_p~10 eV the electron wavevector k_p~1,6×10^{10} m^{-1}, which is of the order of the Brillouin zone in $\vec{k}$ -space). Hence, at electron excitation both direct (vertical) and indirect electron transitions from filled to empty bands are possible.

This paper is aimed at the investigation of slow monoenergetic electron interaction with silicon surface.

Silicon is the principal material applied in modern semiconductor electronics. Its properties are relatively well studied both theoretically and experimentally, including low-energy electron spectroscopy [See e.g. 3–5].

Silicon unit cell contains two atoms with four valence electrons each, i.e. 8 electrons per unit cell. This amount of electrons is sufficient for full occupation of four Brillouin zones. For Si in the Brillouin zone center (Γ, k=0) four allowed energy bands are located: Γ_1, Γ_{25}, Γ_{15}, Γ_2. The first (lowest) Γ_1 band contains two electrons. Somewhat higher is Γ_{25} band, which is 6-times degenerated (with the account of spin), where the remaining 6 electrons are located. Γ_{15} and Γ_2 bands at T=0 K are completely empty.

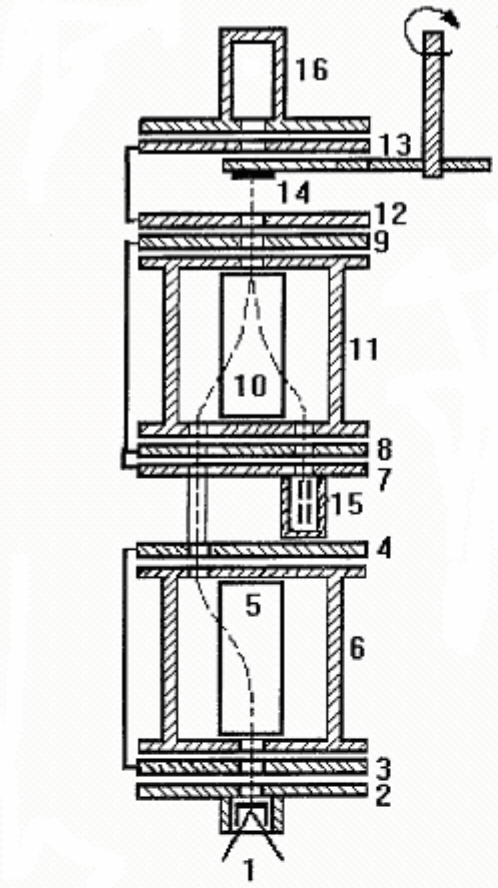

Fig. 1 Schematic diagram of a hypocycloidal electron spectrometer for the low-energy electron backscattering studies: (1) indirectly heated oxide cathode; (2) extracting electrode; (3,4) entrance and exit electrodes of the monochromator; (5,6) inner and outer electrodes of the cylindrical capacitor of the monochromator; (7-9) entrance and exit electrodes of the analyzer; (10,11) inner and outer electrodes of the cylindrical capacitor of the analyzer; (12,13) accelerating electrodes of the spectrometer; (14) sample; (15) collector of backscattered electrons; (16) collector of the primary electron beam

The experiments were carried out using a high-vacuum setup with oil-free pumping out, consisting of the following major units: a superhigh-vacuum chamber where a hypocycloidal electron spectrometer is located, a special goniometric device with the samples under investigation, an electron heating unit, a quartz lamp for heating, electron spectrometer power supply unit, a multichannel system for primary and scattered electron current registration. Outside the chamber Helmholtz rings are located, providing uniform longitudinal magnetic field inside the chamber, required for the spectrometer operation.

In order to obtain monoenergetic electron beam and to analyze elastically and inelastically scattered electrons we used a hypocycloidal electron spectrometer whose schematic layout is shown in Fig. 1. The design and operating principles of the spectrometer are described in detail in [6, 7]. It consists of two consequently located electron energy analysers, the first of them serving as a monochromator, and the second one being used as an analyser of elastically and inelastically scattered electrons. This is enabled by the fact that in crossed electric and magnetic fields electrons, besides the longitudinal motion, also drift in transverse direction, i. e. in the direction normal to **E** and **H**. The drift value in this case is independent of the electron velocity vector. Therefore backscattered electrons, having passed the crossed fields of the analyser, are displaced by a certain value from the primary beam axis. A collector located at this distance can detect elastically backscattered electrons. Inelastically scattered electrons can be detected due to a segment-shaped diaphragms in the analyser electrodes.

The main spectrometer characteristics are the following: primary beam current ~10^{-8} A, backscattered electron current ~10^{-10}–10^{-11} A, the beam diameter ~0.5 mm, full width (FWHM) of the electron energy distribution in the beam ~14–20 meV, energy resolution of the analyser 50 meV. The unique feature of the device consists in its ability to work at very low energies (from practically 0 eV), primary electron beam intensity being practically independent of energy. The spectrometer transmittance is ~ 95%.

Before the measurements the electron spectrometer and the sample were heated at the temperature T~1050 K in vacuum 10^{-6} Pa during 50-60 h, followed by the surface

cleaning by high-energy electrons. The vacuum in the chamber at the measurements was ~10^{-7} Pa. The surface quality was checked by the presence of fine structure at the measured plots.

We have performed studies of elastic backscattering of slow electrons and energy loss spectra at different energies of incident electrons for Si-p (100) surface.

At certain energy value of primary electrons a sharp increase of excitation probability for one-particle and collective states in solids is known to occur [1, 2]. This results in the decrease of the elastically scattered electron flux and a minimum is observed at energy dependences of elastic scattering intensity. Accordingly, in the energy loss spectra at the same energy a maximum is observed. This is confirmed by the results obtained here. Figs. 2, 3 present the energy dependence of the intensity of elastic scattering of electrons by 180° and energy loss spectra at electron backscattering by Si-p (100) surface.

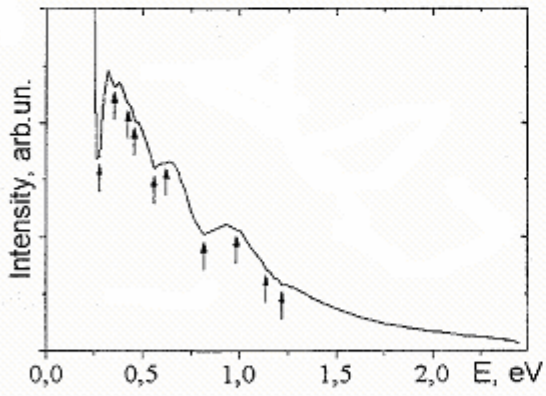

Fig. 2. Energy dependence of the intensity of elastic electron scattering at 180° by the Si-p(100) surface.

Energy loss spectra at the backscattering were studied for different incident electron energies from 0-5 eV. Excitation of electrons in the range 0–1 eV, related to the surface electron states was shown to be of resonant character [7]. Interband electron transitions have appeared to be very sensitive to the energy of the exciting electrons as well. Therefore, the increase of the primary electron energy results in the fine structure weakening in the lower enrgy range. With the incident electron energy increase from 0 to 5 eV the primary electron penetration depth sharply devreases [2], this meaning the reduction of the contribution of interband transitions in the bulk with respect to the contribution of electron transitions in a thin subsurface layer. Hence, depending on E_0, the same features in the loss spectra can reveal in different way.

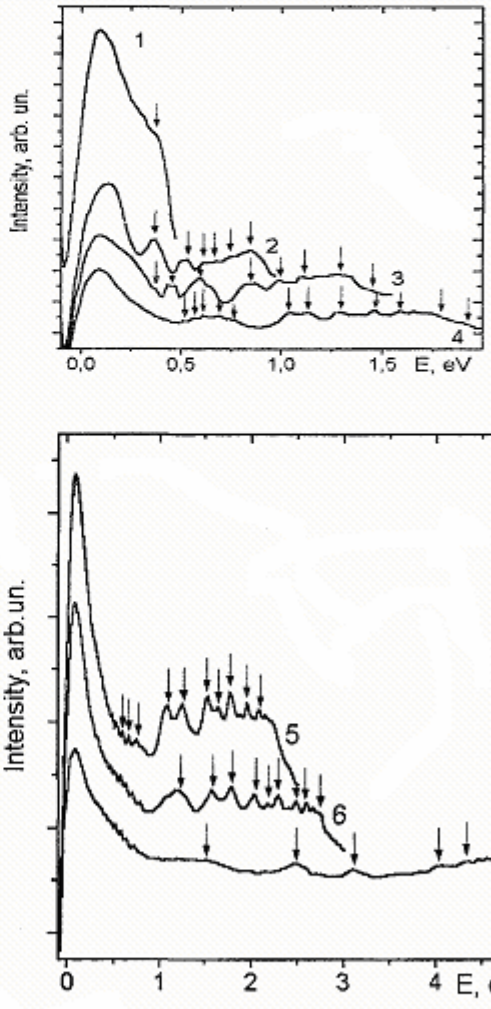

Fig. 3. Energy-loss spectra at the electron backscattering by the Si-p(100) surface at different incident electron energies E_0: 1 - E_0=0.5 eV; 2 - E_0=1.0 eV; 3 - E_0=1.5 eV; 4 - E_0=2.0 eV; 5 - E_0=2.5 eV; 6 - E_0=3.0 eV; 7 - E_0=5.0 eV.

The most characteristic energy loss spectra at electron scttaering by Si-p (100) surface for various incident electron energies (from 0.5 eV to 5 eV) are shown in Fig. 3. As seen from the figure, the shape of the energy loss spectra is very sensitive to the incident electron energy. This confirms the assumption of the resonant character of the incident electron energy loss for excitation of surface electron states and interband transitions.

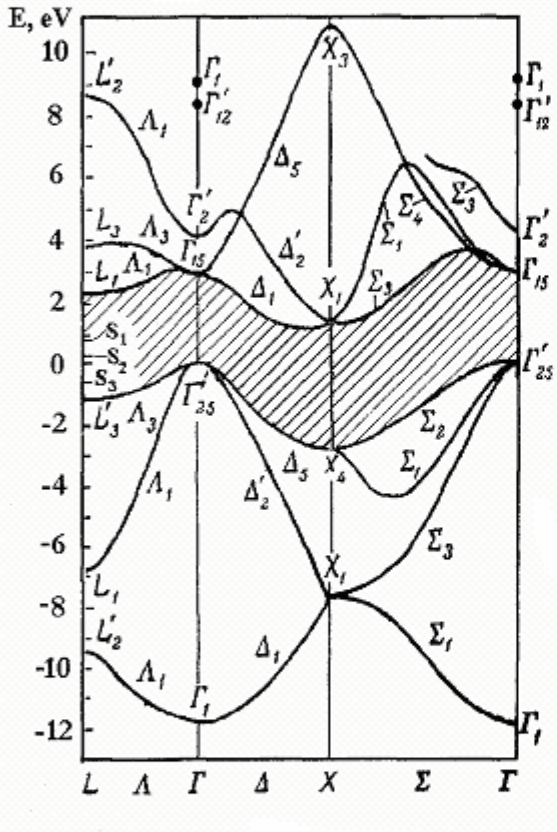

Fig. 4. Silicon band structure calculated by empiric method of orthogonalized plane wave method [9].

In order to illustrate the correlation of the peculiarities in the spectra obtained by different techniques for silicon surface, the data on the singular points in the spectra (Figs. 2, 3) are listed in the Table. The obtained results imply that the energy positions of the features in different spectra are in good agreement, their mean values differing from each other within the setup spectral resolution which in the case of scattering by silicon surface was less than 50 meV.

While earlier [8] we had been able to find specific features only in the energy loss spectra, in this experiment the resolution improvement enabled us to observe fine structure at the energy dependences of elastic scattering intensity as well (Fig.2).

The energy positions of high-symmetry points in the reduced Brillouin zone for the bulk are determined from Fig. 4 [9 (Fig.11b and Table 7)]. The data on the silicon surface states are taken from [10].

Supposed in Γ'_{25} point the valence band being split into a light-hole band $\Gamma'_{25}(l)$ and a heavy-hole band $\Gamma'_{25}(h)$ and the conduction band minimum being located apart from the Brillouin zone boundary in X_1 point (the corresponding energy differences being of the order of 0,1 eV), the obtained energy dependences are in a good agreement with the theoretical calculations of silicon band structure using an empirical orthogonalized plane wave method provided that for low-energy electron backscattering spectra optical selection rules being not valid and direct and indirect transitions of the excited electrons being almost equally probable.

It is seen from the comparison of the obtained results with the data of [9, 10] that almost all features in the energy dependences of elastic scattering intensity and energy loss spectra are not only in good agreement with the results of other authors obtained by various ultraviolet and X-ray electron spectroscopy techniques and field effect, but also essentially complement them.

We know no other technique being so sensitive to the features of non-filled bands and capable of so exact determination of energy differences between the high-symmetry points of the valence band and conduction band as well as between the surface states.

Table 1. Energy position of singularities in elastic and inelastic electron backscattering spectra by silicon surface and their possible relation to intraband and interband transitions of excited electrons.

Possible transition of excited electrons [9,10]	Transition energy calculated by empirical orthogonalized plane wave method, eV [9]	Transition energy, experiment, eV [9]	Elastic scattering singularities, eV (Fig.2)	Energy loss, mean values, eV (Fig.3)
			0.27	0.23
		0.34	0.36	0.35
			0.43	0.42
$S_1 - S_2$		0.49	0.46	0.52
$\Gamma'_{25}(l) - S_3$			0.56	0.59
$\Gamma'_{25}(h) - S_3(p-type)$		0.65	0.62	0.66
$S_1 - \Gamma'_{25}(h)$				0.74
$S_1 - \Gamma'_{25}(l)$		0.83	0.8	0.83
$X_1(\Delta_1) - S_2$	0.97		0.98	1.00
$X(\Delta_1) - \Gamma'_{25}(h)$	1.3	1.1	1.14	1.10
$X_1(\Sigma_3) - \Gamma'_{25}(h)$ $X_1(\Delta_1) - \Gamma'_{25}(l)$			1.22	1.26
$S_1 - S_3$		1.48		1.43
				1.54
				1.64
$L_1 - S_2$	1.86			1.76
$X_1(\Delta_1) - S_3$	1.96			1.93
$X_1(\Sigma_3) - S_3$				2.04
$\Gamma'_{25}(h) - L_1$	2.2	1.9		2.17
$\Gamma'_{25}(l) - L_1$				2.27
$L'_3 - X_1(\Delta_1)$	2.51			2.49
$L'_3 - X_1(\Sigma_3)$				2.59
$\Gamma'_{25}(l) - X_4$				2.67
$\Gamma'_{25}(h) - X_4(p-type)$	2.77			2.73
$\Gamma_{15} - \Gamma'_{25}(h)$	2.8	3.4		2.88
$\Gamma_{15} - \Gamma'_{25}(l)$				2.98
$L_1 - L'_3$	3.4	3.2		3.11
$L_3 - \Gamma'_{25}$ $\Gamma'_2 - \Gamma'_{25}$ $L'_3 - \Gamma_{15}$ $X_1 - X_4$	3.8 4.05 4.0 4.08	3.8; 4.18 4.1		4.05
				4.36
$\Gamma'_2 - S_3$				4.66

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ОСОБЛИВОСТІ РОЗСІЮВАННЯ ПОВІЛЬНИХ ЕЛЕКТРОНІВ ПОВЕРХНЕЮ Si-p(100)

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За допомогою гіпоциклоїдального електронного спектрометра відповідно до розроблених методик проведено дослідження пружного відбивання на 180° та спектрів енергетичних втрат повільних (0–5 еВ) моноенергетичних електронів поверхнею Si-p(100). Знайдено чітку кореляцію енергетичних положень особливостей пружного відбивання та спектрів енергетичних втрат. Поєднання досліджень такого роду в одному експерименті дало змогу одержати інформацію як про можливі міжзонні переходи, так і про збудження поверхневих електронних станів у твердих тілах.