Electronic conductivity of Si(111)-7×7

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Recent electron-energy-loss measurements on Si(111)-7×7 have been analyzed to obtain the temperature-dependent surface resistivity, which is found to take the form $\rho=\rho_0+\alpha T$ where T is the temperature and $\alpha\approx 174\ \Omega/\mathrm{K}$.

Electronic transport (conductivity) at semiconductor surfaces is a fundamental problem which deserves detailed study. All the reconstructed semiconductor surfaces with a small unit cell are found to be semiconducting at zero temperature, i.e., there is a band gap separating filled surface bands from the empty ones.[1] On the other hand, the 7×7 reconstructed Si (111) (Ref. 2) and Ge (111) (Ref. 3) surfaces, as well as Si (111)-Ge (5×5) (Ref. 3) are probably metallic. These surfaces have a large unit cell which contains an odd number of electrons and photoemission measurements show that they have a density-of-states peak in the middle of the bulk band gap which seems to pin the Fermi energy at the surface. However, the resolution of the photoemission measurements (~0.1 eV) is not high enough to really tell whether there is a nonzero density of states at E_F. On the other hand, using electron-energy-loss spectroscopy (EELS), it is possible to probe the electronic structure with much higher resolution. In particular, by studying the temperature-dependent broadening of the quasielastic peak in EELS, one can obtain the temperature-dependent surface resistivity[4] (strictly speaking, this is not the dc resistivity but the ac resistivity at a frequency corresponding to a few meV energy).

In this note, I analyze some recent EELS data from Si (111)-7×7. The silicon surface is treated as a two-dimensional electronic system characterized by the surface polarizability

$$\chi(q_{||},\omega)=\frac{e^2 n}{m^*\omega(\omega+i/\tau)}q_{||}^2 \tag{1}$$

where n is the number of free carriers per unit *area*, m^* their effective mass, and τ a relaxation time determined by, e.g., the electron-impurity and electron-phonon interactions. In an earlier work,[4] we analyzed EELS data from Si (111)-7×7 assuming that $1/\tau$ can be neglected in (1). In this case, the broadening of the quasielastic peak results from excitation of (undamped) two-dimensional plasmons. To explain the experimental data using this model requires $m^*\approx 60 m_e$, where m_e is the free-electron mass. It was argued in Ref. 4 that such a large effective mass (corresponding to very flat electron bands if a one-particle picture can be used) should lead to a Hubbard splitting into a lower filled Hubbard band and an upper empty Hubbard band, i.e., a magnetic and insulating ground state, in disagreement with the experimental data.

In this note I assume instead that the opposite limit holds, i.e., $\hbar\omega\sim 1\ \mathrm{meV} \ll h/\tau$ so that (1) takes the form

$$\chi(q_{||},\omega)=-i\frac{ne^2\tau}{m^*\omega}q_{||}^2=-\frac{i}{\rho\omega}q_{||}^2\ , \tag{2}$$

where ρ is the surface resistivity. The quasielastic peak in EELS from an insulating (or semiconducting) substrate having a surface polarizability of the form (2) has been shown to be a Lorentzian[4] (if $CH/2<<1$)

$$P(\omega)=\frac{1}{\pi}\frac{\Gamma/2}{\omega^2+(\Gamma/2)^2}\ , \tag{3}$$

where the full width at half maximum is given by $\Gamma=2CHk_BT$. Here C is a dimensionless number given by

$$C=\frac{4.7}{(\varepsilon+1)(E_0)^{1/2}\cos^2\alpha}\ , \tag{4}$$

where E_0 is the kinetic energy of the incident electrons measured in units of eV, α is the angle of incidence and $\varepsilon\approx 11.7$ is the zero-frequency dielectric function of Si. The function H is related to another parameter ξ via Eq. (30) or Table II in Ref. 4. The surface resistivity can be obtained from ξ via

$$\rho=1.9\times 10^5\frac{\xi}{(\varepsilon+1)(E_0)^{1/2}}\ , \tag{5}$$

where ρ (the two-dimensional resistivity) is measured in Ω and E_0 in eV. Note (see Table II in Ref. 4) that there are always two solutions, ξ_1 and ξ_2, for any given H. Only one of these solutions is physically correct, but it is usually not hard to decide which to choose.

The circles in Fig. 1 show the surface resistivity of Si

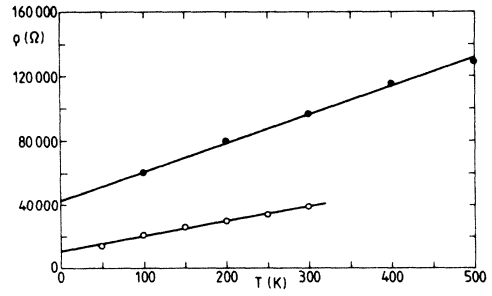

FIG. 1. The temperature-dependent resistivity of the Si (111)-7×7 surface as deduced from the experimental data of Demuth *et al.* (Ref. 4) (open circles) and from the data of Stroscio and Ho (Ref. 5) (solid circles).

(111)-7×7 as deduced from the temperature-dependent linewidth measurements of Demuth *et al.*[4] (open circles) and of Stroscio and Ho[5] (solid circles), respectively. These measurements were performed on *n*-type B-doped silicon ($n=1.3\times10^{15}$ cm^{-3}) and on As-doped silicon ($n=6.6\times10^{12}$ cm^{-3}), respectively. The bulk doping of the latter crystal is so small that it cannot in itself contribute to the quasielastic linewidth while a small contribution from excitation of surface plasmons is expected for the crystal studied by Demuth *et al.* (the exact magnitude of this contribution is not so easy to estimate as it depends on the band bending at the surface).

According to Fig. 1, the resistivity varies linearly with temperature

$$\rho=\rho_0+\alpha T ,$$

where, for the sample studied by Stroscio and Ho, $\rho_0=4.3\times10^4$ Ω and $\alpha=174$ Ω/K. It is likely that ρ_0 is caused by electron scattering against lattice imperfections while α is determined by the electron-phonon interaction. Thus one would expect ρ_0 to vary between different Si crystals (with different surface perfections) while α should be essentially constant. However, α is about 45% smaller for the crystal analyzed by Demuth *et al.* There are two possible explanations for this. First, as pointed out above, for the crystal studied by Demuth *et al.* one might expect some contribution to the linewidth from excitation of surface plasmons (see Appendix C in Ref. 4). Subtracting away this contribution would tend to increase ρ_0 and α. Secondly, the slopes in Fig. 1 are only accurate to within ±20% or so, since the analysis requires a knowledge of the instrumental resolution which in the present case was obtained by extrapolating the experimental data to zero temperature. An uncertainty in the instrumental linewidth by ~0.5 meV corresponds to an uncertainty in α by 10–20%. It would be very desirable if more EELS studies on Si (111)-7×7 (low-doped sample) could be performed to definitely prove if α is an universal constant.

I note, finally, that the surface resistivities deduced above are very large, of similar magnitude as the so-called maximum metallic resistivity $\rho\sim10\hbar/e^2\sim3\times10^4$ Ω. It is not obvious to me, however, what the physical origin and implications of this result might be.

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[1]Photoemission measurements indicate that the Ge (001)-2×1 surface is metallic at room temperature. However, the metallic surface states disappear at low temperatures. See S. D. Kevan and N. G. Stoffel, Phys. Rev. Lett. **53**, 702 (1984); S. D. Kevan, Phys. Rev. B **32**, 2344 (1985).

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