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ELECTRON–PHONON COUPLING IN HIGHLY DOPED *n* TYPE SILICON*

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The effect of free electrons on the optical phonon of silicon at the center of the Brillouin zone is studied using the Raman scattering technique. Heavy doping gives rise to a continuous electronic Raman scattering and makes the phonon line shape assymetric. The profile factor which is related to the dissymetry, is shown to have the signes of the matrix elements of the electron–phonon interaction.

THE EFFECT of free electrons on the optical phonon of silicon at the center of the Brillouin zone is investigated using the Raman scattering technique. Heavy doping ($n \gtrsim 10^{20}$ cm^{-3}) gives rise to a continuous electronic Raman scattering, and affects the position of the one phonon line shape. In contrast to p type silicon, which exhibit a dissymmetry on the high side of the phonon peak maximum,[1,2] n type silicon shows a low energy side dissymmetry. The dissymmetry of the line in p type silicon was attributed in reference 2 to the interference between scattering processes on interband transitions and on optical phonons. (Fano interaction.[3]) In this letter the line shape in n type silicon will also be expressed in terms of the Fano interaction. However, the comparative analysis of the symmetry of the electron states in p and in n type silicon shows, that the difference in the line dissymmetry is connected with the negative sign of the Fano profile factor q in n type silicon.

The measurements reported here were performed at room temperature on arsenic and phosphorus doped silicon. The exciting laser sources are the 4480 Å argon laser line and the 6471 Å krypton one, silicon has been doped by diffusion at high temperature.

Figure 1 shows the Raman spectrum of pure silicon, and of silicon containing 2.3×10^{20} P/cm^{-3} and 7×10^{20} P/cm^{-3}, the dotted line represents the Raman intensities difference between the doped and the pure silicon. The dotted line clearly exhibit the interference pattern between the continuum and a discrete state, the minimum is on the high energy side of the phonon peak, and the continuum extends on a wide range of frequencies.

The continuum Raman scattering arises from electronic transitions between heavy and light hole bands in p type and between Δ_1 and Δ_2' bands in n type silicon. Figure 2 shows the band diagram of n type silicon.[4] The vertical distance between Δ_1 and Δ_2' bands equals $\Delta E = 0.35$ eV[5] (according to reference 4, $\Delta E = 0.5$ eV). The minimum frequency of the scattering by the continuum excitations depends upon the Fermi energy, via.

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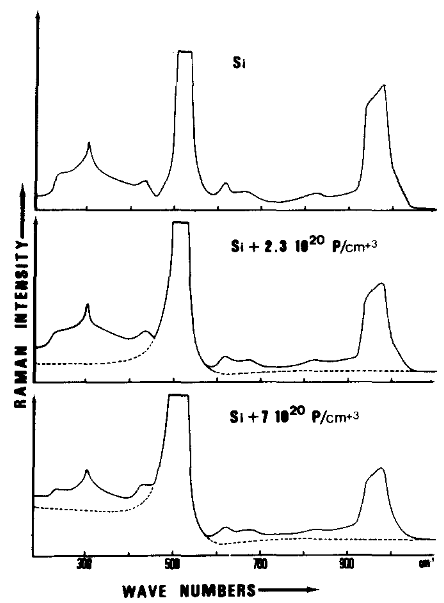

FIG. 1. Raman scattering of silicon containing 2.3 x 10^{20} and 7 x 10^{20} phosphorus donnors per c.c. The laser wavelength is 4880 Å at room temperature. The dotted line is the scattering intensity out of which the double phonon intensity has been deduced.

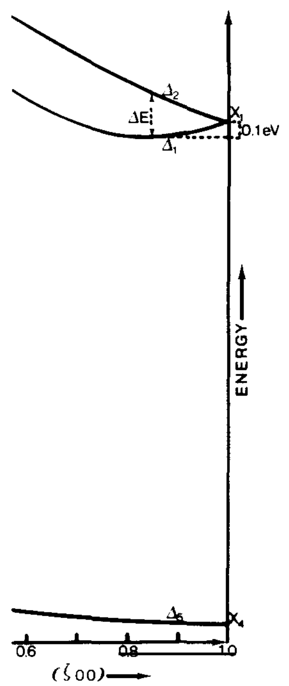

FIG. 2. Conduction bands of silicon along the direction (1 0 0) near the edge of the Brillouin zone.

$$\hbar\omega_{\min} \simeq 2(\Delta E/4 - E_F).$$

The interference is possible only if the optical phonon frequency Ω

$$\omega_{\min} < \Omega < \omega_{\max} \simeq \Delta E.$$

The condition is satisfied for $n > 7 \times 10^{19}$ cm^{-3}.

The line shape in the presence of the interference can be expressed by

$$I(\omega) = \frac{(q+\epsilon)^2}{1+\epsilon^2}, \qquad \epsilon = \frac{\Delta\omega - \Omega}{\Gamma} \tag{1}$$

$\Delta\omega$ is the scattering frequency, Ω is the dressed phonon frequency, Γ is the phonon damping.

The profile factor of the line, q can be expressed through the ratio of the Raman tensors for purely lattice (R_{lat}) and purely electronic (R_{el}) Raman scattering[2,3]

$$q = \frac{R_{lat}}{R_{el}\,\overline{V}_{ep}} \tag{2}$$

Here V_{ep} is interband matrix element of the electron–phonon interaction between the states which contribute to the interference.

In silicon the phonons with the symmetry Γ'_{25} contribute to the one phonon Raman scattering. For the phonon polarisation X the only non-zero lattice Raman tensor component is R_{lat}^{YZ}. Therefore the interference phenomenon is determined by the corresponding component of purely electronic scattering R_{el}^{YZ}. In p type silicon the main contribution to R_{el}^{YZ} comes from the virtual transition between Γ'_{25} and Γ_{15} bands, so that

$$R_{el,\Gamma}^{YZ} \sim \frac{\langle XZ|P_Z|X\rangle\langle X|P_Y|XY\rangle}{E_{c\bar{p}}^{\Gamma} - E_{v\bar{p}}^{\Gamma} - \hbar\omega_i} \tag{3}$$

In n type silicon the main contribution to R_{el}^{YZ} is determined by the virtual transition between X_1 and X_4 bands

$$R_{el,X}^{YZ} \sim \frac{\langle X_1|P_Y|X_4\rangle\langle X_4|P_Z|\bar{X}_1\rangle}{E_{c\bar{p}}^{x} - E_{v\bar{p}}^{X} - \hbar\omega_i} \tag{4}$$

Here $X_1, \bar{X}_1, X_4$ are degenerated states at the Brillouin zone boundary which develop into Δ_1, Δ'_2, and Δ_5 states, correspondingly.

The symmetry of the Γ and X_{YZ} points gives the possibility to determine the relative sign of $R^{YZ}_{el,\Gamma}$ and $R^{YZ}_{el,X}$. In Γ point

$$\langle XZ|P_Z|X\rangle = \langle XY|P_Y|X\rangle$$

so that

$$R^{YZ}_{el,\Gamma} \sim \frac{|\langle XY|P_Y|X\rangle|^2}{E^{\Gamma}_{c\bar{p}} - E^{\Gamma}_{v\bar{p}} - \hbar\omega_i} \qquad (5)$$

The analysis of the symmetry of the states in X point of the space group O^7_h, which includes nontrivial translations gives the relation[4]

$$\langle X_1|P_Y|X_4\rangle = -\langle \bar{X}_1|P_Z|X_4\rangle$$

from which if follows

$$R^{YZ}_{el,X} \sim -\frac{|\langle X_1|P_Y|X_4\rangle|^2}{E^X_{c\bar{p}} - E^X_{v\bar{p}} - \hbar\omega_i}. \qquad (6)$$

Equation (1) shows, that the sign of q determines the dissymmetry of the line. Therefore the sign of q is different for p and for n type silicon.

According to equation (1) the profile factor q can be deduced from the experimental curve

$$q = \frac{\Gamma_{HF} + \Gamma_{LF}}{\Gamma_{HF} - \Gamma_{LF}} \qquad (7)$$

where Γ_{HF} and Γ_{LF} are respectively the width of the high frequency side of the maximum and the width of the low energy side of the maximum. When the free carrier concentration increases from 2×10^{20} cm^{-3} to 7×10^{20} cm^{-3} the interference increases and q decreases from 12 to 9, which approves the electronic nature of the interference observed.

All the experiments[1,2] show, that q does not change its sign with the doping. Consequently R_{lat} does not also change its sign with doping. It follows from the equations (5) and (6), that experimentally established difference between the profile factor sign for p and n type silicon can be attributed to the difference between the signs of the electronic Raman tensors of the scattering in Γ point (p type) and in X point (n type). From this fact we conclude that the sign of the matrix element of the electron–phonon interaction is the same for Γ'_{25} and X_1 states.

According to equation (2) the line shape is a function of the exciting laser energy. As it was shown in reference 2 the frequency dependence of R_{lat} can be approximated by the function $R_{lat} \sim (E^{\Gamma}_c - E^{\Gamma}_v - \hbar\omega_i)^{-3/2}$ However, the frequency dependance of R_{el} in n type silicon differs from that of the p type. The difference between the forbidden gap width in X point ($E^{X_1}_c - E^{X_1}_v = 4.1$ eV) and the energy of the exciting light is much larger than the scattering frequency $\Delta\omega \sim \Omega$. Therefore R_{el} can be apparently better approximated by the function $R_{el} \sim (E^X_c - E^X_v - \hbar\omega_i)^{-1}$, which corresponds to nonresonant scattering case. Thus,

$$\frac{q(\omega_1)}{q(\omega_2)} = \frac{(E^X_c - E^X_v - \hbar\omega_1)(E^{\Gamma}_c - E^{\Gamma}_v - \hbar\omega_2)^{3/2}}{(E^{\Gamma}_c - E^{\Gamma}_v - \hbar\omega_1)^{3/2}(E^X_c - E^X_v - \hbar\omega_2)}. \qquad (8)$$

The calculated ratio $q(\omega_1)/q(\omega_2) = 1.6$ is in good agreement with the experimental value of 1.6.

Thus, the shape of the spectrum, the concentrational and frequency dependance indicate the existence of the interference of the phonon and electronic scattering in n type silicon. The sign of the profile factor evidences the coincidence of the signs of the matrix elements of electron–phonon interaction in p and in n type silicon.

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