

TWO-ELECTRON BAND TO BAND TRANSITIONS IN SILICON*

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Radiative two-electron band to band transitions are investigated experimentally in silicon. The question of phonon-participation is investigated. It turns out that at low temperature the phononless transitions dominate, whereas above room-temperature the phonon-assisted transitions become more important. A theoretical discussion leads to the conclusion that at least one participating phonon is an acoustical one.

1 INTRODUCTION

IN PREVIOUS PAPERS we reported radiative two-electron band to band transitions in Si^{1,2}. In one of the papers,¹ we considered the possibility of phonon participation at high temperatures, whereas at low temperature we had experimental evidence for a phononless transition.² In this paper we report measurements in bulk material at various temperatures. These measurements indicate that at low temperature phononless transitions dominate, whereas at higher temperature the phonon-assisted transitions become more important.

High purity Si was excited by a GaAs injection laser. The detection and registration of the luminescence was carried out in the same manner as described in reference 1.

Figures 1–3 show the observed spectra. The theoretical lineshapes of phononless (full line) and phonon-assisted (dashed line) transitions are drawn in the figures. The lineshapes of the phononless transitions are calculated by phase-space integration,^{1,2} using band data from Haynes *et al.*³ As was pointed out in reference 1, only a two-phonon transition may be comparably strong as the phononless transition, because only two

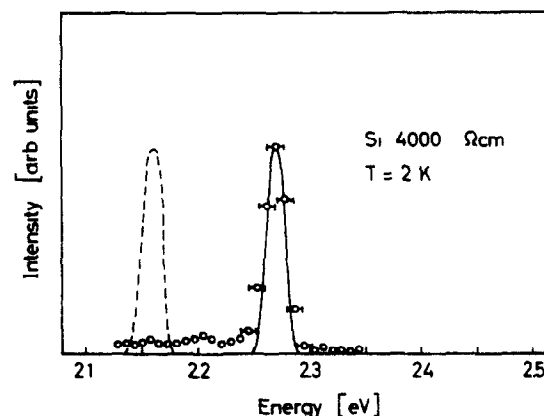


FIG. 1 Two-electron transition spectra at 2 K. The points give the experimental data with corresponding error bars. The full lines are theoretical calculations of phononless transitions, the dashed lines show theoretical calculations of two-phonon-assisted two-electron transitions.

phonons can avoid the large momentum transfer in the electron–electron scattering. Therefore we have calculated the dashed lines under the assumption of two-phonon participation. Furthermore, we have assumed that these phonons are those which dominate in the radiative one-electron transition, i.e., TO-phonons. This assumption may be wrong because of other symmetry selection rules. Under these assumptions we have calculated the lineshape of the phonon-assisted transitions. In Fig. 1 we shifted a phase space integration

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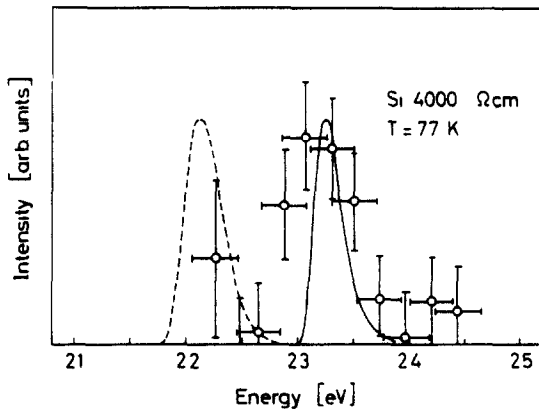


FIG 2. Two-electron transition spectra at 77 K. The points give the experimental data with corresponding error bars. The full lines are theoretical calculations of phononless transitions, the dashed lines show theoretical calculations of two-phonon-assisted two-electron transitions.

without momentum conservation by two TO phonon energies. At higher temperatures we calculated the lineshapes by a convolution integral of the E_g -luminescence using data from Haynes *et al.*³ (Fig 2) and Haynes and Westphal⁴ (Fig 3).

As can be seen from Fig. 1, at He-temperature only a phononless transition appears. The background towards lower energies is caused by the radiative recombination of Auger-electrons which is well understood.⁵ At N₂-temperature (Fig 2) a strong zero-phonon line appears, whereas no information for the lower energy-part could be obtained because of the cut-off of the photomultiplier and the low intensity. At room-temperature both processes obviously participate in the radiative transition. The best fit is obtained with an integral contribution of 57% for the phononless transitions and 43% for the phonon-assisted transitions (dashed-dotted line in Fig 3).

The discrepancy to earlier published data¹ originates from the use of diodes as samples and the use of useless E_g -spectra in that paper. With diodes we get agreement with these bulk measurements only in the case of pin-diodes with a large r -region.

For a theoretical calculation of the temperature dependence three influences have to be considered: the temperature dependence of the phase space integration, the temperature dependence of the screening

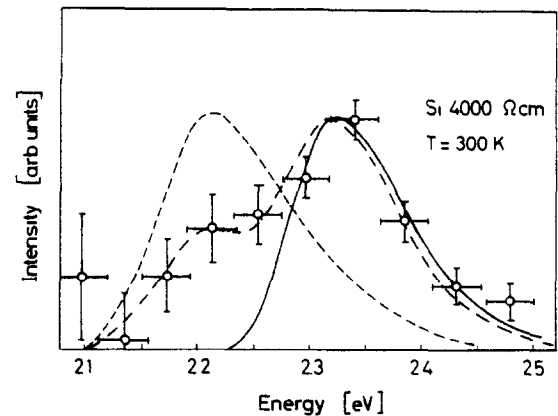


FIG 3. Two-electron transition spectra at 300 K. The points give the experimental data with corresponding error bars. The full lines are theoretical calculations of phononless transitions, the dashed lines show theoretical calculations of two-phonon-assisted two-electron transitions. The dashed-dotted line is a fit with 57% phononless and 43% phonon-assisted transitions.

length, and the temperature dependence of the phonon-participation. The temperature dependence of the enhancement by electron-hole correlation is equal in both cases and therefore not considered, because we got no absolute transition probabilities.

The temperature dependence of the phase space integration was calculated in reference 1. For phononless transitions it turned out that the transition probability decreases with temperature as $T^{-1.5}$ in the case of nondegeneration. Below the Fermi-temperature the transition probability is constant. For phonon-assisted transitions no temperature dependence arises from the phase space integration over the electronic states.

Considering the screening length one must remember the reason why we have taken into account the phonon-participation. According to Beattie and Landsberg⁶ the electron-electron scattering part of the second order transition matrix-element for two-electron transitions is proportional to $(\Delta k^2 + \lambda^2)^{-1}$, i.e. the transition probability is proportional to $(\Delta k^2 + \lambda^2)^{-2}$, where Δk is the transferred momentum and λ is the screening constant. In the case of no phonon participation, Δk is large and nearly constant, so that the transition probability is very small and no temperature dependence arises from this cause. To avoid this large momentum transfer we consider a two-phonon-assisted transition. In this case the squared matrix-element is

very much larger (by about ten orders of magnitude and therefore may weight up the two times higher perturbation order) and is proportional to λ^{-4} . In the case of nondegeneration, the screening constant is the inverse Debye-length, which is proportional to $T^{0.5}$. The K -space integration then leads to a dependence of the transition probability proportional to λ^{-1} or $T^{0.5}$. Below the Fermi-temperature also in this case the transition probability is constant.

It should be mentioned that the dependence of the screening length on the carrier density leads to a deviation from a fourth order reaction kinetic. This is neglected in this paper assuming nearly constant excitation densities in the experiments. In the case of Auger-recombination, it explains the $p^{-1.5}$ dependence of the minority carrier lifetime in Ge reported in an earlier paper.⁷ This is a further argument to assume a phonon-assisted Auger-recombination as we have done in several papers,^{8,9} and as recently was considered by Huldt¹⁰ also.

The two discussed influences lead to a temperature dependence of the ratio between phononless to phonon-assisted two electron transitions proportional to T^{-2} at high temperature and a constant ratio below the Fermi temperature. Taking a Fermi temperature of 150 K for the carrier condensation in Si one expects a ratio variation of 1–4 between He-temperature and room-temperature.

The experiments indicate a stronger dependence. Therefore we must consider a contribution of the phonon occupation to the temperature dependence. This means that our assumption of participation of two TO phonons is wrong. To avoid this discrepancy we must consider the participation of at least one acoustical phonon with a Debye-temperature below the room-temperature. The assumption of participation of one acoustical and one optical phonon would agree with the interpretation of subsequent Auger and optical transition in an earlier paper.⁵

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