Observation of $P_{1/2}$ resonant states and Fano resonances of the deep gold acceptor in silicon

M. Kleverman, J. Olajos, and H. G. Grimmeiss
Department of Solid State Physics, University of Lund, Box 118, 221 00 Lund, Sweden
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Optical transitions from the ground to excited states of the midgap gold acceptor in silicon have been studied by photoconductivity. Our data verify the close similarity between the line spectra of gold and those of group-III acceptors through the observation of $P_{1/2}$ excited states. It is also shown that Fano resonances of $P_{3/2}$ states involve only the Γ phonon (519 cm^{-1}) as in the case of group-III acceptors.

INTRODUCTION

Gold introduces into silicon an amphoteric center which has three different charge states. The ground state of the acceptor lies 545 meV below the conduction band and that of the donor 350 meV above the valence band.[1] Although the gold centers have been extensively studied, their electronic properties are still not fully understood. Recently, a series of excited $P_{3/2}$ states was observed in absorption[2] originating from bound-to-bound hole transitions of the deep acceptor. The series was shown to be very similar to the one observed for indium, a group-III acceptor. In this article we report on additional studies of the gold acceptor level obtained from photothermal ionization spectroscopy (PTIS) measurements. In particular, data will be presented which, for the first time, reveal transitions from the $P_{3/2}$ ground state to resonant $P_{1/2}$ states and strong Fano resonances involving excited $P_{3/2}$ states. This shows that the overall spectral features of deep acceptors agree very well with those for group-III acceptors.

EXPERIMENTAL DETAILS

The samples were lapped, polished, and etched in $HF + H_2O$ prior to gold evaporation of an approximately 300-nm-thick gold layer. The samples were introduced into an evacuated and then sealed quartz ampoule and heat treated for 16 h at about 1250 °C. After diffusion the surface layer was lapped and polished. Good Ohmic contacts were obtained by rubbing Ga-Al onto parts of the surface. All spectra were measured with a Bomem DA 3.01 Fourier-transform infrared spectrometer and the sample temperature was about 10 K. To improve the transparency of our spectra the PTIS data were divided by an averaged background signal.

RESULTS AND DISCUSSION

A typical spectrum obtained from a PTIS measurement of Si:Au is presented in Fig. 1. The dominating excitation process in the spectral region which is of interest for our studies is a two-step excitation process (i.e., excitation from the valence band into the acceptor level and then from the acceptor level into the conduction band). Bound-to-bound-state ($P_{3/2}$) transitions absorb photons but do not contribute to photoconductivity. If such transitions decrease the number of photons which otherwise are accessible for more effective excitation processes they are observed as dips in the background signal. The energy positions of the $P_{3/2}$ lines obtained are close to the ones recently observed in absorption measurements.[2]

At higher photon energies the $P_{3/2}$ spectrum shows an additional structure, in particular, a doublet at 5309 and 5320.5 cm^{-1} which is very close to the energy where the $2p'$ transition is expected (notations from Ref. 3). The energy spacing between these two lines is about 12 cm^{-1}. Considering that the energy spacings of $P_{3/2}$ lines observed for gold in silicon are very close to those of the corresponding lines for group-III acceptors, it is quite obvious that the doublet cannot be identified as $2p'$ and $3p'$ lines since the observed energy spacing of these two lines is about 24 cm^{-1} for group-III acceptors. Comparing the gold spectrum in silicon with data obtained for indium (see lower curve in Fig. 1) we therefore suggest that the

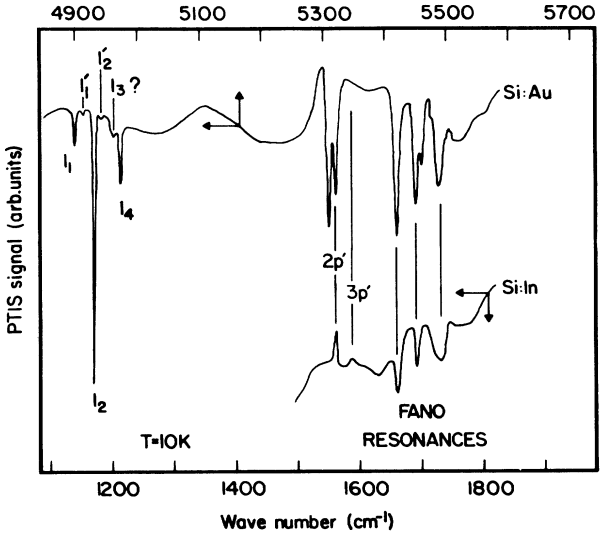

FIG. 1. PTIS measurements of Si:Au showing a series of excited $P_{3/2}$ states at about 4950 cm^{-1} originating from the gold acceptor. At higher energies the $P_{1/2}$ and Fano resonances in Si:Au are compared with those of Si:In. The assignment of the $2p'$ and $3p'$ lines is valid for Si:In.

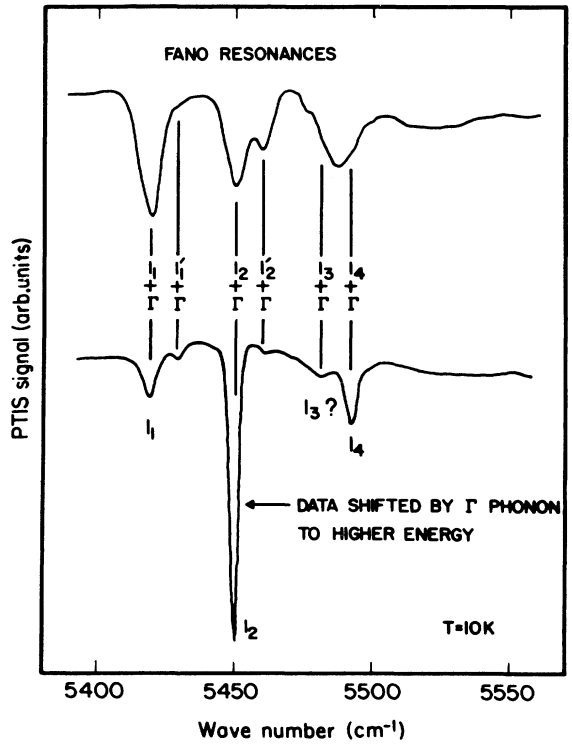

FIG. 2. Fano resonances of the $P_{3/2}$ excited states. The lower curve is the original spectrum of the series of excited $P_{3/2}$ states shifted to higher energies by one Γ phonon.

doublet at 5309 and 5320.5 cm^{-1} is caused by excitations from the $P_{3/2}$ ground state to the $2p'$ resonant $P_{1/2}$ state in the valence band and that the splitting may be caused by a lower symmetry of the center than T_d since similar splittings have been observed for other lines. This interpretation is in agreement with studies of the thermal emission rate for the gold acceptor under stress.[4,5] A closer inspection of the $P_{3/2}$ lines in Fig. 1, for example, reveals low-intensity partners with an energy separation equal to the one observed for the $2p'$ doublet. Since the final state of the $2p'$ transition is believed to be a spin doublet and since the energy separations between the different lines of the $P_{3/2}$ doublets and the $2p'$ lines are equal, we believe that the doublet structure originates from a splitting of the ground state. The large differences in the relative intensities are probably not caused by the Boltzmann factor, since the initial state of the low-intensity partners of I_1 and I_2 are expected to originate from the deeper component of the ground state. The differences in intensities may thus be caused by differences in transition probabilities.

TABLE I. Fano resonances for the $P_{3/2}$ transitions.

Transition	Transition energy (cm^{-1})	Transition energy + Γ phonon (cm^{-1})	Observed Fano resonance (cm^{-1})
I_1	4898.2	5417.2	5419.2
I_2	4929.1	5448.1	5449.5
I_3	4961.0	5480.0	5478.0
I_4	4971.8	5490.8	5488.0

Fano resonances have been observed for substitutional shallow[6,7] and deep centers.[6,8–10] The assignment of the resonances for chalcogens in silicon[6,8,9] has recently been confirmed by independent measurements.[11] For acceptors, only the Γ phonon (519 cm^{-1}) has been reported to be involved in the resonances process. Adding the Γ-phonon energy to the observed $P_{3/2}$ lines of gold in silicon, a spectrum is obtained which is almost identical to the one experimentally observed in our samples at higher energies, as shown in Fig. 2. We therefore conclude that the structure seen at about 5450 cm^{-1} is due to Fano resonances of bound-to-bound-state $P_{3/2}$ transitions (Table I). It is interesting to note that the I_2 Fano resonance exhibits a similar doublet as the I_2 line in the $P_{3/2}$ series. In addition to the acceptor line spectra presented in this report, similar structures previously reported in Refs. 2 and 12 were also observed.

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