Observation of Fano resonance in heavily doped p-type silicon at room temperature

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We report the observation of a resonance in the infrared-absorption spectrum of heavily boron-, aluminium-, and gallium-doped silicon at room temperature. This resonance occurs near the frequency of the zone-center optical phonon (517 cm^{-1}) and is attributed to a discrete-continuum Fano-type resonant interaction between the optical phonon and direct inter-valence-band transitions of holes. The optical-phonon transitions are allowed due to the disruption of symmetry of the crystal lattice by acceptor atoms. The dependence of the resonance on doping level is investigated.

I. INTRODUCTION

Fano resonances (antiresonances) (Ref. 1) have been observed as an electron-phonon coupling in silicon.[2-9] A resonant interaction of the optical phonon with photoexcitation of the acceptors has been observed at low temperatures (6–100 K) by infrared-absorption spectroscopy[2-5] and photoconductivity.[6] A resonance between the optical-phonon and free-carrier absorption in heavily doped Si has been observed by Raman scattering at $T = 300$ K.[9]

Reported here is an observation of a resonance in the infrared-absorption spectrum of heavily boron-, aluminium-, and gallium-doped silicon at room temperature. This resonance occurs as a sharp dip in the absorption spectrum near the frequency of the zone-center optical phonon ($\sim$517 cm^{-1}). This dip is attributed to a discrete-continuum Fano-type resonant interaction between the optical phonons and direct inter-valence-band transitions of holes. These free-hole interband transitions have not been directly observed in the infrared-absorption spectrum of Si [unlike Ge (Ref. 10)] because of masking by the indirect intraband transitions, but become detectable at high doping levels due to resonant interaction with the optical phonons.

II. EXPERIMENT

The transmission spectra were measured at room temperature using a Nicolet-520 Fourier transform infrared (FTIR) spectrometer with a spectral resolution of 4 cm^{-1}. The samples used had heavily B-, Al-, and Ga-doped layers formed on float zone, $\langle 100 \rangle$, single-crystal Si substrates of thickness 0.028 cm with a residual impurity (boron) concentration of 10^{14} cm^{-3}. B-doped layers of depth 0.05–0.5 μm were diffused on both surfaces of the substrates. The maximum B concentrations in the layers varied from 2×10^{19} to 10^{20} cm^{-3}. Al- and Ga-doped layers of thickness 1–5 μm were grown by epitaxy, with acceptor concentrations ranging from 10^{18} to 10^{19} cm^{-3}.

III. RESULTS AND DISCUSSION

The transmission spectra of the specimens doped with B, Al, and Ga are shown in Fig. 1. The background comes from the free-hole absorption (Fig. 2) and Si lattice absorption. A prominent peak at about 517 cm^{-1} is attributed to a Fano-type interaction between the optical phonons and the continuum of free-carrier intervalence-band transitions (Fig. 2). Near-zone-center optical phonons with wave vectors $\vec{g}$ distributed away from $\vec{g}=0$ are allowed[2] to participate in the interaction. The possibility of excitation of the optical phonons is due to the presence of acceptor atoms which destroy the symmetry of the Si lattice. Represented as a ratio of the Fano absorption to the free-carrier absorption, the spectrum shows (Fig. 3) a sharp dip (antiresonance) and a further increase in absorption at lower photon energies (resonance). The behavior of the absorption spectra of Al- and Ga-doped samples is analogous. This line shape is in good agreement with that reported earlier.[2-3,9,11] Fano[1] gives a line-shape formula as a ratio $R(\varepsilon, q)$ for the transition probabilities from a modified discrete state to the unperturbed continuum
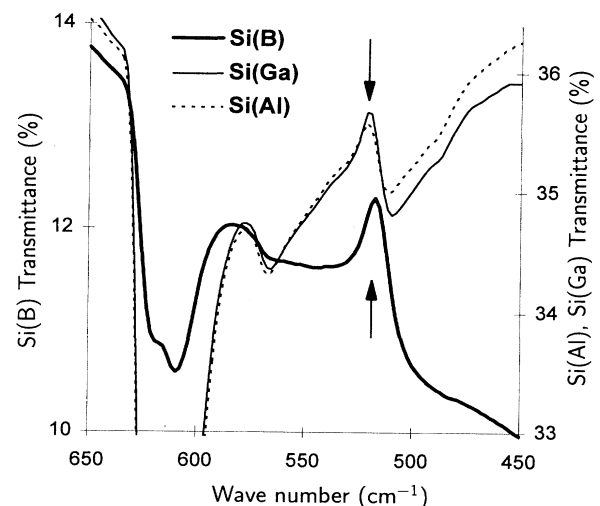

FIG. 1. Infrared transmission spectra at room temperature for silicon substrates with a 1-μm-thick gallium-doped film ($\sim 7 \times 10^{18}$ cm^{-3}), a 3-μm-thick aluminium-doped film ($\sim 4 \times 10^{18}$ cm^{-3}), and 0.25-μm-thick boron-doped layers ($\sim 5 \times 10^{19}$ cm^{-3}) on both surfaces.
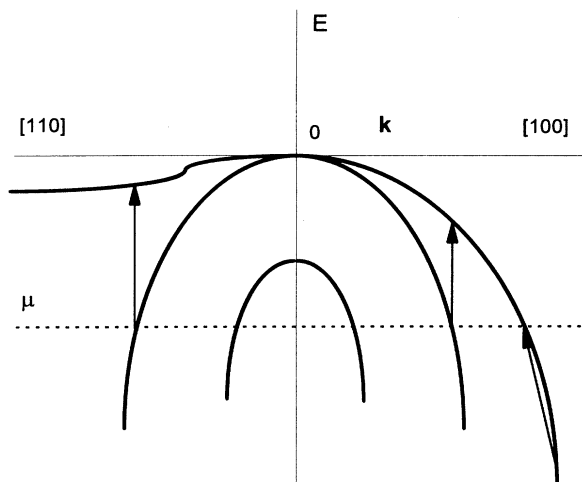
FIG. 2. The structure of the silicon valence band. Examples of interband (vertical arrows) and intraband (oblique arrow) electronic transitions are indicated. Here μ stands for the Fermi energy.

FIG. 4. Parameters Γ (full symbols) and q (open symbols) from Fano ratio vs free-carrier concentration. Squares, circles, and triangles indicate B, Al, and Ga acceptors, respectively.

$$R(\varepsilon,q) = (q+\varepsilon)^2/(1+\varepsilon^2) , \tag{1}$$

with

$$\varepsilon = (h\nu + E_1)/(\Gamma/2) , \tag{2}$$

where q is the line-shape parameter, $h\nu$ is the energy of the IR photon, E_1 is the sum of the resonance energy E_0 (energy of the optical phonon in our case) and its shift due to the configuration interaction, and Γ represents the strength of the configuration mixing between the discrete state and the continuum. The quantity q^2 represents the transition probability to the discrete state (modified by the continuum) divided by the transition probability to a bandwidth Γ of the unperturbed continuum state.[1]

Figure 4 shows the dependence of Γ and q (full and open symbols, respectively) on free-carrier concentration N_{fc}. The two increasing regions in these dependences are attributed to different mechanisms of excitation of the optical phonons, and will be discussed separately.

(i) We propose that at moderate doping levels ($10^{18} \leq N_{fc} \leq 3.5 \times 10^{18}$ cm^{-3}) the majority of optical phonons participating in a Fano resonance are those permitted due to the presence of the neutral acceptor atoms. It is known[12–14] that in silicon at room temperature in the doping range from about 10^{17} to about 5×10^{19} cm^{-3}, the dopant atoms are not completely ionized, and the majority-carrier concentration can be significantly lower than the doping concentration. Calculated using a model proposed in Ref. 12 and plotted in Fig. 5 is a fraction of neutral (unionized) boron atoms versus total free-carrier concentration (for Al and Ga acceptors this curve is simi-
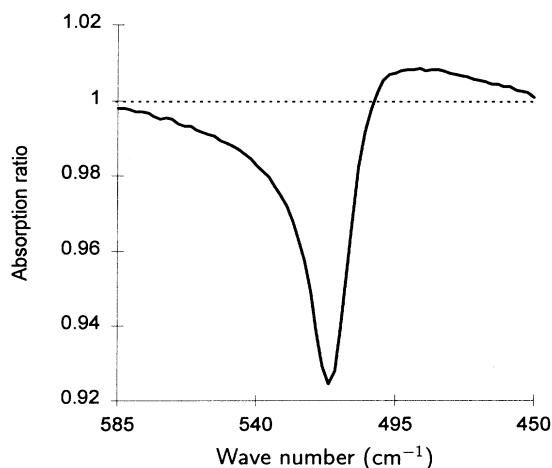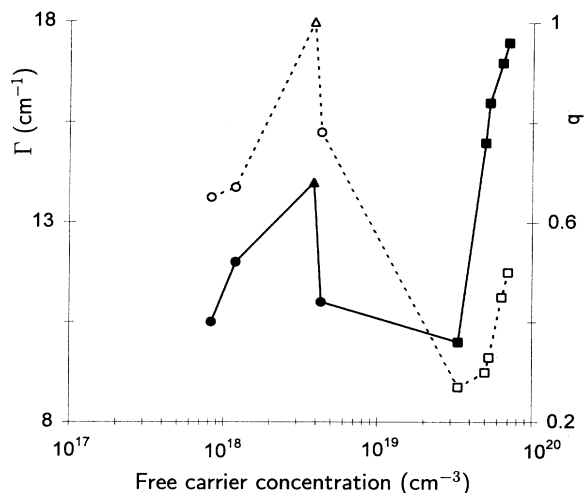

FIG. 3. Fano resonance for the Si(B) specimen corresponding to Fig. 1. The spectrum is normalized to the background absorption.
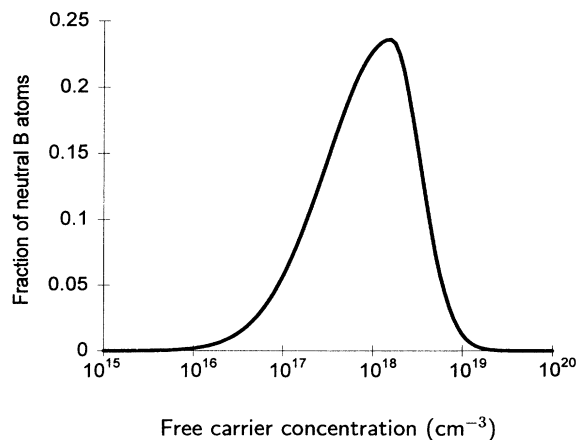

FIG. 5. Fraction of neutral (unionized) boron atoms in silicon vs free-carrier concentration at room temperature.

lar). These neutral atoms are mostly localized in regions with a carrier concentration of about 3×10^{18} cm^{-3}. As the fraction of neutral acceptors increases, the interaction strength (Γ) increases as well, and achieves a local maximum at $N_{fc} \sim 3.5 \times 10^{18}$ cm^{-3} (Fig. 4). After reaching a maximum at higher N_{fc}, Γ decreases in accordance with the decrease in the fraction of neutral acceptors, as seen in Fig. 5. In the N_{fc} range under consideration, the excitation of the optical phonons due to the presence of ionized acceptor atoms was shown to be undetectable.[3,15]

(ii) In heavily doped samples with $N_{fc} \geq 3.5 \times 10^{19}$ cm^{-3}, the fraction of neutral acceptors is negligible (Fig. 5), and the dominant mechanism of excitation of the optical phonons is that due to the disruption of symmetry of the crystal lattice by ionized acceptor atoms.[15] At these high doping levels, one can see a rapid increase of Γ with the increase in doping level (Fig. 4).

The behavior of parameter q is similar to that of Γ over the whole range of N_{fc}. An important difference is that the values of q in region (i) are much greater than those in region (ii). This means that the excitation of the optical phonons due to the presence of neutral acceptors is more likely than that due to the ionized acceptors.

Finally, as evidence that the free valence hole absorption participates in the resonance, rather than the photoionization of the acceptor, is the fact that the resonance we observe does not depend on the kind of dopant and occurs in boron-, aluminium-, and gallium-doped silicon (see Fig. 1). While the photoionization continuum of B in Si, starting at the energy $E_i \cong 44$ meV, overlaps with the energy of the optical phonon (64 meV) and leads to the resonance,[2] the photoionization continua of Al ($E_i \cong 69$ meV) and Ga ($E_i \cong 73$ meV) do not.

IV. CONCLUSION

In summary, at room temperature we have observed a resonance at approximately 517 cm^{-1} as a dip in the infrared-absorption spectra of heavily acceptor-doped layers on pure silicon substrates. The observed resonance is attributed to a discrete-continuum Fano-type interaction between the optical-phonon transitions and the continuum of inter-valence-band transitions. These direct interband transitions are normally not observed in the infrared-absorption spectrum of p-type Si because of strong indirect free-carrier absorption, but become detectable at high doping levels due to the resonant interaction with the optical phonons. The optical-phonon transitions are allowed due to the presence of the acceptor atoms. Both ionized and neutral (unionized) acceptors destroy the symmetry of the silicon lattice, permitting the optical-phonon transitions. These two mechanisms of excitation of the optical phonons have been observed separately via Fano resonance. The resonance is shown not to depend on the acceptor species and occurs in boron-, aluminium-, and gallium-doped silicon. The dependence of the resonance on the doping level is investigated. This type of study may provide a direct method of studying the properties of the optical phonons and free carriers in such systems.

ACKNOWLEDGMENTS

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