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POLARIZATION DEPENDENCE OF THE PIEZOREFLECTANCE IN Si AND Ge

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(Received 19 July 1965)

Previous high-precision measurements of the piezoreflectance of Si,¹ based on the technique used by Philipp, Dash, and Ehrenreich,² have been extended to include the dependence on the polarization of the radiation. Here, results of static and low-frequency measurements are given for the reflection peaks of Ge and Si near 2 and 3.4 eV, respectively, and a microscopic theory for the dependence of the effect on the orientation of the stress axis and on the polarization is described. A more comprehensive discussion is given elsewhere.³ These data allow one to deduce the symmetry of the transitions responsible for the reflection peaks and the deformation-potential constants. The results are also of interest with regard to more recent measurements^{4,5} obtained by an ac technique using piezoelectric transducers.

In both Si and Ge, the stress axes have been chosen to be parallel to the [001] and the [111] directions, and light has been linearly polarized parallel and perpendicular to the stress axes. All curves have been taken at room temperature on crystals immediately after etching in CP4. The data which were reproducible to $\Delta R/R = 3 \times 10^{-4}$ (error in the relative position of the curves to each other is $\Delta R_{rel} = \pm 0.5\%$) reveal effects not observed in previous static measurements.² Also, dynamical measurements have been carried out on Ge by applying a sinusoidal alternating stress at about 100 cps with narrow-band phase-sensitive detection. These give results in good agreement with the static measurements.

The results for the 2-eV peaks of Ge are shown in Fig. 1. In the case of the [001] axis [Fig. 1(a)], there is a polarization-independent energy shift of the reflectivity peaks, whereas a shift with a marked polarization dependence is observed in the [111] case [Fig. 1(b)].

If we assume that transitions with k along $\langle 111 \rangle$ axes of the type $\Lambda_4 + \Lambda_5 - \Lambda_6$, $\Lambda_6 - \Lambda_6$ (double group notation) are primarily responsible⁶ for the 2-eV peaks, then [001] stress affects all $\langle 111 \rangle$ axes equally and causes no polarization-dependent splitting in energy, as observed. On the other hand, under [111] stress, the eight $\langle 111 \rangle$ levels divide into two groups of two and six levels. The energy shifts of the two groups depend on their orientation to the stress axis. The contributions of the two groups of $\langle 111 \rangle$ levels to the intensity of the transition are determined by the respective orientations of the polarization vector. The observed dependence of the energy shift on polarization for stress thus supports the above assignment.

From the observed energy shifts one can determine the deformation-potential constants⁷⁻⁹ $E_{1c}^{\Lambda} - E_{1v}^{\Lambda} = -5.7 \text{ eV} \pm 5\%$, $E_{2c}^{\Lambda} = +5.1 \text{ eV} \pm 20\%$, where c and v refer to the conduction and valence bands, respectively. The value for $E_{1c}^{\Lambda} - E_{1v}^{\Lambda}$ is the same as that deduced from hydrostatic measurements by Paul.¹⁰

In addition to the energy shifts of the reflectivity peaks, there is a strong strain-induced change in the magnitude of the peaks [Fig. 1(a)]. To explain this effect, we consider the imaginary part of the dielectric constant, ϵ_2 , which shows essentially the same structure as the reflectivity in the region of strong absorption. Both the joint density of states¹¹ and the transition matrix elements contribute to ϵ_2 . Each of these factors may change by the application of uniaxial stress. In the case of [001] stress, the reflectivity of the 2.1-eV peak increases, and the reflectivity of the 2.3-eV peak decreases for light polarized parallel to the compression axis, whereas the converse occurs for the perpendicular polarization (Fig. 1). The change in the joint density of states caused by [001]

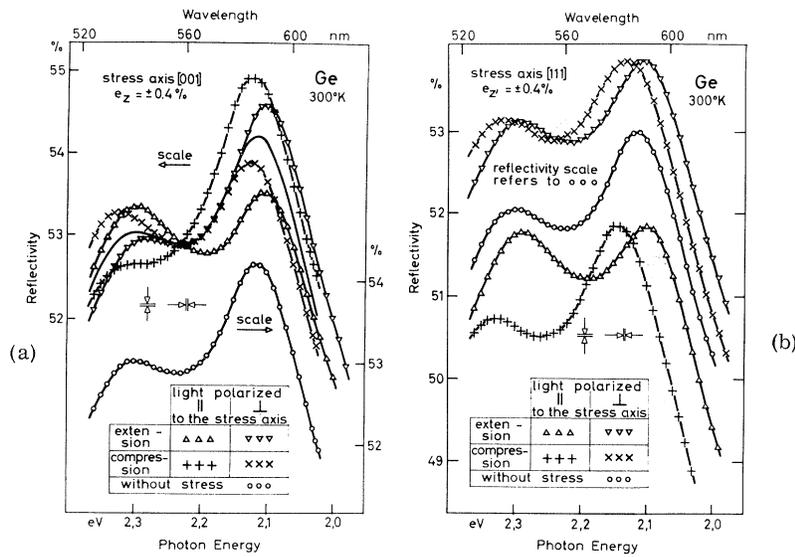


FIG. 1. The reflectivity of unstressed and uniaxially stressed Ge crystals at 300°K near 2 eV. The stress axis is [001] (a) and [111] (b). The light is linearly polarized parallel and perpendicular to the stress axis, and the strain component along the stress axis is 0.4%. The arrows show the reproducibility and the resolution. The curve in the lower part of (a) (unstressed crystal) is repeated in the upper part. In (b), the curves taken on the stressed crystal are shifted arbitrarily in direction of the reflectivity scale.

stress is the same for all equivalent Λ transitions. Thus, it cannot account for the observed behavior. We therefore conclude that the change in the reflectivity is due to a change in the transition matrix elements. The selection rules for light polarized parallel and perpendicular to a $\langle 111 \rangle$ crystal axis are shown in Table I for the cubic crystal. These rules are broken only to second order by the applied strain, but in first order equivalent oscillator strengths become inequivalent. Summing over the $\langle 111 \rangle$ axes, one can then show that the reduction in crystal symmetry accounts for the changes in magnitude of the double peaks.³ The data of the peak near 3.4 eV in silicon are given in Fig. 2. For compression (or extension) along [001], the sign of the energy shift of the

peak depends on the polarization, whereas compression along [111] always shifts the peak to higher energies [Fig. 2(b)]. Using arguments similar to those given above, one concludes that the main contribution to this peak is given by transitions with k along $\langle 100 \rangle$ axes, i.e., $\Delta_6 \rightarrow \Delta_6$ and $\Delta_7 \rightarrow \Delta_6$. The broadening of the curves, which have been taken with light polarized perpendicular to the stress axis, compared to the curves with parallel orientation, is probably caused by a strain-induced splitting of the valence bands Δ_6 and Δ_7 . This strain splitting is larger than the spin-orbit splitting, which is of order 0.01 eV near Γ . The broadening is of the same order of magnitude as the splitting of the degenerated energy bands Γ_8^+ by stress, which has been measured by cyclotron resonance.¹² This implies that the peak is due to critical points along the Δ axes near Γ . The assignment of this peak, based on symmetry arguments, is a new one,¹ but it has also been obtained independently in refined pseudopotential calculations by Brust.¹³

Table I. Selection rules for Λ transitions. The entries indicate the components of the momentum matrix elements, which are different from zero. π and σ refer to the components parallel and perpendicular to the $\langle 111 \rangle$ axes, respectively.

	Λ_4	Λ_5	Λ_6
Λ_4	π		σ
Λ_5		π	σ
Λ_6	σ	σ	π, σ

We may summarize the foregoing detailed arguments as follows. Strain-induced changes in reflectivity are of two kinds, depending both on shifts in energy levels and changes in matrix elements. In all cases studied so far, symmetry arguments at the critical points account

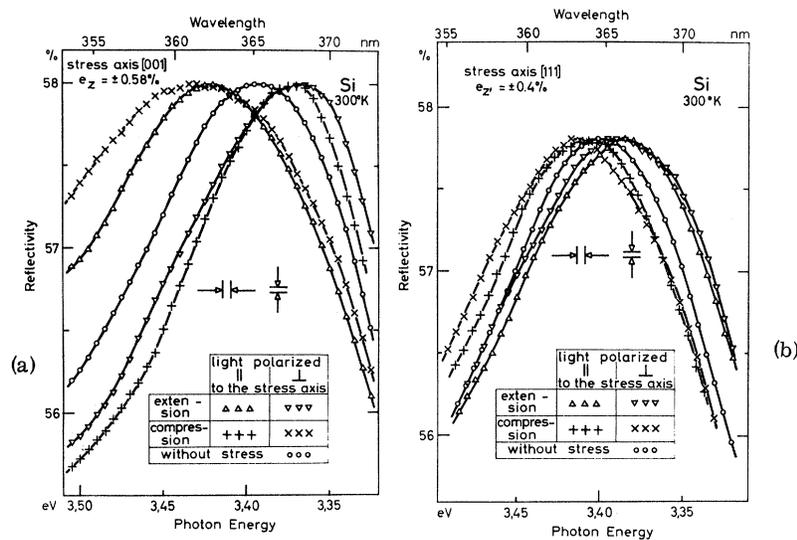


FIG. 2. The reflectivity of unstressed and uniaxially stressed Si crystals at 300°K near 3.4 eV. The notation is the same as that used in Fig. 1.

for the orientation and polarization dependence of the data. On the other hand, deformation potentials and temperature coefficients, which also have been used to assign the transitions,^{14,15} may not be so simply interpretable. This may be especially so for interband edges derived from critical points which are not fixed at symmetry points but may be displaced, e.g. along a symmetry line, as in the cases discussed above. Thus both the deformation potential¹⁴ and the temperature coefficient¹⁵ of the 3.4-eV edge in Si appear to be anomalously large for the neighborhood of Γ , where the critical points are placed by our symmetry arguments. These anomalies may also be related to the second-order reflectivity changes which are evident, for example, in Fig. 2(a). More extended discussion of these anomalies is given in reference 3.

I would like to express my gratitude to Professor W. Martienssen for his excellent advice and instruction. I also appreciate valuable discussions with Mr. H. Leonhardt and Professor J. C. Phillips.

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