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OPTICAL PROPERTIES OF SEMICONDUCTORS UNDER HYDROSTATIC PRESSURE—II. SILICON*

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Abstract—The pressure coefficient of the optical absorption edge due to indirect transitions has been measured in silicon over a pressure range of 1–8000 kg/cm². A value of $(dE/dP)_T = -1.3 \times 10^{-12}$ eV/dyne cm⁻² was obtained, in agreement with other optical and resistivity measurements. The lack of an observable change of shape of the edge with pressure implies that a simple displacement of the (100) conduction-band minima relative to the (000) valence-band maximum takes place with change of pressure.

INTRODUCTION

THE variation of the optical energy gap in germanium with hydrostatic pressure has been discussed by us in a preceding paper.⁽¹⁾ In this paper we shall present similar results for silicon, but since much of the technique of measurement and interpretation is common to both experiments, we refer the reader to the germanium discussion for many of the details.

The band structure of silicon is shown schematically in Fig. 1. Our primary concern in this paper will be with the pressure shift of the fundamental absorption edge at low absorption coefficients, i.e. with the absorption edge caused by indirect optical transitions from the top of the valence band (E_v) to the conduction-band minima (E_c) in the (100) direction, where the (000) minimum in the conduction band (E_{c0}) is a possible intermediate state. Other details of the band structure, discussed elsewhere,⁽²⁾ will not concern us here.

As we discussed in the introduction to our paper on germanium, it is not feasible at present to compare experimental measurements of the energy-gap change with pressure with a theoretical coefficient deduced from a deformation potential

analysis. We can only try to fit our results on the measurement of resistivity and other parameters into a consistent pattern. Several estimates for

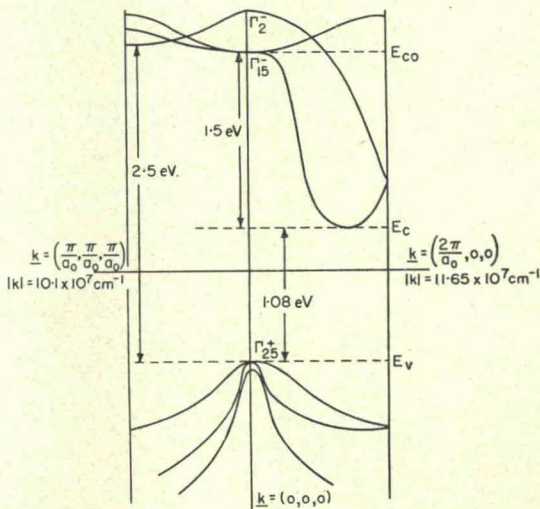


FIG. 1. Band structure of silicon in the (111) and (100) directions.

the pressure variation of the energy gap have already been reported. PAUL and PEARSON⁽³⁾ cite a value $(dE/dP)_T = -1.5 \times 10^{-12}$ eV/dyne cm⁻² derived from resistivity measurements under the

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assumption of no mobility changes. This value is in agreement with our optical value, previously reported briefly,⁽⁴⁾ and with the value obtained optically by NEURINGER⁽⁵⁾ over a smaller pressure range. NATHAN and PAUL⁽⁶⁾ arrived at a value of -2×10^{-12} eV/dyne cm^{-2} from pressure measurements on a gold level in silicon. However, FAN *et al.*⁽⁷⁾ observed an increase rather than a decrease in the optical energy gap with pressure.

METHOD

The discussion of the apparatus, experimental techniques, and treatment of sources of errors in the previous paper⁽¹⁾ is also pertinent here. The sample was an optically polished plane-parallel slab of 25–35 Ω cm *p*-type silicon, 0.0109 in. thick. Carbon disulfide was again used as hydraulic

using the second and third order of a 300 lines/mm blazed grating mounted in a Perkin-Elmer spectrometer in order to obtain sufficient resolution and angular dispersion. Suitable filters were used to eliminate overlapping orders.

The smallness of the shifts dictates that we examine carefully the following possible sources of error in the measurement.

- (1) Source-intensity change with time.
- (2) Source-spectral-dependence change with time.
- (3) Detector-gain change with time.
- (4) Detector-spectral-sensitivity change with time.
- (5) Refractive-index changes with pressure:
 - (a) Sample-reflection correction.
 - (b) Effect of sample-index change on beam geometry.
 - (c) Change of index of refraction of fluid.

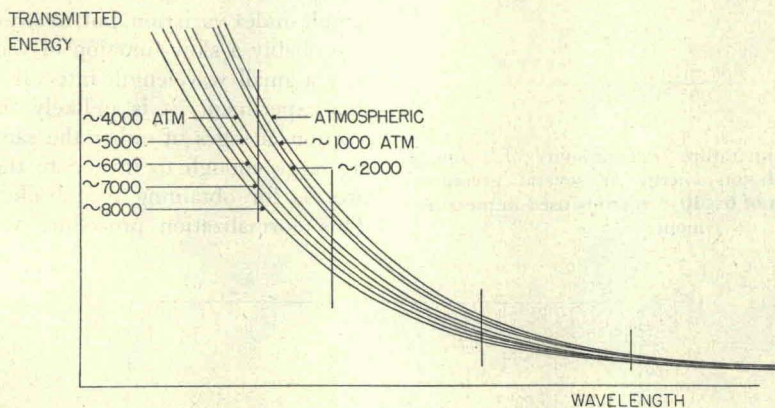


FIG. 2. Transmitted energy versus wavelength at several pressures for a silicon sample.

fluid because of its transparency in the near infrared. The pressure range in these experiments was from 1 to 8000 kg/cm^2 .

Since some question seems to exist concerning the direction of the edge variation with pressure, and since the direction deduced may depend on the manner of reduction of results, we present in Fig. 2 tracings of the original recordings of the unnormalized transmitted energy of a sample as measured, with pressure as a parameter. No spectrum was taken at 3000 kg/cm^2 . The vertical lines represent specific wavelengths on the spectra which have been matched on the combined tracing.

Because the edge shift is small over the available pressure range, further experiments were done,

- (6) Window distortion with pressure.
- (7) Changes at reference wavelength (when used).
- (8) Spectrometer resolution.

These are reproduced from the paper on germanium. From the discussion there, we have to examine most carefully sources 5 and 8. We consider error source 8 first.

Transmissivity as a function of pressure at a 500 micron slit width is shown in Fig. 3. The second order resolution at 1 micron for this slit width is 6×10^{-3} microns. In Fig. 4 transmissivities are shown for 2000 micron slit widths, i.e. at 3×10^{-2} micron resolution. This resolution is comparable to that of Fig. 2, where a glass prism was used. The two sets of curves are identical to

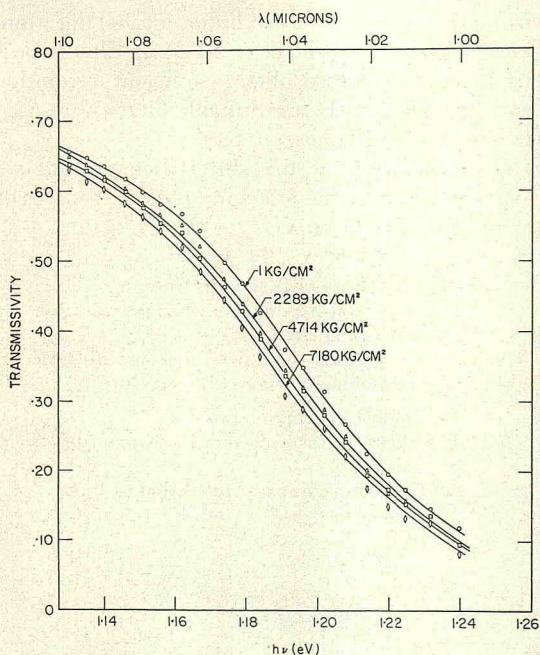


FIG. 3. Room-temperature transmissivity of a silicon sample versus photon energy at several pressures. Spectral slit-width of 6×10^{-3} microns used in measurement.

within other experimental errors, such as the detector sensitivity variation. Thus, for resolution of 3×10^{-2} microns or better, the same, presumably correct, shape and movement of the absorption edge is observed.

We consider error source 5 next. Errors 5(b) and 5(c) remain uncorrected only if there is a strong spectral-dependence of the fluid or sample-index variation. The change of the refractive index of silicon with pressure, calculated from a translation of the index-versus-frequency curve along the frequency axis by the amount of the energy-gap change with pressure,⁽³⁻⁶⁾ is of the order of 0.1 per cent in 5000 kg/cm². Experimentally, a 5 per cent increase in unnormalized transmission at long wavelengths over a pressure range of 5000 kg/cm² was observed. It is not yet determined whether this change occurs because of fluid- or sample-index variation, but, in any case, the change is probably a slow function of wavelength. Since only a small wavelength interval is of interest in this experiment, it is unlikely the index of refraction changes of either the sample or the CS₂ are large enough to invalidate the normalization process for obtaining the absolute transmission. This normalization procedure was described in

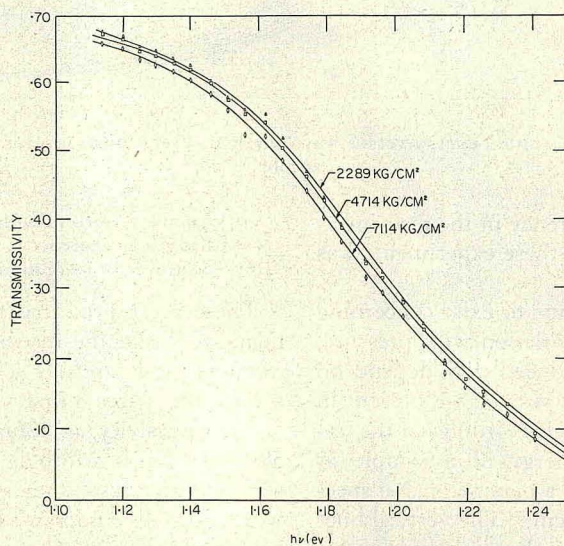


FIG. 4. Room-temperature transmissivity of a silicon sample versus photon energy at several pressures. Spectral slit-width of 3×10^{-2} microns used in measurement.

the paper on germanium. The absorption coefficients were similarly determined using values of the refractive index and extinction coefficient averaged from several sources.⁽⁸⁾ Fig. 5 shows our atmospheric data compared to that of other workers.^(7,9)

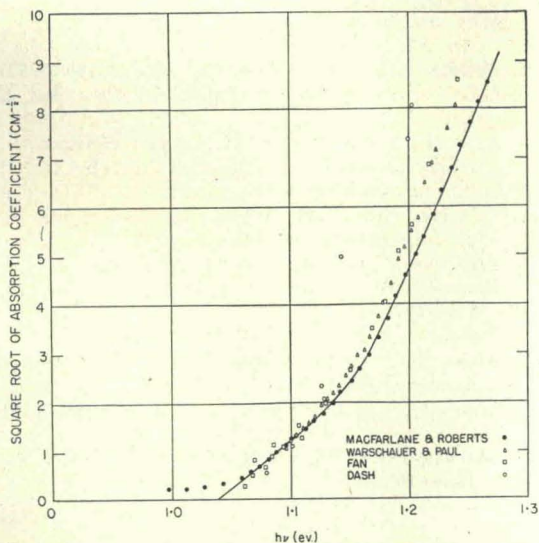


FIG. 5. Comparison of silicon room-temperature low-absorption coefficients versus photon energy with the work of other investigators.

RESULTS

As can be seen from either Fig. 3 or 4, the shift of the edge wavelength at any value of transmissivity is small as a function of pressure, and careful examination reveals no detectable change in the shape of the edge over this range of absorption constant and pressure. Thus, the pressure coefficient of the energy gap can equally well be found from isoabsorption or isotransmission curves, or from an extrapolation of the absorption coefficient curves to zero absorption coefficient. Although we have chosen to use curves of transmissivity to obtain the pressure coefficient of the energy gap, the corresponding absorption coefficients can easily be found by using Fig. 5. Fig. 6 shows an isotransmission plot derived from the curves of Fig. 3. The average pressure coefficient obtained from these curves, which were taken at room temperature, is $(dE/dP)_T = -1.3 \times 10^{-12}$ eV/dyne cm^{-2} . This is seen to be in agreement with the values obtained by other workers cited earlier,⁽³⁻⁶⁾ but not with that of Fan *et al.*⁽⁷⁾ The fact that the

isotransmission lines are approximately parallel to within the experimental accuracy verifies the lack of observable shape change in the absorption edge.

From the comparison of our absorption-coefficient range with that obtained by other

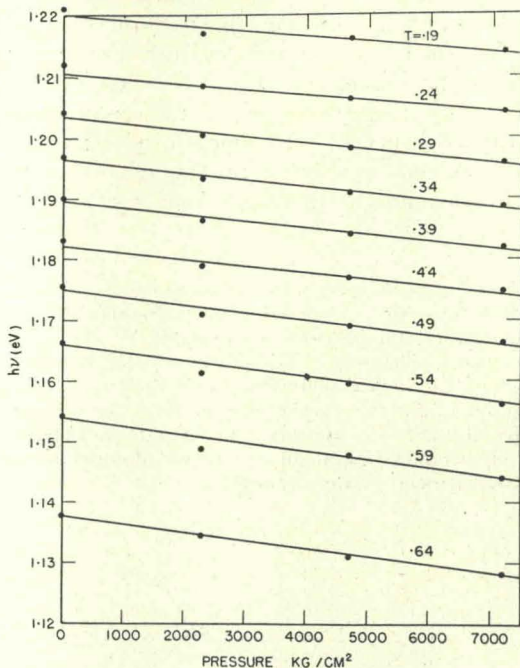


FIG. 6. Isotransmission curves for silicon at room temperature.

workers, as shown in Fig. 5, we interpret our measurements as pertaining to indirect optical transitions between E_v and E_c of Fig. 1. E_{co} may play a role as a virtual state in this process, but since its height above E_c and E_v is large, any movement of this minimum should have only a very small effect* on the value of $[d(E_c - E_v)/dP]_T$ as determined from the experiment. The good agreement between the above optical coefficient and the resistivity-derived values^(3,6) indicates the extent of validity of this view. The more elaborate examination of the effects of pressure carried out on the germanium data has not been attempted here because of the lack of indication of any change in the shape of the absorption edge with pressure.

* See the discussion of the effect of energy denominator on absorption coefficient given in reference (1).

CONCLUSIONS

Our earlier measurements of the pressure coefficient of the optical energy gap $(dE/dP)_T = -1.3 \times 10^{-12}$ eV/dyne cm^{-2} have been confirmed, in agreement with resistivity measurements^(3,6) and with the value of NEURINGER.⁽⁶⁾ The lack of change of shape of the absorption edge with pressure and the agreement of the coefficient with that derived from resistivity measurements indicate that the shift in the range of absorption measured can be attributed primarily to a simple displacement of the (100) conduction-band minima relative to the (000) maximum in the valence band.

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