

Characterization of a bulk semiconductor's band gap via a near-absorption edge optical transmission experiment

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(Received 8 July 1992; accepted 7 December 1992)

An experimental setup that employs lock-in detection to measure the optical transmission data on a bulk semiconductor sample is described. A straightforward manipulation of these data yields the semiconductor's absorption coefficient α in the energy range near its absorption edge ($0 < \alpha < 100 \text{ cm}^{-1}$). The theory of optical transitions in semiconductors required to analyze the resulting absorption spectra is presented. It is shown that a model based on an indirect optical transition involving a single phonon accurately describes data taken on a silicon sample. Based on this analysis, a value of $(1.098 \pm 0.004) \text{ eV}$ for silicon's indirect band gap and an energy of $(51 \pm 4) \text{ meV}$ for the involved phonon is deduced. Conversely, it is shown that data taken on a gallium-arsenide sample are consistent with a model based on a direct optical transition involving exponential band-tail states. A value for the band-tail's Urbach slope of $E_0 = (6.7 \pm 0.2) \text{ meV}$ is found. All of these results accurately agree with published values. This laboratory demonstrates important concepts in solid state physics via universally applicable experimental techniques at a level appropriate for upper-division undergraduates.

I. INTRODUCTION

The most direct and perhaps simplest method for probing the band structure of a semiconductor is to measure its optical absorption spectrum. In the absorption process, a photon of known energy excites an electron from a lower to a higher energy state within the semiconductor. Thus, by inserting a wafer of semiconducting material into a monochromatic light beam and studying the changes in transmitted optical intensity as a function of wavelength, one can investigate some of the possible quantum-mechanical transitions that the semiconductor's electrons can make and learn much about the distribution of allowed electronic energy levels.

A bulk semiconductor's optical absorption coefficient α can be directly calculated from optical transmission data. When light of intensity I_0 and wavelength λ is incident on a semiconducting wafer of thickness x , a transmitted intensity I emerges at the opposite face. Accounting for multiple reflections that occur within the wafer, the transmission coefficient $T \equiv I/I_0$, is given by¹⁻³

$$T = [(1-R)^2 \exp(-\alpha x)] / [1 - R^2 \exp(-2\alpha x)], \quad (1)$$

where R is the reflection coefficient at the air-semiconductor interface. Near its band edge, the imaginary part of a semiconductor's index of refraction $k = \lambda\alpha/4\pi$ is much smaller than the real part n ; thus the reflection coefficient becomes

$$R = [(n-1)^2 + k^2] / [(n+1)^2 + k^2] \\ \approx [(n-1)/(n+1)]^2. \quad (2)$$

For example, in the experiment described below, the largest α considered is 100 cm^{-1} , while $\lambda \sim 1 \mu\text{m}$. Consequently, $k \leq 10^{-2}/4\pi \approx 10^{-3}$. Since $n = 3.4$ for both Si and GaAs, the approximation of Eq. (2) is clearly valid.

The dominant mechanism for optical absorption in a semiconductor of band gap E_g is valence band-to-conduction band electronic transitions.^{1,2,4} Assuming parabolic bands, it has been shown that if a photon of energy

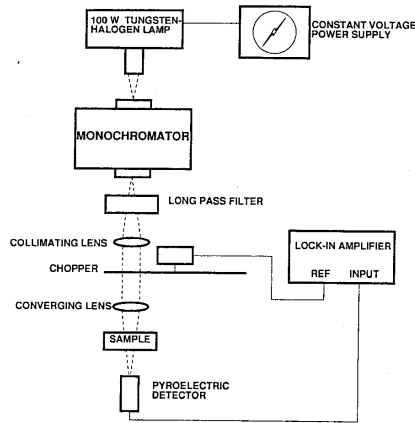


Fig. 1. Block diagram of optical transmission measurement system.

E directly creates an electron-hole pair (as at the band edge in a direct gap semiconductor), the absorption coefficient is given by

$$\alpha = A(E - E_g)^{1/2}, \quad (3)$$

where the constant A depends only on material properties. However, quite commonly in direct gap semiconductors, disorder due to impurity and temperature effects will cause exponential band-tails of electronic states to extend into the semiconductor's forbidden gap. Then, near the absorption edge, optical transitions from a parabolic band to an exponential band-tail state are manifested by an exponentially varying absorption coefficient,

$$\alpha = B \exp(E/E_0), \quad (4)$$

where B is a constant and E_0 is the Urbach slope, a parameter describing the steepness of the exponential band-tail. On the other hand, if a phonon of energy E_p is required to conserve momentum in the optical production of an electron-hole pair (as at the band edge in an indirect semiconductor), assuming parabolic bands,

$$\alpha = \alpha_a + \alpha_e, \quad (5)$$

where α_a is the absorption coefficient due to transitions involving the absorption of a phonon

$$\alpha_a = C(E - E_g + E_p)^2, \quad E > E_g - E_p, \quad (6)$$

and α_e is the absorption coefficient due to transitions involving the emission of a phonon

$$\alpha_e = D(E - E_g - E_p)^2, \quad E > E_g + E_p, \quad (7)$$

where the constants C and D depend on material properties and temperature. Note that in the α_a process, a photon along with a thermally available phonon creates an excited electron, while in the α_e process, a photon creates both a phonon and an excited electron. Thus the latter process has a greater optical energy threshold.

A recent paper presented an optical transmission laboratory designed for thin-film semiconductor samples.⁵

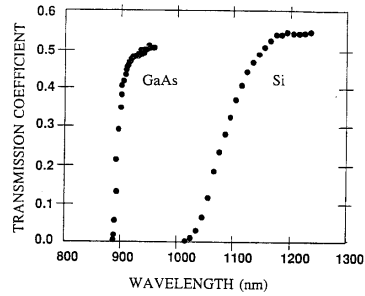


Fig. 2. Transmission coefficient vs optical wavelength data taken on silicon and gallium-arsenide samples.

The analysis for this experiment utilized the interference pattern apparent in the transmittance data to extract the sample's complex refractive index and, subsequently, the semiconductor's band gap. In this paper, we report an alternate experimental method that employs lock-in detection to directly determine a bulk semiconductor's absorption coefficient α near its band edge ($\alpha < 10^2 \text{ cm}^{-1}$). Straightforward analysis of this data reveals the nature of the semiconductor's band gap (whether direct or indirect), yields accurate values for parameters that describe band structure features (e.g., E_g, E_0) and, in the case of an indirect gap, determines the phonon energy involved in the optical transition. We demonstrate the application of this technique with data taken on silicon and gallium-arsenide samples.

II. EXPERIMENT

Figure 1 illustrates our experimental system, optimized for the investigation of samples with E_g in the near infrared. A 100-Watt tungsten-halogen source illuminates the 280- μm -wide entrance slit of a 1/8-m monochromator (Oriel 77264SPR) equipped with a 600-lines/mm diffraction grating (Oriel 77299). Exiting light passes through a 280- μm -wide slit followed by an externally mounted 800-nm long-pass interference filter (to eliminate second-order wavelengths) and condensing lens, producing a collimated monochromatic beam of variable λ in the range of 800–1600 nm with a bandpass of 4 nm. This beam is mechanically chopped (typically at 4 Hz, the lowest frequency available from our Ithaco 230 chopper, in order to maximize our detector output) then focused onto an Eltec 404VM pyroelectric detector (chosen for its wide spectral response and low cost). The pyroelectric detector's output, which is proportional to the modulated light intensity, is monitored by a PAR 5209 single-phase lock-in amplifier. For a given λ , the incident intensity I_0 is measured with the sample withdrawn. Then, with the sample placed in front of the detector, the transmitted intensity I is measured and the transmission coefficient $T(\lambda) \equiv I/I_0$ is calculated. The entire setup is mounted on a 3 \times 1 ft Newport breadboard and is immune to environmental influences such as room lighting and nearby heated bodies (e.g., students) by virtue of the lock-in detection method.

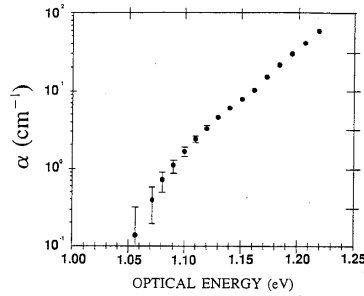


Fig. 3. Semi-log plot of absorption coefficient α vs optical energy for silicon sample. Dominant cause of α -uncertainty in the low- and high-energy range due to uncertainty in reflectivity R and transmitted intensity I , respectively.

Our silicon sample is a 1-in.-diam, (1.00 ± 0.02) mm-thick disk that is optically polished on both sides and conveniently mounted in a Newport filter holder. Such samples, stocked as IR windows, are readily available from several optical companies. With a 1-mm sample thickness, our optical system allows sensitive detection for values of α up to about 50 cm^{-1} . Alternately, we obtained good results by optically polishing a 0.5-mm-thick silicon wafer (of the type used in device fabrication) in a geology thin-sections lab. This smaller thickness increased our sensitivity to α by a factor of two. Our gallium-arsenide sample is a commercially purchased 2-in.-diam (0.50 ± 0.03) mm-thick undoped wafer, optically polished on both sides.

III. ANALYSIS AND RESULTS

Figure 2 shows $T(\lambda)$ data taken on our samples at wavelengths ranging from the transparent regime ($\alpha \approx 0$) to the limits of detectability in the absorptive region ($\alpha \approx 100 \text{ cm}^{-1}$). For Si and GaAs, this range corresponded to data from $\lambda = 1300\text{--}900 \text{ nm}$ in 10-nm increments and $\lambda = 960\text{--}892 \text{ nm}$ in 2-nm increments, respectively.

To extract $\alpha(\lambda)$ from these measurements, we exploited the fact that n and, therefore, R [see Eq. (2)] are only slightly varying over the narrow energy range of our data.⁶ Thus we deduced a value for R from the long-wavelength portion of the data and used this value in analyzing all of our measurements. From Eq. (1), we see that when $\alpha = 0$,

$$T = (1 - R)/(1 + R). \quad (8)$$

Averaging values calculated in the transparent region of 1300–1200 nm for silicon and 960–950 nm for gallium-arsenide, we obtained a value of $R = 0.31 \pm 0.01$ and $R = 0.33 \pm 0.01$ for Si and GaAs, respectively. These figures are consistent with published values for the near-absorption-edge index of refraction in silicon and gallium arsenide.⁶

Armed with this knowledge of R , the measured $T(\lambda)$ data, the known thickness of our samples and the following solution derived from Eq. (1):

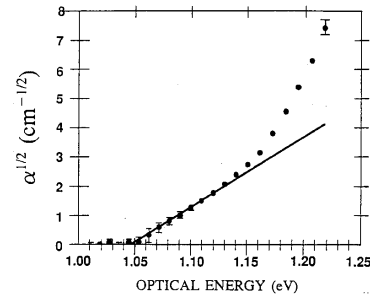


Fig. 4. Plot of $\alpha^{1/2}$ vs optical energy for silicon sample. Least-squares fit for low-energy linear region (due to phonon-absorption process) shown with extrapolation to higher energies. x-intercept is $E_g - E_p = (1.047 \pm 0.004) \text{ eV}$.

$$\alpha = -x^{-1} \ln \left(\left[\frac{(1-R)^4 + 4T^2R^2}{(1-R)^2 + 2TR^2} \right]^{1/2} \right), \quad (9)$$

we calculated the value of α at each wavelength in the absorptive regime. Applying the rules of propagation of errors to Eq. (9), we found that the calculated value of α varied by only a few percent for ± 0.01 uncertainties in R , except when $\alpha \approx 0$, i.e., in the transparent region. Significant uncertainties also occurred at our largest α values due to the low signal-to-noise ratio of transmitted intensity measurements in that regime.

Figure 3 displays the absorption spectrum that was obtained on our silicon sample. We demonstrate that indirect optical transitions between parabolic-shaped band edges are responsible for producing this spectrum by the following analysis.

A. Phonon-absorption transition

Equations (5)–(7) predict that for optical energies $E < E_g + E_p$, $\alpha = \alpha_a$ only. Thus, for an indirect gap semiconductor, a linear region should appear in the low-energy portion of a plot of $\alpha^{1/2}$ vs E . From Eq. (6), the x-intercept of this straight-line portion is $(E_g - E_p)$. Figure 4 displays

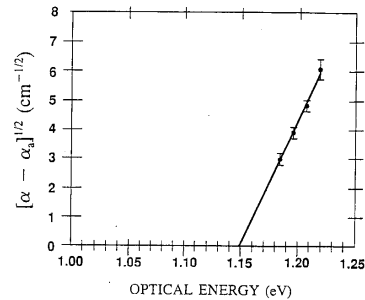


Fig. 5. Plot of $\alpha^{1/2} - \alpha_d^{1/2}$ vs optical energy for silicon sample. Linear least-square fit yields x-intercept of $(E_g + E_p) = (1.148 \pm 0.005) \text{ eV}$.

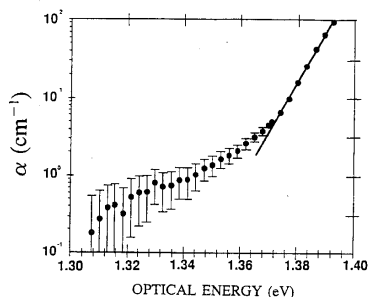


Fig. 6. Semi-log plot of absorption coefficient α vs optical energy for gallium-arsenide sample. Linear region above 1.37 eV indicates exponentially varying region of α . Linear least-squares fit yields slope of $E_0^{-1} = (149 \pm 5) \text{ eV}^{-1}$.

such a plot and identifies the low-energy linear regime. A weighted linear least-squares fit for these data yields an x -intercept value of $(1.047 \pm 0.004) \text{ eV}$. Also, using the slope and y -intercept of this fitted line, the extrapolation of α_a absorption to higher ($E > E_g + E_p$) optical energies is shown.

B. Phonon-emission transition

For optical energies $E > E_g + E_p$, Eq. (5) indicates that α_e can be found by subtracting the extrapolated α_a (determined above) from the measured α . Equation (7) then predicts that a plot of $(\alpha - \alpha_a)^{1/2}$ vs E will yield a straight line with an x -intercept of $(E_g + E_p)$. Figure 5 reveals that such a plot does indeed produce a straight line. A weighted linear least-squares fit results in a x -intercept value of $(1.148 \pm 0.005) \text{ eV}$ for this fitted line.

The value of silicon's indirect band gap and the momentum-conserving phonon's energy now can be easily calculated. One-half of the sum and difference of the two above x -intercepts yield the following values:

$$E_g = (1.098 \pm 0.004) \text{ eV},$$

$$E_p = (0.051 \pm 0.004) \text{ eV}.$$

These results are consistent with published values^{2,7} based on the single-phonon model that we have employed. (A four-phonon model, which accounts for the four branches of the phonon dispersion relation at a given k -value, has been employed by G. G. MacFarlane *et al.*³ to analyze the temperature dependence of absorption-edge spectra, yielding a value of $E_g = 1.121 \text{ eV}$ for silicon.)

It is interesting to compare our findings with information known from independent techniques. Cyclotron resonance measurements demonstrate that silicon's conduction band minima lie in the [100] directions. Comparison of our experimentally determined range of $E_p = (47-55) \text{ meV}$ with the measured phonon dispersion relation for silicon⁸ identifies this energy interval as characteristic of either a longitudinal acoustical or longitudinal optical phonon with a wave vector k at 80%-100% of the zone boundary in the [100] direction. Thus, based on our analysis, we deduce that the conduction band minima occur at a momentum value that deviates by at most 20% from the zone edge.

This conclusion is in qualitative agreement with band structure calculations that place silicon's conduction band minima at about 80% of the way to the zone boundary.

Figure 6 displays the absorption spectrum that was obtained on our gallium-arsenide sample. This plot displays the very steeply rising absorption edge (beginning at about 1.37 eV) that is characteristic of a direct gap semiconductor. Noting the straight-line character of the absorption edge on the semi-log plot, we conclude that α is proportional to $\exp(E/E_0)$ in the region of $1 \text{ cm}^{-1} < \alpha < 100 \text{ cm}^{-1}$. Equation (3) then leads us to conclude the GaAs is a direct gap semiconductor with significant band-tailing into its forbidden gap. A linear least-squares fit of our data yields an Urbach slope value for the exponential band-tail of $E_0 = (6.7 \pm 0.2) \text{ meV}$. This result agrees with published reports,^{1,9,10} which attribute a (5-7) meV band-tail to potential fluctuations caused by ionized impurities in undoped GaAs.

IV. CONCLUSION

Using an experimental setup and data-analysis appropriate for an upper-division laboratory, we have demonstrated that optical transmission data taken on silicon is consistent with a model based on indirect optical absorption between parabolic band edges. We calculate the indirect band gap to be about 1.10 eV, with the conduction band minima occurring fairly near the zone boundary. Conversely, we have shown that data taken on gallium-arsenide agrees with a model based on direct optical transitions involving exponential band-tails. This upper-division laboratory allows undergraduates to gain insight into the interaction of light with matter as well as valuable experience with experimental techniques such as lock-in detection and data modeling.

ACKNOWLEDGMENTS

We would like to thank Ron Brown of California Polytechnic University, San Luis Obispo, for helpful discussions and Fred Pool of Jet Propulsion Laboratory for the donation of our GaAs sample. This work was funded by a generous gift from Captain and Mrs. Fred Bates and NSF-ILI Grant No. USE-91-50979.

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