

Examination of the Optical Band Gap of various Semiconducting Materials

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(Dated: March 7, 2010)

In this experiment, we examine the band structures of three different semiconducting materials, silicon, gallium-arsenide, and cadmium-telluride. Using a monochromator and a lock-in detection method, measurements of the optical transmission data for each material were taken. The data was examined in order to determine a model for each semiconductor's absorption coefficient near its band edge ($0 < \alpha < 100 \text{ cm}^{-1}$). The data obtained for the silicon sample suggests an indirect-gap model of a semiconductor with transitions involving a single phonon. The band-gap energy, E_g , and the phonon energy, E_p , were determined as follows.

$$E_g = 1.090 \pm 0.008 \text{ eV} \quad E_p = 0.048 \pm 0.008 \text{ eV}$$

The data obtained for both the gallium-arsenide and cadmium-telluride samples suggest a direct-gap model of a semiconductor with transitions involving exponential band-tail states. The band-tail's Urbach slope for each sample was determined as follows.

$$E_0^{ga} = 0.121 \pm 0.004 \text{ meV} \quad E_0^{ca} = 0.672 \pm 0.004 \text{ meV}$$

The energy values obtained for silicon accurately agree with published values, however the Urbach slope values for gallium-arsenide and cadmium-telluride do not. Possible sources or error are discussed in the conclusion.

INTRODUCTION

The optical absorption spectrum of a semiconductor may be examined by directing a monochromatic beam of light through a thin wafer of semiconducting material. When a photon is incident on the surface of a semiconductor, it can be reflected, transmitted through the material, or absorbed. When a photon is absorbed, it excites an electron to a higher energy state within the semiconductor (often into the conduction band, allowing electrons to move freely within the semiconductor, allowing it to conduct current). By studying the transmitted optical intensity as a function of the wavelength of light incident on the sample, much can be learned about the absorption process of a particular semiconductor. This method of probing the band structure allows one to investigate the allowed energy levels and quantum mechanical transitions of electrons within various semiconducting materials.

THEORY

When light of intensity I_0 is incident on the surface of a thin wafer of semiconductor material, a portion of the light is transmitted through the wafer, exiting the material with intensity I . The rest of the light is either absorbed by the material or reflected off of its surface. These interactions are governed by the transmission, reflection, and absorption coefficients of the material, T , R , and α respectively. Given the thickness x of a sample, the transmission coefficient, T , may be represented by the following equation.

$$T = \frac{(1 - R)^2 e^{-\alpha x}}{1 - R^2 e^{-2\alpha x}} \quad (1)$$

Across the transparent regime of a semiconductor, $\alpha \approx 0$. Thus, we can simplify the above equation for the transparent regime to the following.

$$T = \frac{1 - R}{1 + R} \quad (2)$$

Reversing this equation, we get an equation for the reflection coefficient, R , given values for the transmission coefficient, T , over the transparent regime.

$$R = \frac{1 - T}{1 + T} \quad (3)$$

The reflection coefficient, R , can also be represented by the following equation where n is the real part of the semiconductor's index of refraction and $k = \lambda\alpha/4\pi$ is the imaginary part.

$$R = \frac{(n - 1)^2 + k^2}{(n + 1)^2 + k^2} \quad (4)$$

However, near the band edge of a semiconductor, $k \ll n$, making the reflection coefficient R relatively constant over the range of energies around its band edge. We may thus use the value of R determinable for the transparent regime for all our calculations concerning the energies around the band edge.

Given values of T then, and determining a constant value for R around the band edge, we can then rewrite

our original equation to solve for the absorption coefficient, α , near the band edge, in terms of T , R , and the sample thickness, x .

$$\alpha = -\frac{1}{x} \ln \frac{[(1-R)^4 + 4T^2R^2]^{1/2} - (1-R)^2}{2TR^2} \quad (5)$$

Valence-band to conduction-band electronic transitions represent the dominant mechanism responsible for optical absorption in semiconductor materials. Assuming parabolic bands, at the band edge of a direct-gap semiconductor, band gap E_g , a photon of energy E will create an electron-hole pair, absorbing or emitting a phonon of energy E_p in the process in order to conserve momentum. This interaction may be described by the following equations where α_a and α_e represent the absorption coefficient due to absorption or emission of a phonon respectively. C and D represent constants determined by material properties.

$$\alpha = \alpha_a + \alpha_e \quad (6)$$

$$\alpha_a = C(E - E_g + E_p)^2 \quad E > E_g - E_p \quad (7)$$

$$\alpha_e = D(E - E_g - E_p)^2 \quad E > E_g + E_p \quad (8)$$

For an indirect-gap semiconductor we may represent the absorption coefficient, α with the following equation.

$$\alpha = A(E - E_g)^{1/2} \quad (9)$$

However, impurities and temperature effects will often cause exponential band-tails of electronic states to extend into a direct-gap semiconductor's forbidden gap. The transitions from a parabolic band to these exponential band-tail states cause the absorption coefficient to vary exponentially, as represented by the following equation.

$$\alpha = B e^{E/E_0} \quad (10)$$

In this equation, E_0 represents the Urbach slope, a parameter describing the steepness of the exponential band-tail.

EXPERIMENT

The entire setup for our experiment is mounted on Newport Breadboard and is relatively immune to optical noise and environmental influences by virtue of our lock-in detection method in which we chop the beam at a specific frequency and only measure data received at that same frequency. Figure 1 shows the experimental setup.

To begin with, a 100-Watt tungsten-halogen source is powered by a Kepco Power Supply set to 12-Volts. The light from the source is directed through the entrance

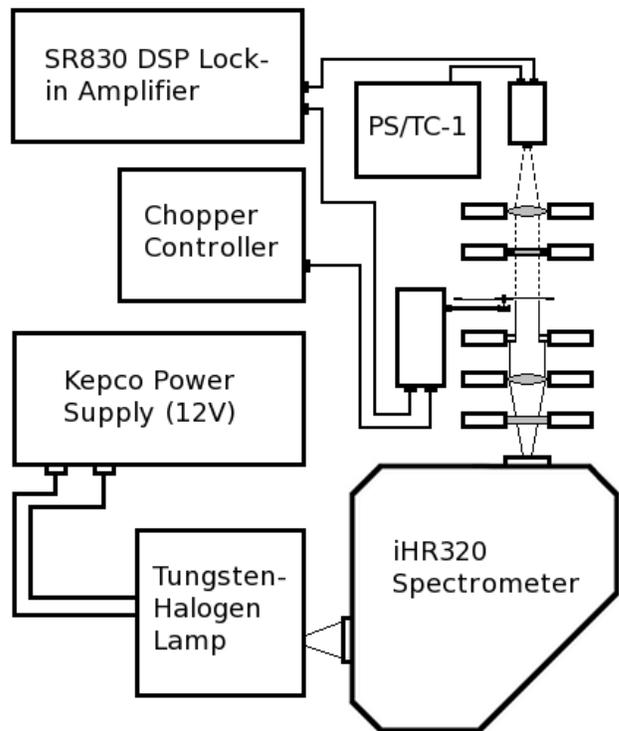


FIG. 1. Experimental Setup

slit of an iHR320 Spectrometer (Serial No. 0071-08-06). Within the spectrometer the light is reflected across a 600-lines/mm diffraction grating (blazed for 1500-nm) before exiting the spectrometer through an exit slit (both entrance and exit slits are set at 0.2-mm wide). The light is then passed through a long-pass interference filter set to block out wavelengths below 850-nm in order to eliminate second-order wavelengths. A KPX094 condensing lens ($f = 150\text{-mm}$, $f\# = 3.9$), producing a collimated beam of monochromatic light.

The beam is then passed through a Newport Aperture (1D-1.0) in order to decrease the beam's diameter to the size of the sample (preventing any light from hitting the surrounding sample container and appearing in our data to have been absorbed by the sample). The beam is then mechanically chopped at a frequency of 150-Hz as set by a Stanford Research Systems Inc. Chopper Controller (Model No. SR540). This frequency is fed into a Stanford Research Systems Inc. DSP Lock-in Amplifier (Model No. SR830) for use in our lock-in detection method. The beam is then directed through a Newport filter holder where it is incident any one of our semiconductor samples.

The resulting beam is then incident on a converging lens with an Electro-Optical Systems Inc. H Series Photodiode/Receiver (Model No. IGA-020-TE2-H) positioned at its focal point. The photodiode is connected to an Electro-Optical Systems Inc. PS/TC-1 temper-

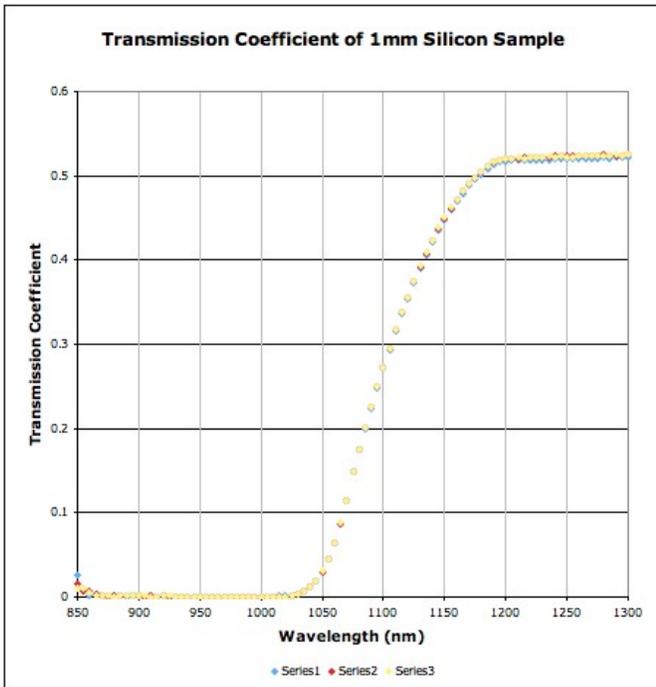


FIG. 2. Plot of transmission coefficient vs. wavelength for 1-mm silicon sample.

ature control device which keeps the photodiode's circuitry from heating up. The lock-in amplifier is connected across the photodiode to take measurements of the voltage corresponding to the chopped frequency.

A LabVIEW driver (Monochromator Scan.vi) is used to drive the Spectrometer and take measurements off of the lock-in amplifier. The wait time on the LabVIEW program is set to 3000-ms, ten times the time constant of 300-ms set on the lock-in amplifier.

The silicon sample is a 1-mm thick, optically polished, disk approximately 1-in in diameter. Three sets of measurements were taken over a range of wavelengths, 850-1300 nm, at 5-nm intervals. Similar measurements were taken with a cadmium-telluride sample, 1.75-mm thick and also optically polished on both sides.

Originally, a 3-mm thick sample of gallium-arsenide was used, however, second-order terms made the data difficult to analyze. For this reason, further measurements were taken on a 0.5-mm un-doped wafer of gallium-arsenide, approximately 2 -in in diameter and optically polished on both sides. Three sets of measurements were taken over a range of wavelengths, 850-1300 nm, at 5-nm intervals. However, the sharp band edge of the data led us to take a second set of measurements over a range of wavelengths, 850-1000 nm, at 2-nm intervals in order to get more accurate results.

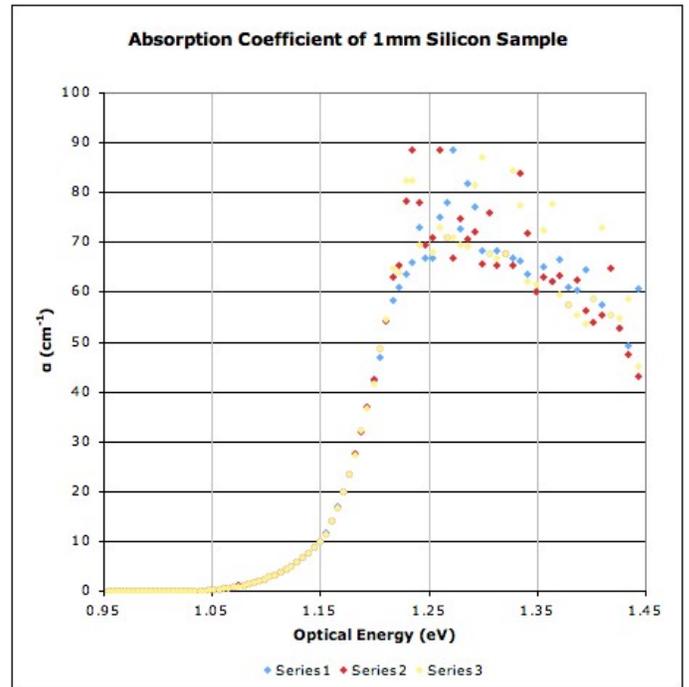


FIG. 3. Plot of absorption coefficient vs. optical energy for 1-mm silicon sample.

RESULTS AND ANALYSIS

The voltage measured across the photodiode is directly proportional to the intensity of light incident on its surface, $V I$. By taking measurements of the voltage both with a given sample in the sample container (V) and without any sample at all in the sample container (V_0), we were able to experimentally determine the transmission coefficient, T for each sample over a range of wavelengths using the following equation.

$$T = \frac{I}{I_0} = \frac{V}{V_0}$$

Figure 2 shows the three data sets we collected for silicon as measurements of the transmission coefficient, T , as a function of wavelength. In Figure 3, the absorption coefficient, α , of silicon is plotted against the optical energy associated with each wavelength. This energy value was determined using the following equation for each value of λ where h is Planck's constant and c is the speed of light.

$$E = \frac{hc}{\lambda}$$

Averaging values for T across the transparent regime ($\lambda = 1200$ to 1300 nm for silicon), we used equation (3) to determine the value of the reflection coefficient, R , for each of the samples of semiconductor material.

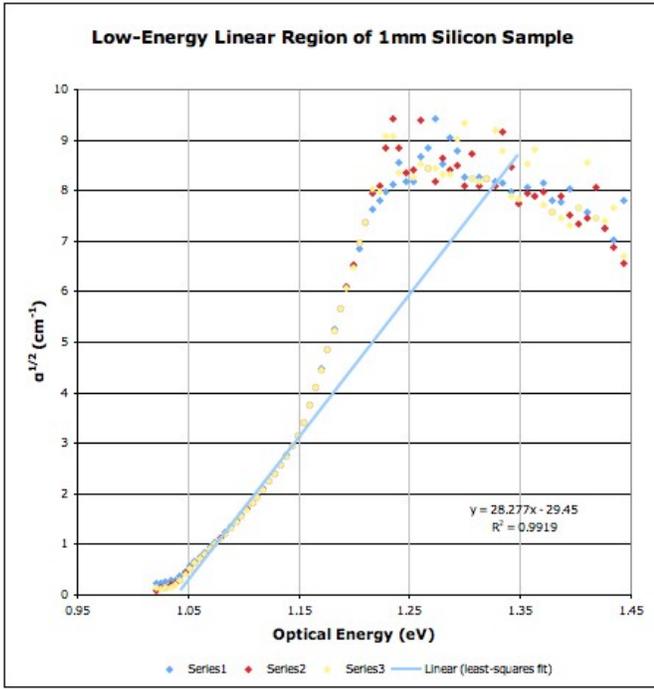


FIG. 4. Plot of $\alpha^{1/2}$ vs. optical energy for 1-mm silicon sample. Least-squares fit for low-energy linear region ($\alpha_a^{1/2} = 28.277E - 29.45$).

$$R_{si} = 0.31 \pm 0.02$$

$$R_{ga} = 0.35 \pm 0.02$$

$$R_{ca} = 0.24 \pm 0.02$$

These values are consistent with published values for each material.[1] Using these values for the reflection coefficient of each of the samples, we calculated values for the absorption coefficient of each over a range of wavelengths using equation (5).

Silicon

Equations (6) - (8) tell us that for $E_g - E_p < E < E_g + E_p$, $\alpha = \alpha_a$. Thus, for an indirect gap semiconductor, there should be a low energy region of the band edge for which a plot of $\alpha^{1/2}$ vs. optical energy should yield a linear relationship describing α_a , Figure 4 shows such a graph for silicon. By extrapolating values for α_a into the higher energy region of the band edge using our linear least-squares fit, we can make a similar plot of $\alpha_e^{1/2} = (\alpha - \alpha_a)^{1/2}$. This plot should similarly yield a linear relationship in the high energy region, $E > E_g + E_p$. Figure 5 shows such a graph for silicon with a linear least-squares fit over the high energy region.

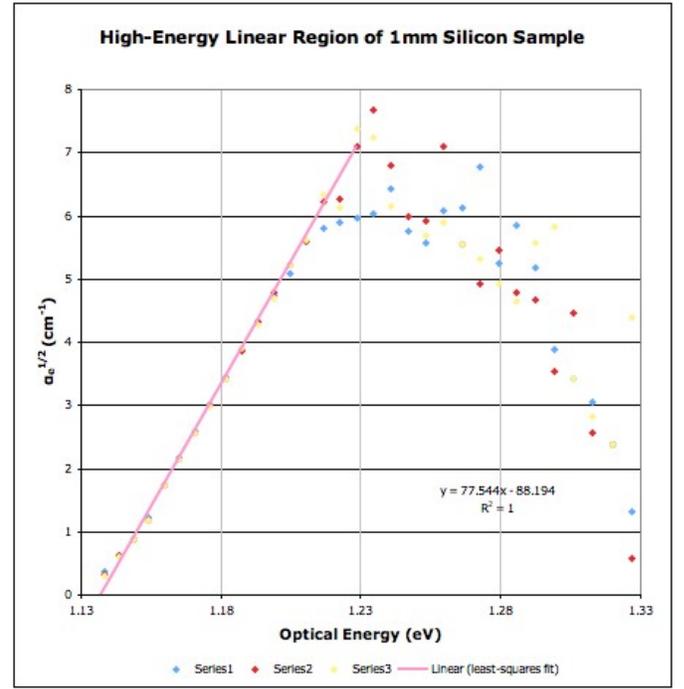


FIG. 5. Plot of $[\alpha - \alpha_a]^{1/2}$ vs. optical energy for 1-mm silicon sample. Least-squares fit for high-energy linear region ($\alpha_e^{1/2} = 77.544E - 88.194$).

Using our linear fits for α_a and α_e , we can calculate values for E_g and E_p . The x-intercept of our linear fit for α_a can be described using equation (7) as $x[y = 0] = (E_g - E_p)$. Similarly, the x-intercept for α_e can be described using equation (8) as, $x[y = 0] = (E_g + E_p)$. Given our x-intercept values then, we can calculate E_g and E_p as follows.

$$x[y = 0]_a = 1.042 \text{ eV} \quad x[y = 0]_e = 1.137 \text{ eV}$$

$$E_g = 1.090 \pm 0.008 \text{ eV}$$

$$E_p = 0.048 \pm 0.008 \text{ eV}$$

These values are consistent with published values based on a single-phonon model.[1][2]

Gallium-Arsenide

Originally, three data sets were taken on an un-doped wafer of a gallium-arsenide semiconductor 3-mm thick. However, the thickness of the sample allowed second order phonon interactions to significantly affect our data. Figure 6 shows the plot for the transmission coefficient obtained from this sample. Additional data sets were taken on a 0.5-mm sample, producing a much cleaner band edge as seen in Figure 7.

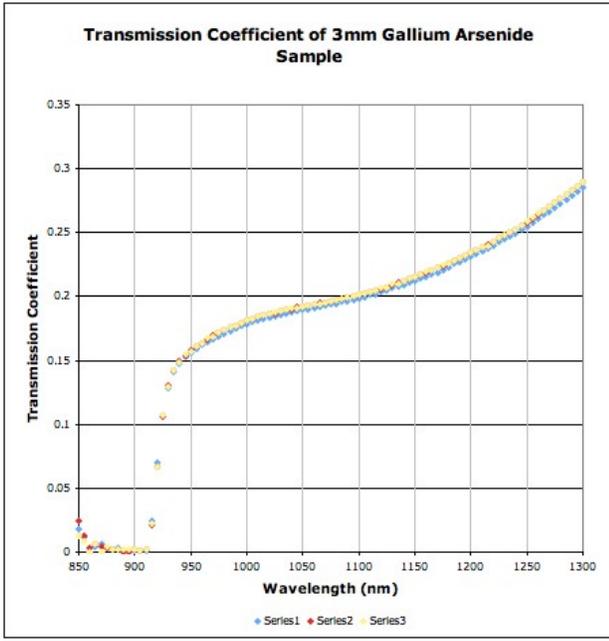


FIG. 6. Plot of transmission coefficient vs. wavelength for 3-mm gallium-arsenide sample.

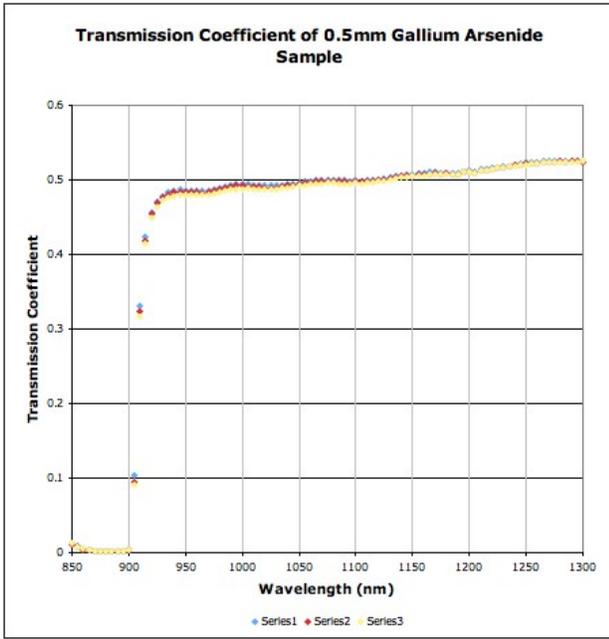


FIG. 7. Plot of transmission coefficient vs. wavelength for 0.5-mm gallium-arsenide sample.

Figure 8 shows our graph of α vs. optical energy for further data sets taken on this 0.5-mm sample of gallium-arsenide at 2-nm intervals. A linear region is apparent in the steeply rising absorption edge this plot, characteristic of a direct-gap semiconductor, and suggesting an exponentially varying absorption coefficient as described

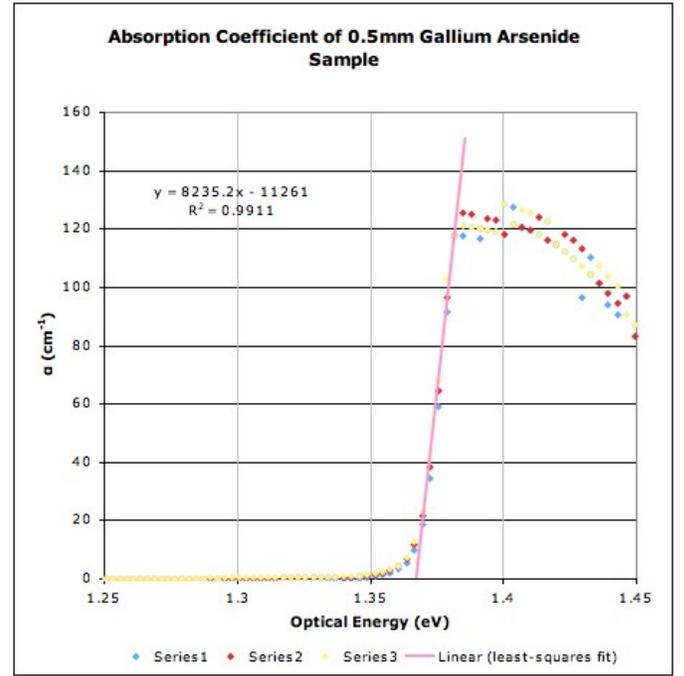


FIG. 8. Plot of absorption coefficient vs. optical energy for 0.5-mm gallium-arsenide sample. Linear least-squares fit ($\alpha = 8235.2E - 11261$).

in equation (10). Taking a linear least-squares fit of our data, we can determine the Urbach slope of the exponential band-tail.

$$m = 8235 \text{ eV}^{-1} = E_0^{-1}$$

$$E_0 = 0.121 \pm 0.004 \text{ meV}$$

This value is not consistent with published values attributing 5-7 meV band-tails due to impurities in undoped samples of gallium-arsenide semiconductors.[1][3]

Cadmium-Telluride

Figure 9 shows our graph of α vs. optical energy for the data sets taken on our 1.75-mm sample of cadmium-telluride. Like the gallium-arsenide, a linear region is apparent in the steeply rising absorption edge. This suggests that cadmium-telluride is another direct-gap semiconductor and should have an exponentially varying absorption coefficient like gallium-arsenide. Taking a linear least-squares fit of our data, we can determine the Urbach slope of the exponential band-tail.

$$m = 1488 \text{ eV}^{-1} = E_0^{-1}$$

$$E_0 = 0.672 \pm 0.004 \text{ meV}$$

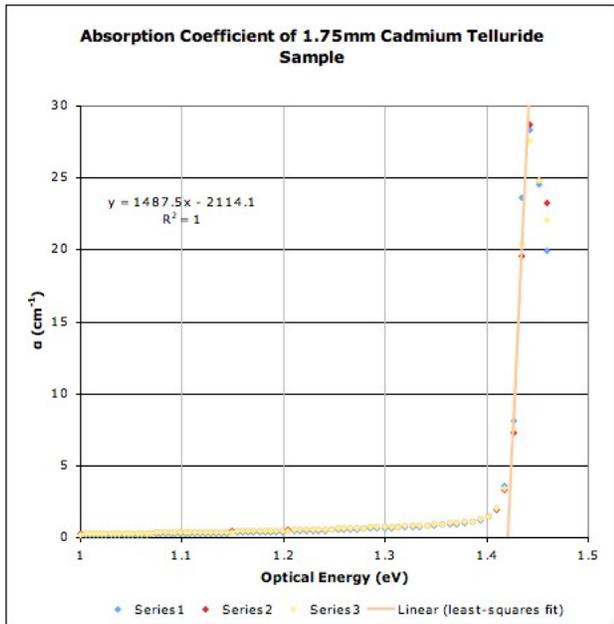


FIG. 9. Plot of absorption coefficient vs. optical energy for 1.75-mm cadmium-telluride sample. Linear least-squares fit ($\alpha = 1487.5E - 2114.1$).

CONCLUSION

Examining the optical absorption spectra for various semiconductive materials, we have shown that three com-

mon semiconductors (namely silicon, gallium-arsenide, and cadmium-telluride) follow standard theoretical models. The optical transmission data obtained for the 1-mm silicon sample is consistent with the model for an indirect-gap semiconductor. The energy of the band gap for silicon was calculated to be about 1.10-eV.

Gallium-arsenide and cadmium-telluride were shown to follow a model for direct-gap semiconductors involving exponential band-tails. However, the Urbach slopes we calculated for both semiconductors were an order of magnitude smaller than published values. Because the data still clearly indicates direct-gap behavior, this may suggest some systematic error in our experimental procedure. However, the lack of inaccuracy in our data for silicon means that the error was somehow confined to the gallium-arsenide and cadmium-telluride data.

Further experimentation could take more data over the narrow band edge of these direct-gap semiconductors in order to obtain more accurate calculations of their Urbach slopes.

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- [1] J. M. Essick and R. T. Mather, *American Journal of Physics* **61** (Dec 1993).
 - [2] J. J. Low, M. L. Kreider, D. P. Pulsifer, A. S. Jones, and T. H. Gilani, *American Journal of Undergraduate Research* **7** (Dec 2007).
 - [3] J. I. Pankove, *Phys. Rev.* **140**, A2059 (Dec 1965).