Experiment 16

Absorption Band-edge Thermometry of Semiconductors

16.1 Purpose

1. To explore several forms of thermometry.
2. To become familiar with some fundamental properties of semiconductors.
3. To understand and familiarize yourself with optical spectroscopy as a measuring tool.

16.2 Introduction

In this experiment, you will be characterizing the absorption edge of semiconductor samples at different temperatures. One application of this technique is the measurement of the process temperature of semiconductors under ultra-high vacuum where other methods fail [1,2]. Absorption bandedge thermometry was studied extensively at UBC, and has now been commercialized.

16.3 Theory

The Semiconductor Bandgap

Crystalline solids may be categorized as conductors or insulators depending on the distribution of electrons [3,4,5]. In a simple picture, the outer electrons in a metal, instead of remaining attached to their home ion, are delocalized over the entire crystal. Electrons in an insulator are more tightly bound. A semiconductor is both a poor conductor and a poor insulator.

![Band structure of different solids: a) Copper. b) Gallium arsenide (GaAs) near the Γ point (the origin in k-space) — labelled are the conduction band, two valence bands and the split-off band.](image)

A more rigorous treatment requires considering electrons not in real space but in momentum (or wavevector) space, referred to as k-space, as well as quantum and statistical physics. Wavevector
space is the Fourier transform of real space, and states there are indexed by their crystal momentum \( \mathbf{p} = \hbar \mathbf{k} \) instead of \( \mathbf{r} \). In \( k \)-space, a solid is defined using band structure: a band describes energy levels \( \varepsilon(\mathbf{k}) \) where electrons are allowed, as shown by the curves in Fig. 16.1. These bands are combinations of orbitals on all atoms in the crystal, and can only accommodate as many electrons as could be accommodated in their component real-space orbitals.

The energy of the highest occupied electronic state at zero temperature is called the Fermi level, \( \varepsilon_F \). If the Fermi energy falls in the middle of a band (i.e. the band is partially-filled) as in Fig. 16.1a, the crystal is metallic. When this occurs (e.g. band \( \Sigma_1 \) in the upper right), there is always a level slightly higher in energy for the last electron to excite into; hence, in an external field the electron will move and current will flow.

Fig. 16.1b shows part of the band structure of gallium arsenide (GaAs), a semiconductor. For this material, the Fermi level lies somewhere between the “valence” band (downward facing parabola) and the “conduction” band (upward facing parabola), and the highest-energy electron lies at the very top of the valence band. The gap between the valence and conduction bands is the forbidden energy gap, normally called the bandgap and labelled \( \varepsilon_g \). There are no states at any momentum in this energy range. Under a moderate electric field, there are no allowed energy levels to move to, hence the material is insulating. For a pure GaAs crystal [4,6], the external field would have to exceed the energy of the bandgap in order to excite electrons to the conduction band and allow current to flow.

For the remainder of the discussion, we will only consider the band structure shown in Fig. 16.1b. As mentioned above, electrons could be excited from the valence band to the conduction band with a sufficiently strong electric field, but this can also be done with light. If a photon impinges on the crystal with an energy less than \( \varepsilon_g \), then it cannot be absorbed and will pass unmolested, just as visible light goes through a window pane. However, if the energy of the photon exceeds \( \varepsilon_g \), it can be absorbed by the material, exciting an electron from the valence band into the conduction band, and the material will be opaque to light of that particular color (this is why regular window glass protects us from ultraviolet light). Hence, an experiment using transmission of light can determine the bandgap of a material — the material would be completely transparent below \( \varepsilon_g \) and completely absorbing above \( \varepsilon_g \), leading to a step function absorption spectrum.

This can be summarized as follows:

\[
\begin{align*}
    h\nu & \geq \varepsilon_g; \quad \alpha \geq \alpha_g \\
    h\nu & < \varepsilon_g; \quad \alpha \to 0
\end{align*}
\]  

where \( h \) is Planck’s constant, \( \nu \) is the frequency of incident light, \( \alpha \) is the optical absorption coefficient in cm\(^{-1}\) and \( \alpha_g \) is the optical absorption coefficient at the band-gap energy. For GaAs, \( \alpha_g = 8000\text{cm}^{-1} \) [7].

The preceding discussion is strictly rigorous for a perfect, infinite crystal at absolute zero. In this experiment, however, we will be dealing with real crystals which are finite and have imperfections, and the experiments will be done near room temperature. Both properties contribute to a broadening of the step function, leading to an absorption band edge known as the Urbach edge [1,2].

The absorption in the Urbach region can be described by:

\[
\alpha(h\nu) = \alpha_s e^{-\frac{h\nu - \varepsilon_G}{\varepsilon_o}}
\]

where \( \varepsilon_o \) is the characteristic energy of the Urbach edge, \( \varepsilon_G \) is the extrapolated optical bandgap energy, and \( \alpha_s \) is again the optical absorption coefficient at the bandgap energy. Note that we
denote the Urbach edge optical bandgap with a capital $G$ subscript to distinguish it from the other definition of the bandgap; in practice, we can consider the two quantities to be the same for the purposes of this laboratory. This equation is **only** valid for $h\nu < \varepsilon_G$; in practice, the region where $\alpha \sim 30 - 100\text{cm}^{-1}$ can be used to extrapolate for $\varepsilon_G$.

A full quantum mechanical treatment of optical absorption in direct bandgap semiconductor material gives the following relationship between $\alpha$ and $h\nu$:

$$\alpha h\nu \propto \sqrt{h\nu - \varepsilon_g} \quad (16.3)$$

Hence, a plot of $(\alpha h\nu)^2$ versus $h\nu$ should give an extrapolated value at $\alpha h\nu = 0$ that corresponds to the bandgap. This equation is **only** valid for $h\nu > \varepsilon_g$. In practice, this last method will work well when one can extract good values of $\alpha$ but will not work when $\alpha$ is obscured, for instance due to normalization or dark signal uncertainties. In summary, there are three methods that can be used to obtain a bandgap from optical absorption measurements.

In quantum theories of the Urbach edge for crystalline semiconductors, both $\varepsilon_o$ and $\varepsilon_G$ are proportional to the phonon population — phonons are quantized acoustic waves (vibrations of the crystal lattice). Using the Einstein model for phonons, the width of the Urbach edge is

$$\varepsilon_o = S_o k_B \theta_E \left[ \frac{1 + X}{2} + \frac{1}{e^{\frac{\theta_E}{T}} - 1} \right] \quad (16.4)$$

where the dimensionless parameter $X$ is a measure of the structural disorder, $\theta_E$ is the Einstein temperature, $S_o$ is a dimensionless constant related to the electron-phonon coupling, and $k_B$ is the Boltzmann constant. $X$ is expected to be zero for a perfect crystal. The temperature dependence of the band gap is given by

$$\varepsilon_G(T) = \varepsilon_G(0) - S_g k_B \theta_E \left[ \frac{1 + X}{2} + \frac{1}{e^{\frac{\theta_E}{T}} - 1} \right] \quad (16.5)$$

where $S_g$ is a dimensionless coupling constant and $\varepsilon_G(0)$ is taken as the published band gap at liquid-He temperature.

**Optical Absorption Measurements**

In this experiment, the absorption coefficient will be extracted from optical transmission of light through the sample. The spectrum read by the computer is a convolution of the incident light intensity reaching the detector and the detector response. Fig. 16.2 shows a typical spectral response for a silicon detector. The signal $I(\lambda)$ read by the detector at wavelength $\lambda$, for light incident on a sample of thickness $d$ with wavelength-dependent absorption coefficient $\alpha$ is given by

$$I(\lambda) = S(1 - R)I_o(\lambda)e^{-\alpha d} \quad (16.6)$$

where $S$ is a dimensionless scattering factor, $R$ is the reflectivity of the material and $I_o(\lambda)$ is the intensity of light incident on the sample. For semiconductors near the fundamental absorption edge, we can approximate the refractive index, $n$, to be wavelength independent; $R$ is then

$$R = \left| \frac{n - 1}{n + 1} \right|^2 \quad (16.7)$$

The transmission of light through the sample is thus

$$T = \frac{I(\lambda)}{(1 - R)SI_o(\lambda)} = e^{-\alpha d} \quad (16.8)$$

and can be inverted to extract $\alpha$ when the thickness of the sample is known.
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16.4 Apparatus

The apparatus consists of a diffraction grating spectrometer with a CCD detector (Ocean Optics USB2000) connected to a computer by USB; a type K thermocouple for measuring the sample’s temperature with an HP 3455A voltmeter to measure its voltage; a Dewar flask (thermos); a halogen lamp with a cooling fan; a variac to control the lamp intensity; and a heat gun to change the sample temperature. Be careful with the thermocouple as it’s fragile.

Fig. 16.3 is a schematic diagram of the apparatus. The copper sample holder contains a hole in which the fibre optic’s lens is mounted. Samples can be mounted to cover this hole and should only be handled with the plastic tweezers provided — the GaAs samples are EXTREMELY fragile.

16.5 Procedure

Task I — The Apparatus

1. Turn on the equipment, ensuring that the cooling fan is on when the halogen lamp is on. There is a desktop icon for the Ocean Optics spectrometer (OOIBase23). You will want to look at the spectral response of the detector with and without incident light. Please save your data in My Documents\PHYS352\[Yourname]. This can be set easily when saving your first spectrum.

2. What spectrum is detected without incoming light (i.e. dark signal)?
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Figure 16.3: Schematic diagram of the apparatus.

3. Qualitatively explain the spectrum obtained with incoming light. With directly incident light, what is the effect of time normalization? What is the effect of averaging over several curves?

4. There are 4 icons in the software labelled S, A, T, and I — explain what they stand for and how you can access the A, T and I functions. Hint: think of normalization and equations 16.6 to 16.8. Will normalization be required for your measurements? Why or why not?

5. Introduce a few material samples in front of the empty sample block (plastic, glass, hand,...) and look at the spectral response (you may need to adjust the integration time). Plot and explain your observations.

6. Explain the thermocouple circuit and the use of Dewar flask. What do you measure for room temperature?

7. What are the temperature precision and accuracy of this thermocouple? Are they temperature dependent? Hint: see part II of reference 8 or 9.

Task II — Bandgap of GaAs from Absorption Measurements

1. Measure the optical transmission through the GaAs sample (handle the sample with care and plastic tweezers). Extract its absorption coefficient.

2. For the sample provided, which has one unpolished side, scattering reduces the detected signal. How can you normalize its transmission to obtain reliable values of \( \alpha \)? Hint: consider what transmission you should expect for all values of \( \alpha \), which is wavelength dependent.

3. What is the bandgap of GaAs at room temperature? Is it what you expected? Which definition of the bandgap appears to give the best results? Why?

4. Repeat for different GaAs wafer temperatures. Does the temperature dependence behave as expected? Hint: refer to references 1 and 2.
16.6 References


6. To make semiconductors useful, impurities are incorporated (doped) into the crystal, in order to make them n-type (conduction by electrons in the conduction band) or p-type (conduction by “holes” or absence of electrons in the valence band). Consult references 1-2 for more information.


8. The PDF documents are named *Practical T meas part I*... and *Practical T meas part II*... and come from the Library Reference Edition CD.