Optical Properties Of Solids

Sriyani Jayatilleke

Department of Physics,

University of Cincinnati

Cincinnati,

Ohio 45221.

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Abstract

The analysis of optical spectra is one of the most useful tools for understanding electronic structure of semiconductors. The spectral region of major interest for a semiconductor is in the vicinity of the absorption edge, since it can provide information on the optical gap, E_g, as well as on the density of states within the gap. In this report, I discuss about optical absorption. Under this topic, I discuss about photon absorption and phonon absorption of solids as well as features of the optical absorption spectrum in semiconductive materials such as amorphous semiconductors and crystalline semiconductors.

I. INTRODUCTION

The most natural method to study electronic transitions is to measure the absorption spectrum, the levels being localized or not. The optical absorption spectra in crystals are observed by the band to band transition, i.e., the electronic exitation from the valence band into the conduction band. The threshold at the low energy side of the optical absorption spectra is called optical absorption edge, i.e., the separation in energy between the bottom of the conduction band and the top of the valence band. When the bottom of the conduction band and the top of the valence band are located at the same wave vector $\overrightarrow{k}$ in the k space, direct transitions are possible. When they are located at different positions in the k space, indirect transitions accompanying emission and/or absorption of phonons are observed.

II. ABSORPTION COEFFICIENT (α)

If I is the flux density of incident light and z is the distance measured from incident surface of a sample then;

$$\alpha = -\frac{1}{I}\frac{dI}{dz} \tag{1}$$

$$\Rightarrow I = I_0 exp(-\alpha z) \tag{2}$$

The Bloch functions of the conduction band and the valence band can be written as,

$$|c, \overrightarrow{k} >= u_{ck}(\overrightarrow{r}) exp(i\overrightarrow{k}.\overrightarrow{r}) \tag{3}$$

$$|v, \overrightarrow{k\prime} >= u_{ck\prime}(\overrightarrow{r}) exp(i\overrightarrow{k\prime}.\overrightarrow{r}) \tag{4}$$

For direct transition, matrix element $\overrightarrow{M_{vc}}$ is expected by

$$\overrightarrow{M_{vc}} = \frac{1}{\Omega}\int_{\Omega} u^*_{ck}(\overrightarrow{r})\overrightarrow{e}.\overrightarrow{p}u_{vk}(\overrightarrow{r})dr \tag{5}$$

$\overrightarrow{e}$- polarization vector of light
$\overrightarrow{p}$-electron momentum
Ω-volume of a unit cell
When n is the refractive index;

$$\alpha = \frac{\pi e^2}{n\epsilon_0 cm^2\omega}\sum_{\overrightarrow{k}\overrightarrow{k\prime}} |\overrightarrow{M_{vc}}|^2 \delta[E_c(\overrightarrow{k}) - E_v(\overrightarrow{k}\prime) - \hbar\omega]\delta_{\overrightarrow{k}\overrightarrow{k}\prime} \tag{6}$$

We can replace summation by an integral, using the density of states spectrum N_c(E) and N_v(E)

$$\alpha = \frac{\pi e^2}{n\epsilon_0 cm^2\omega}\int N_v(E)N_c(E+\hbar\omega)dE \tag{7}$$

FIGURES

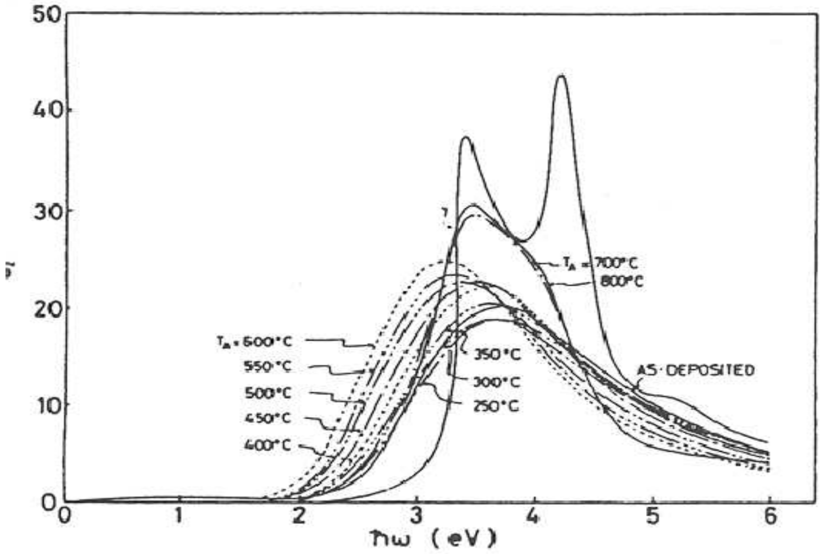

FIG. 1. The spectral dependance of the imaginary part of the dielectric constant ϵ_2 for glow-discharge a-Si:H samples prepared at 300 ^0C. The ϵ_2 curves for the samples annealed at T_A are shown as well as that for crystalline Si.

III. HIGH ENERGY ABSORPTION

The measurments of absorption spectra in the high energy range provide important information about the band structure in crystals. In this energy range, the reflectance spectra are measured instead of absorption spectra (transmission spectra). The absorption coefficient in this energy range is too large to permit the measurment of the transmittance of the sample. Optical constants are obtained through the Kramers-Kronig transformation from measured reflectance as a function of photon energy. In crystalline semiconductors, various sharp peaks are observed in reflectance spectra. In amorphous semiconductors, these peaks are broadened as shown in FIG.1

IV. TAIL ABSORPTION

A tail extending from the absorption edge towards low energy has been generally observed in the optical absorption spectra of amorphous semiconductors. This is called exponential tail, because it has an exponential shape as a function of photon energy. Interaction between the optical phonons and the electronic excitations leads to a spread of the absorption edge being an exponential tail. This tail is given by

$$\alpha(\omega) = exp(\frac{\gamma(\hbar\omega - E_u)}{k_B T^*}) \tag{8}$$

$$T^* = \frac{\hbar\Omega_0}{2k_B} coth(\frac{\hbar\Omega_0}{2k_B T}) \tag{9}$$

for $\hbar\omega \leq E_u$, where $\hbar\Omega_0$ and γ are optical phonon energy and a constant, respectively, and E_u is called Urbach focus.

As an origin of the exponential tail, two models have been proposed: One of them is that temporary self-trapping of excitons by lattice distortions due to thermal vibrations gives a shift and a broadening for exciton absorption and leads to an exponential tail towards low energy. The other is that optical phonons act as internal electric fields for excitons, so that transitions within the band gap are allowed by soaking out of the wavefunction of excitons into the band gap.The exponential tail observed in amorphous semiconductors is shown in FIG.2. As seen from the figure, the exponential tail obviously arises from the following two effects: The temperature effect and the static disorder effect due to amorphous networks.

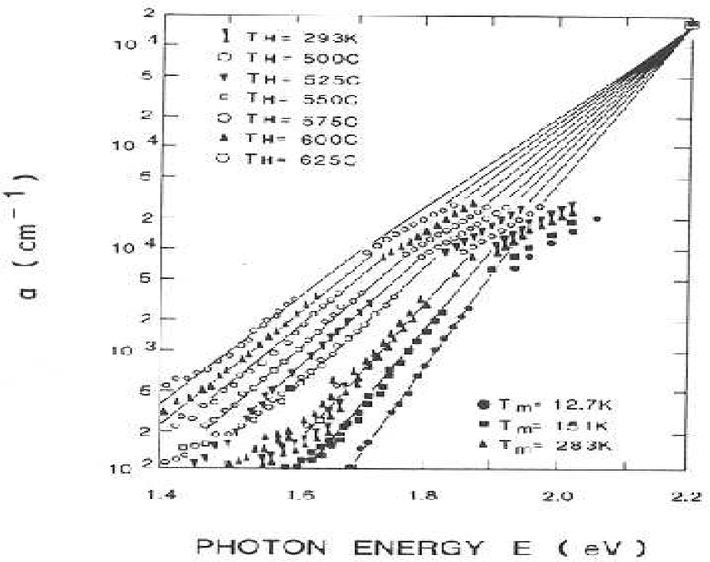

FIG. 2. Optical absorption coefficient, α, as a function of photon energy. The solid symbols refer to data obtained at different measurment temperatures T_m. The open symbols refer to a film that has been isochronally heated at temperature T_H.

V. OPTICAL BAND GAP

When the energy distribution curves are examined, one finds variations in the position and streangth of structure as a result of the conservation of wave vector $\overrightarrow{k}$ in the crystal. However in amophous materials no such variaions had been found in the energy distribution curves. The absence of k space in amorphous semiconductors does not imply that the density of electronic states is not a meaningful concept. The photoemission showed that, just as for crystals, the electronic states fall into bands separated by energy gaps. A schematic illustration of the Density of states N(E) for an amorphous seminconductor compared to that for a crystal, is shown in FIG.3

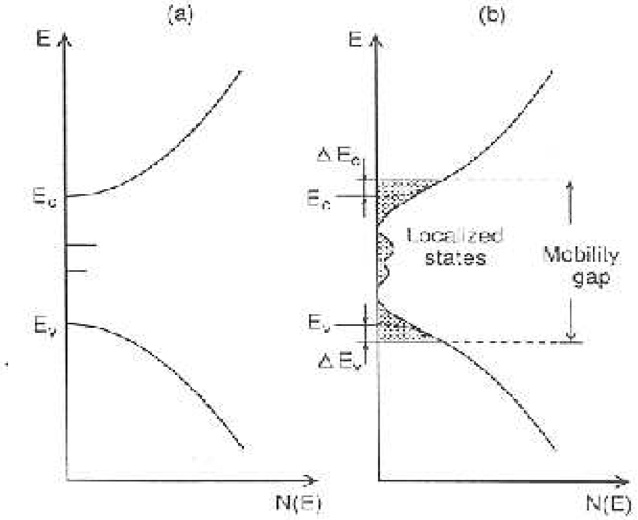

FIG. 3. N(E) as a funstion of energy E for (a) crystaline and (b) amorphous semiconductors. Dotted area indicated localized states. ΔE_c and ΔE_v are band tails due to disorder.

The most noteworthy features found in the electronic states of amorphous semiconductors are :(1) the absence of sharp band edges and tailing in to the gap; (2) localization of states in energy regions where density of states N(E) is low; (3) the existence of broad bands of defect levels in the gap through which hopping conduction may occur. The form of the corresponding optical absorption edge is illustrated schematically in Fig.4. In the strong absorption edge(region A in Fig.4), the absorption coefficient α can be decribed by the relation

$$E\alpha \sim (E - E_g)^m \tag{10}$$

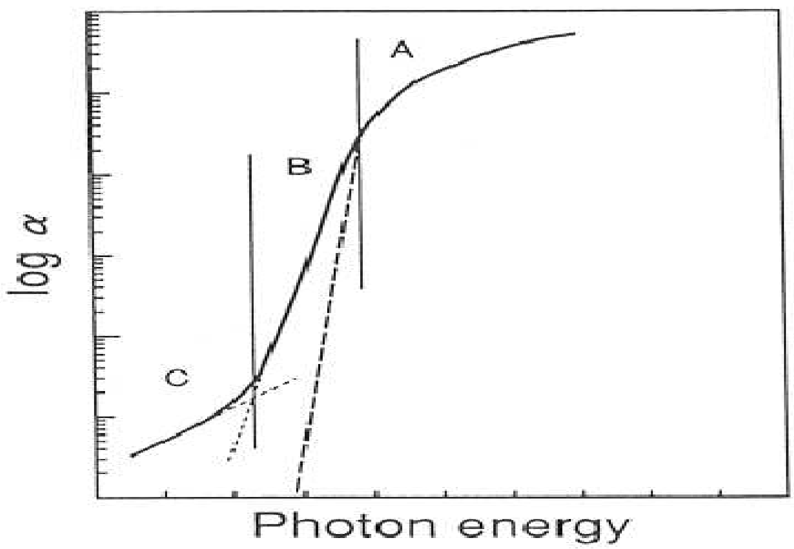

FIG. 4. Three principal regions, A, B, and, C of optical absorption in an amorphous semiconductor. The dashed line represents extrapolation of part A, using Eq.10

Where the constant m is usually equal to 2 or 3, depending on whether the transition is quantum mechanically allowed or forbidden, and E_g is the optical band-gap energy. At lower energy (region B), α shows an exponential tail written in the form:

$$\alpha \sim exp(\frac{E}{E_u}) \tag{11}$$

This region is called Urbach region (Urbach tail) and corresponds to absorption involving one or both of the band tails, with additional broadning expected from any potential fluctuations arising from charged defect states and lattice vibrations (phonons). The absorption edge reflects the tailing of states into the gap region due to fluctuations of bond lengths and bond angles. The exponential factor E_u indicates the width of the band tails of the localized states. The transition probability changes rapidly in the absorption tail as the energy states become increasingly localized. At very low absorption part (region C), one observes another exponential part of the absorption edge where

$$\alpha \sim exp(\frac{E}{E_t}) \tag{12}$$

and the energy E_t is always larger than E_u. This region arises from transitions involving defect states within the gap. In contrast to region B, region C may show a very structure-sensitive property.

VI. CONCLUSION

Unfortunately, there is no well-established physical model owing to the complexity of the electronic states in disordered systems. However, the fact does not change the conclusion that the position and shape of the optical absorption edge and optical absorption coefficient are sensitive and quantitative measures of the structural and electrical disorder of amorphous materials.

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