Photoacoustic and Transmission Studies of SiC Polytypes

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The optical bandgap energies (OBGE) of 3C, 15R, 6H and 4H-SiC have been investigate experimentally by transmission and photoacoustic spectroscopies. The measurements were performed on 470 μm thick wafers. The OBGE obtained from both spectroscopies for different polytypes show very good agreement. In order to have a better understanding of these materials calculations of eletronic band structure were performed by the full-potential linearized augmented plane wave (FPLAPW) method. For the OBGE the results are compared to the measurements agreeing closely over the energies of those polytypes.

1. Introduction

In the past decade techniques have been developed for the fabrication of bulk and epitaxial films of various SiC polytypes[1]. These developments have revived the possibility of SiC system applications in high temperature, high power, and high-speed electronics devices[2,3]. In this work we will discuss the use of photoacustic spectroscopy, a contactless thermal technique, as well as the transmission, to monitor the optical properties of the 3C-SiC, 4H-SiC, 6H-SiC and 15R-SiC polytypes.

Photothermal spectroscopy has achieved great developments in the last two decades, and it has been successfully applied to semiconductors samples in case of powders, non-polished samples, crystalline, polycrystalline or amorphous thin films, multilayered structure, etc. One of the principal advantage of photoacoustic spectroscopy over other optical measurements, e.g. optical absorption, is that produce similar spectra, and may provide direct information of the nonradiative recombination process and, consequently, compliments the absorption and the photoluminescence spectroscopy. In the present work we will investigate the bandgap energies both experimentally and theoretically.

Theoretically by the full potential linearized augmented plane wave (FPLAPW) method.

2. Experimental Technique

Photoacoustic spectroscopy (PAS) is directly related to the periodic heat generated in a sample due to the absorption of modulated light. Generally the PAS experimental set up consists of a sample enclosed in a sealed cell at atmospheric pressure coupled to a sensitive microphone. Therefore the temperature of the encapsulated gas is modulated at the excitation frequency and the microphone detects the resulting dynamic pressure. The signal generated by this process depends on the amount of heat generated in the sample due to its optical absorption coefficient, the non-radioactive processes efficiency, and the thermal diffusivity. The study of the dependence of the sample absorption coefficient on the light source wavelength allows one to determine optical and electronic properties of opaque and transparent materials[4].

In order to minimize the background noise a new designed photoacoustic cell with, double walls was built. This new device consists of two concentric cylindrical wall cell

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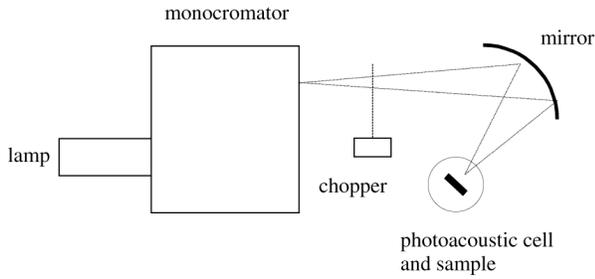
Figure 1. Schematic Experimental Setup.

with uv-quartz windows. The space between the walls was filled with air at atmospheric pressure. The internal cell cavity was gold plated in order to minimize unwanted radiation absorption. Air was used as coupling media between the sample and the microphone. A 1/2-inch condenser microphone (Bruel and Kjær, model 3547) was used to monitor the change in the pressure inside the cell. A 150 Watts Xe lamp, with a ellipsoidal reflector, couple to a 0.22 m double monocromator (Spex model 1680) was used as variable wavelength light source. The light was chopped at a frequency of 5 Hz, to improve the signal/noise ratio. The system was computer controlled. The schematic of the experimental setup is shown in Fig. 1. All the PAS spectra of the samples were normalized to the spectra of a highly absorbing film. PAS has been used to measure the bandgap energy of the polytypes.

The transmission measurements were performed placing the sample, attached to a holder with a 1 mm × 2 mm aperture, in front of the exit slit of the variable wavelength light source used in the photoacoustic experiments. The intensity of the transmitted light was monitored with a Si-photodiode. All the sample transmission spectra were normalized to the spectra of the light transmitted through the sample holder without the sample. The transmission experiment was carried out in the same set of sample studied by PAS.

3. Computation Method

The computational method, for the calculation of the bandgap, full potential linearized augmented plane wave (FPLAPW) method within the density-functional theory and local-density approximation (LDA) and using the correlation potential of Perdew and Wang (PW) [5]. The LDA is known to underestimate the bandgap energy Eg for semiconductors[6].

Because of the incorrect bandgap, one cannot guarantee that the calculations yield an accurate dielectric function. However, it has been shown by Del Sole and Girlanda[7] that the LDA combined with the scissors-operator approximation describes the optical spectrum rather well. We have therefore made an estimate of the correction Δ_g to the

bandgap by using a quasi-particle method proposed by Bechstedt and Del Solo[8]. Their model for the correction is based on the difference in self-energies obtained from the LDA and the W approximation. The correction is given by[6,8]

$$\Delta_g = \frac{e^2 q_{TF}}{2\pi\varepsilon(0)} \int_0^\infty \frac{1}{1-t^2}((1-\alpha_p)f(q_{TF}{}^r A^t) + (1+\alpha_p)f(q_{TF}{}^r A^t))^2 dt \tag{1a}$$

$$f(x) = \frac{1 - 10x^2/3 + x^4}{(1+x^2)^6}; \qquad r_A = r_B = \frac{a}{4\pi \cdot 1.7} \tag{1b}$$

In the equation above q_{TF} is the Thomas-Fermi wave number, $\varepsilon(0)$ is the static dielectric function, α_p the polarity of the interatomic interaction[8] calculated to be 7.67, and a is the lattice constant for each of the polytypes[5].

We have employed experimental values for the lattice dielectric function. For 3C-(6H-) SiC $\varepsilon(0)$ = 9.72 (9.78). The dielectric constant for 6H-SiC are the geometric average values of the transverse and longitudinal components: $\varepsilon(0)_\perp$ = 9.66 and $\varepsilon(0)_\parallel$ = 10.03,

$$\varepsilon(0) = \frac{2\varepsilon(0)_\perp + \varepsilon(0)_\parallel}{3}$$

Furthermore, 4H-SiC and 15R-SiC are presumed to have the same lattice dielectric function as 6H-SiC.

4. Experimental Results

In Figs. 2 and 3, we show the room temperature photoacoustic and transmission spectra respectively. The optical bandgap energies derived from these results are shown
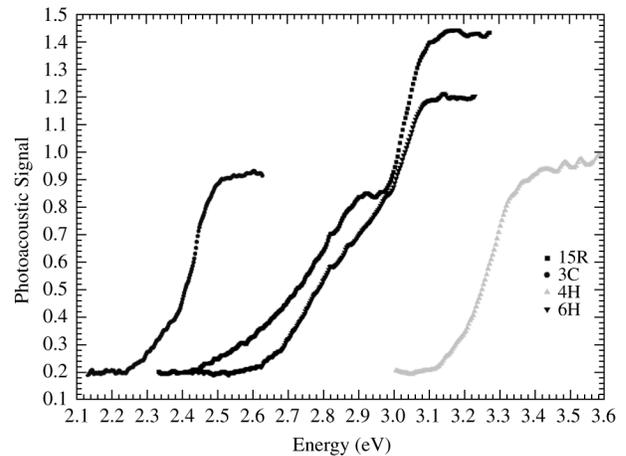
Figure 2. Photoacoustic signals as a function of energy for SiC polytypes.

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Table 1. Obtained values of the bandgap energies for Photoacoustic (PA) and Transmission (TR) measurements. The calculated E_g (C) and quasi-particle correction Δ_g are shown.

Material	E_g (PA) (eV)	E_g (TR) (eV)	E_g (C) (eV)	Δ_g (eV)	$(E_g(C) + \Delta_g)$ (eV)
3C - SiC	2.44 ± 0.02	2.44 ± 0.02	1.30 ± 0.01	1.24	2.54 ± 0.01
15R- SiC	3.02 ± 0.02	3.04 ± 0.02	1.76 ± 0.01	1.23	2.99 ± 0.01
6H - SiC	3.03 ± 0.02	3.05 ± 0.02	1.97 ± 0.01	1.23	3.20 ± 0.01
4H - SiC	3.30 ± 0.02	3.30 ± 0.02	2.17 ± 0.01	1.23	3.40 ± 0.01
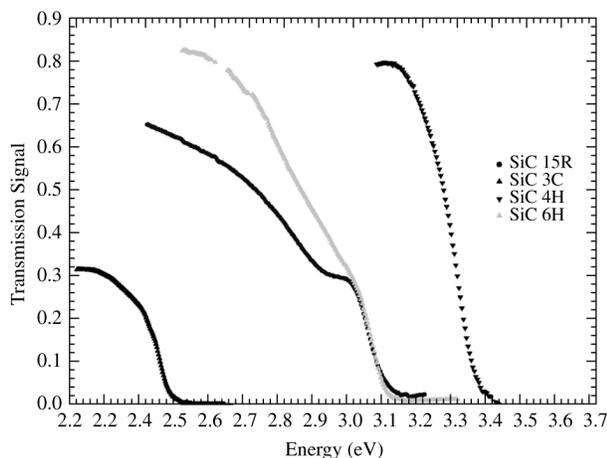
Figure 3. Transmission signal as a function of energy for SiC polytypes.
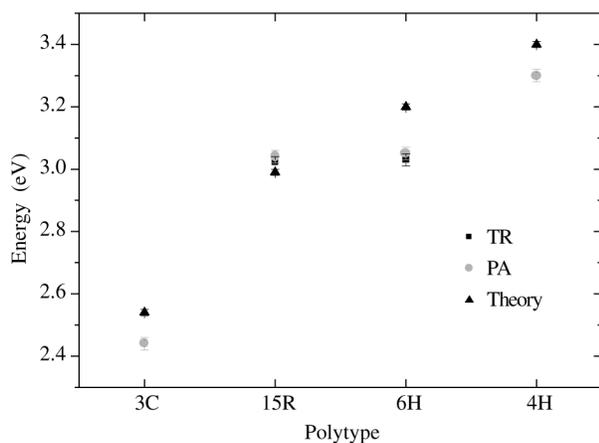
Figure 4. Optical bandgap energies as function of SiC polytypes. (The error in the energies is less than 0.02 eV, so the bars are inside the dots.)

in Table 1 together with the calculated values. The results are compared to the measurements agreeing closely over the energies of those polytypes. They are also shown in Fig. 4.

5. Conclusion

We have measured the optical bandgap energies of 3C-, 4H-, 6H- and 15R-SiC, using photoacoustic and transmission spectroscopies. The results are in good agreement with our full-potential calculations.

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