Optical band gap of the $\alpha$-mercuric iodide

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We investigate by photoacoustic spectroscopy the optical band-gap energy of mercuric iodide, $\alpha$-HgI$_2$, grown by sublimation in a sealed ampoule. Due to its importance as a detector material operating at ambient temperature, the physical properties of $\alpha$-HgI$_2$ have been recently studied. We found, by two different methods, the band-gap energies $E_g = 2.32$ and $2.39$ eV, respectively. These results are in good agreement with recent measurements based on reflection and absorption spectra. © 1995 American Institute of Physics.

Since 1982, when the researches on mercuric iodide celebrated the tenth anniversary of the first article related to its use as a room-temperature detector, much attention has been paid to investigation of this semiconductor toward optical properties and development of crystal growth and device fabrication techniques. The mercuric iodide crystal is a wide-band-gap semiconductor. The band-gap energy has been measured by different methods, varying from $E_g = 2.11$ to $2.397$ eV. Recently Burger and Nason measured $E_g$ by a method based on reflection and absorption spectra. They found $E_g = 2.292$ eV at room temperature. This result differs from other experiments. In the absence of a complete study in $\alpha$-HgI$_2$, further analysis of this system is of much interest.

As the value of $E_g$ is an important parameter in electronic and optoelectronic design, we investigate the optical absorption at the fundamental band edge by the photoacoustic spectroscopy (PAS) technique. PAS has been proved to be a simple and reliable nondestructive method for measuring the optical properties of solids or powder samples. It has the advantage of obtaining directly the spectra of the heat generated in a sample, due to nonradiative deexcitation process, following the absorption of light, on any type of materials.

In order to obtain a high-purity mercuric iodide, we have used the following procedure: iodine and mercury elements from Merck (5N) were placed in a Pyrex ampoule (18 cm length and 15 mm diameter) with a ratio obeying the stoichiometry of $\alpha$-HgI$_2$, resulting in a total mass of 15 g. The ampoule was closed under vacuum. This sealed ampoule was submitted to a temperature of 200 °C during 7 days. The recrystallized compound filled the inferior part of sealed ampoule through a sublimation process. With this method, we obtained polycrystalline $\alpha$-HgI$_2$ of very good optical quality. The sample used in this work is a platelet of this grown material with 1 mm thickness.

The PAS system consists of a tungsten lamp source of 200 W, a monochromator, a chopper with a modulation frequency of 17 Hz, photoacoustic cells, a lock-in amplifier, and a computer. The wavelength range is 300–850 nm. The resultant PA spectra are monitored by the computer, which simultaneously displays the wavelength-dependent signal intensity.

The optical band-gap energy has been estimated from the absorption data obtained as a function of the wavelength.

![PA spectra of $\alpha$-HgI$_2$ as a function of photon energy.](https://example.com/fig1.png)
We use the relation

\[ I h v = A (h v - E_G)^{1/2}, \]

which is valid for allowed direct transition. In Eq. (1), \( I \) is the absorption intensity and \( A \) a coefficient. From the data obtained, a straight-line fitting of \((Ih v)^2\) versus the photon energy \(h v\) and the change in the relative intensity of the absorption confirm that when the linear portion of the plot crosses the \( h v \) axis, we find the energy gap \( E_G = 2.32 \) eV. We also calculate \( E_G \) by the changing of the derivative in the fundamental absorption edge and found \( E_G = 2.39 \) eV. Both values are closer to Burger and Nason’s results, i.e., \( E_G = 2.292 \) eV, than others recorded in the literature.

In Fig. 1 we show the PA spectra for \( \alpha \)-HgI₂, at room temperature, as a function of photon energy. Figure 2 shows the relation \((Ih v)^2\), here denominated as PA intensity, as a function of the photon energy.

In summary we have shown that the PAS technique provides a reliable method to determine room-temperature value of the fundamental band-gap energy \( E_G \) of \( \alpha \)-HgI₂. The value of \( E_G \) is similar to the one obtained recently by a method based on reflection and absorption spectra.