Optical band gap of the α−mercuric iodide

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(Received 8 May 1995; accepted for publication 29 June 1995)

We investigate by photoacoustic spectroscopy the optical band-gap energy of mercuric iodide, α-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 α-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,[1,2] 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.[3,4] The band-gap energy has been measured by different methods, varying from E_G=2.11 to 2.397 eV.[4–7] Recently Burger and Nason[4] 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.[4–7] In the absence of a complete study in a α-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 nonodestructive method for measuring the optical properties of solids or powder samples.[8–11] 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.[8–14]

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 α-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 24 h to obtain a homogeneous material. After this, the sealed ampoule with the material filling it superior part was positioned in a vertical furnace under a thermal gradient from 150 to 100 °C, during 7 days. The recrystalized compound filled the inferior part of sealed ampoule through a sublimation process. With this method, we obtained polycrystalline α-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.

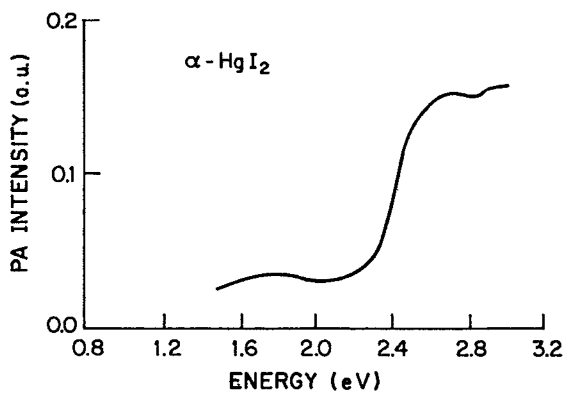

FIG. 1. Room-temperature PA spectra of α-HgI_2 as a function of photon energy.

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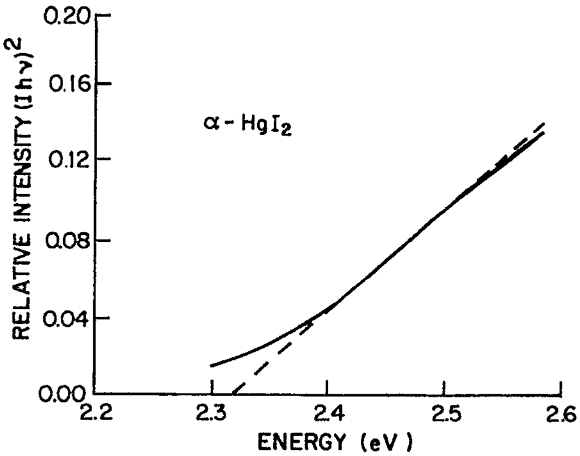

FIG. 2. Relative intensity $(Ih\nu)^2$ vs photon energy near the fundamental absorption edge at room temperature. The dashed line crosses the energy axis at 2.32 eV.

We use the relation

$$Ih\nu = A(h\nu - E_G)^{1/2}, \quad (1)$$

which is valid for allowed direct transition.[15] In Eq. (1), I is the absorption intensity and A a coefficient. From the data obtained, a straight-line fitting of $(Ih\nu)^2$ versus the photon energy $h\nu$ and the change in the relative intensity of the absorption confirm that when the linear portion of the plot crosses the $h\nu$ 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[4] results, i.e., E_G=2.292 eV, than others recorded in the literature.[4–7]

In Fig. 1 we show the PA spectra for α-HgI_2, at room temperature, as a function of photon energy. Figure 2 shows the relation $(Ih\nu)^2$, 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 α-HgI_2. The value of E_G is similar to the one obtained recently by a method based on reflection and absorption spectra.[4]

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