ON DIFFUSE REFLECTION SPECTRA OF V_2O_5

By I. HEVESI

Institute of Experimental Physics, Attila József University, Szeged

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Diffuse reflection spectra of powders prepared from V_2O_5 single crystals show a correlation between the range of linear increase in the spectrum and the range of exponential drop in the tail to the absorption edge of V_2O_5 single crystals. Comparative data are presented.

Band gap width and position of the absorption edge of semiconductors can be estimated with a relatively simple method by using their diffuse reflection spectra $R(\lambda)$ [1]. The evaluation is based on the fact, that the sharp decrease in absorption of powdered semiconductor particles in the neighbourhood of the absorption edge goes hand in hand with a steep increase in reflectivity. The onset of the linear part of the curve, which at the same time represents the region of greatest slope in the reflectivity curve, can be brought into connection with the onset of the exponential drop in the long wave tail to the absorption edge in a number of semiconductors. Though the use of the steepest part of the diffuse absorption spectrum as the base of determining the optical band gap is somewhat arbitrary, this method can give valuable informations, especially in the beginning of more detailed investigations on a semiconductor, while in other cases it is useful for comparing or checking the results.

In our investigations we used single crystals of V_2O_5, which are characterized by relatively low melting point and great band gap width. In determining the band gap of such semiconductors mainly optical methods can be taken into account rather than thermical ones. In two publications [2—3] dealing with optical absorption of V_2O_5 single crystals more in detail, we were able to state that the long wave tail to the absorption edge shows an exponential drop both with photon energy and temperature in accordance with URBACH's rule. The onset of the exponential drop was found to be at about $\lambda = 520\ m\mu$ and $\lambda = 515\ m\mu$ for light polarized parallel to the c axis and to the a axis, respectively. It was to be expected that the onset of the linear part in the diffuse reflection spectrum $R(\lambda)$ of V_2O_5 would to be found near the wavelengths mentioned. This supposition has been confirmed by our measurements.

Diffuse reflection spectra were obtained with the aid of a double beam grating spectrophotometer Type Optica Milano CF4DR, the reflectance head of which was provided with an integrating sphere. The V_2O_5 single crystal plates were ground to powders of different size distribution ($I > II > III \sim 10\ \mu$, see Fig. 1) in an agate pestle and mortar. One of two holders fixed on and easily removable from the surface of the integrating sphere contained the V_2O_5 single crystal powder to be measured, the other containing MgO powder used as reference standard, both

slightly compressed. Reflection spectra of the powdered samples were measured in the spectral range 350 mμ to 650 mμ.

Fig. 1 presents automatically recorded diffuse reflection spectra of three powders of different size distribution. Reflection shows a steep increase in the wavelength range 500 mμ to 580 mμ for each of the three samples. Though the steep increase in reflection becomes the more pronounced the smaller the size of the particles in the powder is, no essential differences can be found in the position

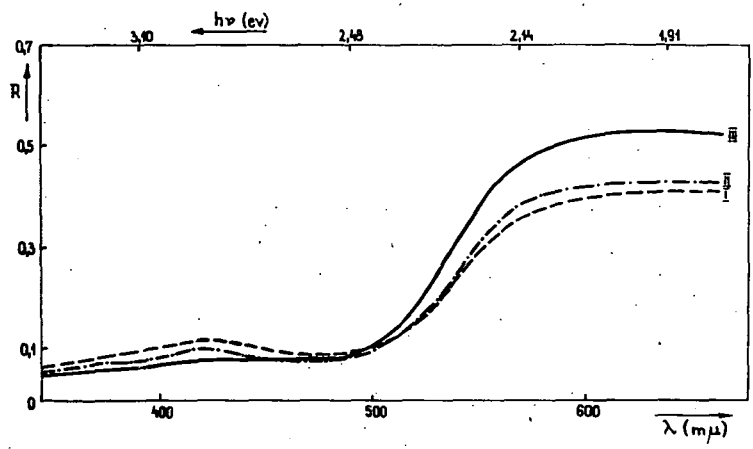

Fig. 1. Diffuse reflection spectra of V_2O_5

of the onset of the linear section in the curves. In the short wave range of the spectrum, *i. e.* in the region of low and nearly constant reflection, a band with a maximum at $\lambda = 425$ mμ can be observed. This increase in reflection is rather pronounced with thick single crystals, while it becomes indistinct with decreasing size of the particles in powdered samples.

On the base of diffuse reflection spectra of V_2O_5 it can be stated that the wavelength range of the linear increase in the spectra $R(\lambda)$ essentially coincides with that of the exponential drop in the tail to the absorption edge of V_2O_5 single crystals, and the onset of the linear increase in the reflection spectrum (~ 530 mμ) is to be found near the onset of exponential drop. Determining the band gap with the method given above, a value of 2,34 eV ($\triangleq 530$ mμ) has been obtained. The agreement of this figure with the values $E_g^{\parallel} = 2{,}30$ eV and $E_g^{\perp} = 2{,}32$ eV found in V_2O_5 single crystals at room temperature according to the polarization of light relative to the crystal axes, on the supposition of direct forbidden transitions [2—3], justifies the above estimate.

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О СПЕКТРАХ ДИФФУЗНОГО ОТРАЖЕНИЯ МОНОКРИСТАЛЛОВ ПЯТИОКИСИ ВАНАДИЯ

И. Хевеши

В работе исследованы спектры диффузного отражения порошков полученных из монокристаллов пятиокиси ванадия. Установлена связь между экспоненциальным участком края основной полосы поглощения и резко возрастающим участком спектров диффузного отражения. Приведены данные для сравнения.