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Optical constants of WSe_2 single crystals

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Abstract. The optical constants n and k for WSe_2 single crystals have been determined from the reflectivity measurements on basal plane of the crystal at wavelengths 5460, 4360 and 4050 Å. From the variation of k with frequency of radiation, the optical energy band gap E_g of the crystal has been evaluated.

Keywords. Optical constants ; optical energy gap ; WSe_2 single crystal.

1. Introduction

Recently dichalcogenides of tungsten have found a potential application in the construction of regenerative electrochemical solar cells. An important parameter for the selection of a material for the cell preparation is the energy band gap. So attempts made to determine this parameter will be quite interesting. In the present work we have carried out measurements of the optical constants of diselenides of tungsten which have enabled us to determine its optical energy band gap.

Tungsten diselenide crystals used in the present work have been grown in this laboratory by a direct vapour transport method. These crystals are semiconducting and are in the form of layer platelets having weak van der Waals, type inter-layer bonding. The as-grown faces are perfectly shining and so can easily lend themselves to reflectivity study in the visible range. Such studies can be used to gain direct information regarding the optical constants such as the refractive index n, the extinction coefficient k and the optical energy band gap E_g, of the crystal. In the present work the optical constants for WSe_2 crystals have been determined from the reflectivity measurements using plane polarised monochromatic radiations from a monochromator, consisting of a Waton mercury vapour lamp with appropriate filters and a sheet of polaroid rotatable about the axis of the beam, which do not give any lateral shift to the beam upon rotation. Standard methods (Avery 1952) were employed to evaluate the optical constants.

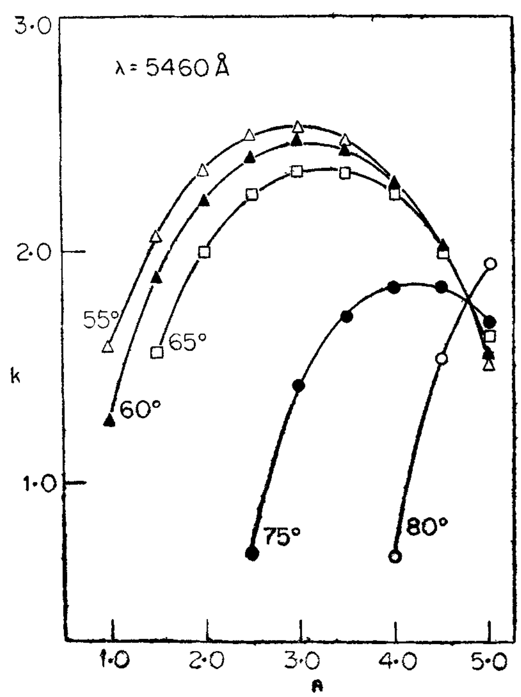
2. Experimental details

The spectrophotometer employed in the present study was constructed by replacing the telescope and the collimator of an ordinary spectrometer with a monochromator and a photomultiplier tube (having a narrow opening). The power supply of the photomultiplier tube and the mercury vapour lamp were energised by a stabilised power line and the constancy of emission was tested by noting the photocurrent for a long period of time. The prism table was replaced by a goniometer on which the crystal was mounted. The linearity of the photomultiplier tube at all the intensity levels and for all the wavelengths was checked by making use of Malu's law.

2.1. *Measurement of optical constants*

Using the expressions for the R_p and R_s components mentioned by Goswami and Rao (1974) curves relating R_p/R_s to n and k, for 12 angles of incidence from 25° to 80° in the step of 5°, for 9 values of n from 1 to 5 in the step of 0·5, and for the 16 values of k from 0 to 3·0 in the step of 0·2 were generated with the help of a computer. The consistency and accuracy of the determination of R_p/R_s at a particular wavelength and at a particular angle of incidence was confirmed by evaluating R_p/R_s repeatedly using different intensity levels of the slightly diverged reflected beam and also by using different portions of the same reflecting surface.

For a particular wavelength and angle of incidence, the value of R_p/R thus determined was used to obtain the pairs of possible values of n and k from the above mentioned curves. Such pairs were evaluated for several angles of incidence at 5460 Å, 4360 Å and 4050 Å wavelengths. The true values of n and k were then determined from the intersection of the curves of k versus n [figures 1 (a), 1 (b) and 1 (c)]. These values are tabulated in table 1 along with the values of the absorption coefficient (α) evaluated by using the expression $\alpha = k\,(4\pi/\lambda)$.



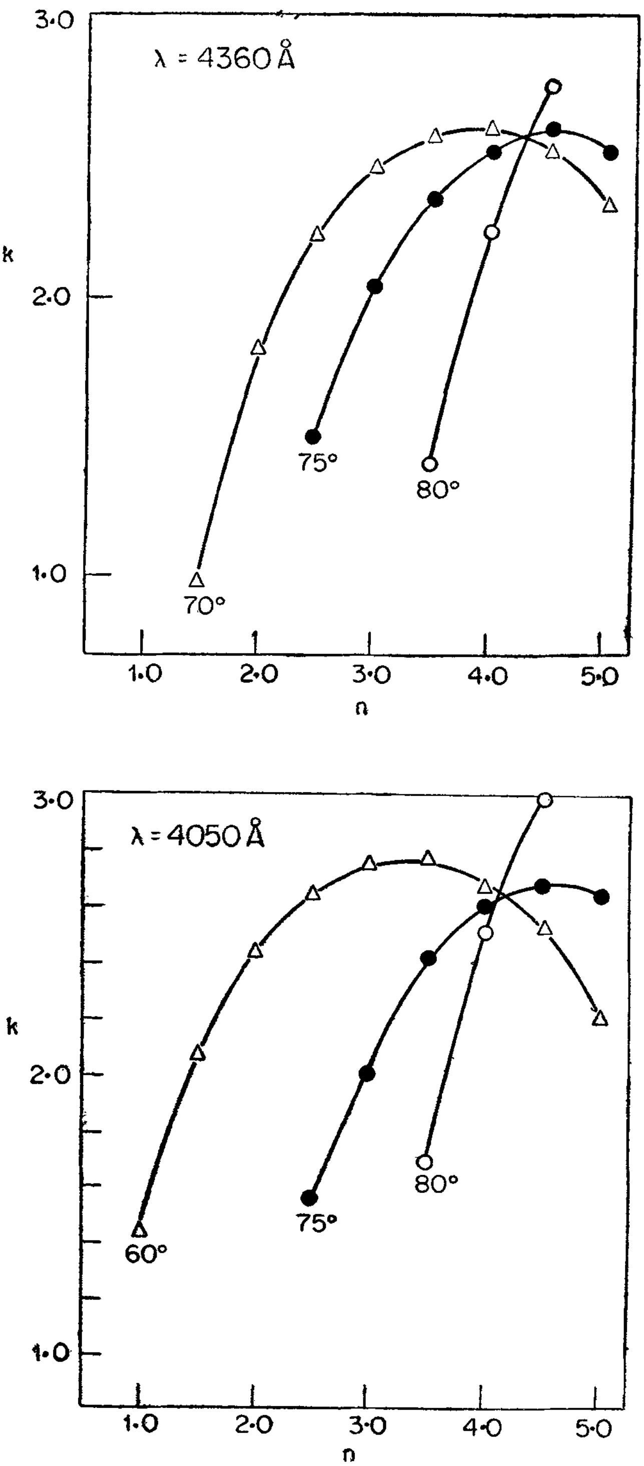


Figure 1. Curves showing the graphical determination of true values of n and k

Table 1. Optical constants.

λ in Å	n	k	a $\times 10^7 m^{-1}$
5460	4·762	1·79	4·12
4360	4·275	2·58	7·43
4050	4·125	2·64	8·19

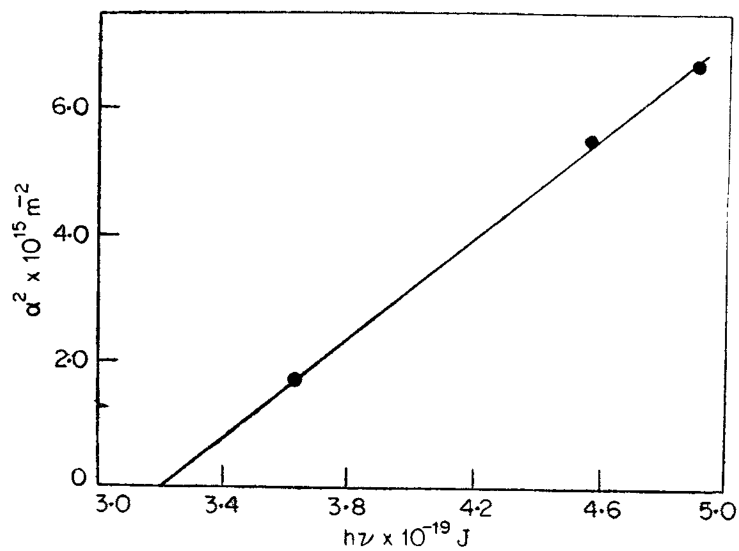


Figure 2. Plot of a^2 with photon energy.

The plot of a^2 vs $h\nu$ is shown in figure 2. It is a straight line as expected from the relation

$$a^2 = h\nu - (E_g)_{opt}.$$

The value of the energy gap $(E_g)_{opt}$ comes out to be $3 \cdot 21 \times 10^{-19}$ J (2·00 eV).

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