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The Dispersion of the Refractive Index and the Birefringence  
of AlN

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Measurements of the spectral dependence of the refractive index of AlN have been reported in (1). The comparison of the magnitude of  $n$  and the birefringence with the theoretical variation of the refractive index may reveal some information on the character of optical transitions and on the type of chemical bond of the substance under discussion.

From various formulae that approximate the dependence of the refractive index on wavelength in a region sufficiently remote from the absorption band, we have chosen the relation

$$n^2 - 1 = \frac{A}{\omega_0^2 - \omega^2} \quad (1)$$

The reason is that the constants  $A$  and  $\omega_0$  appearing in it may be interpreted immediately by the dispersion theory (cf. (2)).

The measured values of the refractive index of AlN are summarized in Table 1 and Fig. 1, together with the values calculated from formula (1). The values of  $A$  and  $\omega_0$  have been computed from experimental data using the method of least squares. The values obtained for the ordinary ray are:

Table 1

$\lambda (\mu\text{m})$	$n_e \text{ exp}$	$n_e \text{ calc}$	$n_o \text{ exp}$	$n_o \text{ calc}$
0.225	2.708	2.509	2.550	2.389
0.250	2.504	2.429	2.408	2.330
0.300	2.350	2.334	2.278	2.260
0.400	2.252	2.253	2.200	2.200
0.500	2.222	2.220	2.172	2.172
0.600	2.206	2.204	2.159	2.158



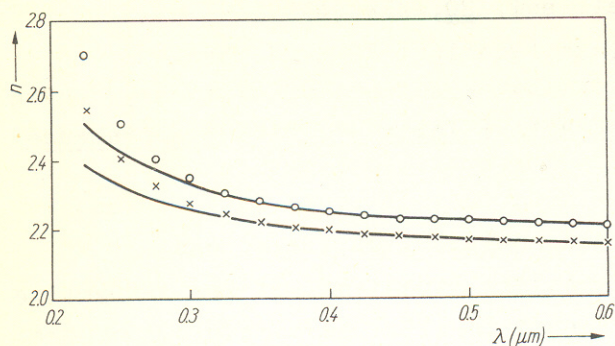


Fig. 1. Refractive index vs. wavelength  
 ○ ○ ○ n<sub>e</sub> (experimental)  
 × × × n<sub>o</sub> (experimental)  
 — computed from equation (1)

$A_o = (992 \pm 81) \times 10^{30} \text{ s}^{-2}$ ,  $\omega_o = (16.8 \pm 0.7) \times 10^{15} \text{ s}^{-1}$  (11.02 eV) and for the extraordinary ray:  $A_e = (854 \pm 46) \times 10^{30} \text{ s}^{-2}$ ,  $\omega_o = (15.2 \pm 0.5) \times 10^{15} \text{ s}^{-1}$  (9.98 eV).

If we interpret the constant A in the usual way, we obtain a value of  $920 \times 10^{30} \text{ s}^{-2}$ . In doing so, we have assumed that there are six optical electrons per AlN molecule.

Formula (1) gives only the mean value of the refractive index. Keffer and Portis (3, 4) have calculated the value of birefringence for crystals with an ideal wurtzite structure. In introducing the electron susceptibilities  $\chi$ , we may write for the case of an ionic bond, if only the anion is polarized (4),

$$\frac{1}{\Delta\chi} = \frac{1}{\chi_o} - \frac{1}{\chi_e} = 0.0075 + 0.2973 \frac{q}{f}, \quad (2)$$

where q is equal to the ionic valence, f is a constant characterizing the polarizability of the given anion. In (4) f is estimated with the aid of the respective value for a rare-gas atom having identical electron configuration (Mueller reports for Ne a value of  $f = 2.37$  (5)). Equation (2) enables one to estimate the effective charge of the anion and, in turn, the type of bond in the given substance.

From the measured refractive indices we obtain for the difference between the inverse electron polarizabilities in the limit  $\omega \rightarrow 0$  the value  $1/\Delta\chi = 0.155$ . In order to achieve an agreement with the theoretical value obtained from equation (2) we must put  $q \approx 1.2$ . In view of the approximations used



this is in reasonable agreement with the fraction of the ionic bond of 39% determined from X-ray analysis by Ugay and Domachevskii (6).

Estimating the effective charge from Szigeti's formula for the difference between the static and optical dielectric constant (7), we find  $q \approx 1.2$ ; this is again in agreement with (6) and with the previous value. In the foregoing, we have used for the energy of the transverse optical phonon  $\hbar\omega = 82.6$  meV (8), and for the dielectric constant  $\epsilon = 8.5$  (3, 9).

Stern (10) has made an examination of the spectral distribution of the refractive index in the vicinity of the absorption edge. The curve of the refractive index will display a maximum in the region of the absorption edge (i.e.  $\partial n / \partial E$  has a local singularity) provided that the absorption edge is determined by direct transitions.

In the case of indirect transitions, the curve will be monotonous in the edge region. The existence of transitions is manifested by an increasing growth of  $n$  with  $\lambda$ .

For AlN, the region of strong absorption starts at about 3000 Å. The deviation of the experimental points from the approximated curve which is evident in this region (Fig. 1) is caused (in accordance with Stern's considerations (10)) by the fact that with the onset of intrinsic absorption an approximation by the dispersion curve of a simple oscillator is no longer satisfactory.

A smooth course of the refractive index curves even in the region of the absorption edge, i.e. the absence of a singularity, confirms the presence of an indirect gap in AlN.

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