

Optical Constants of Magnesium Oxide
in the Far Ultraviolet*

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The refractive indices of many crystals are well known in those spectral regions where the materials are transparent. On the other hand, very few data exist on either the refractive index, n , or the absorption index, k , for these materials beyond their ultraviolet transmission limits. Part of our research program on the electronic spectrum of crystalline magnesium oxide included the intermediate derivation of the optical properties as far as 28 eV.

The experimental procedure consisted of the measurement of the near-normal-incidence reflectance spectrum of freshly cleaved crystals of magnesium oxide from 4 to 28 eV. If the ratio of the reflected and incident light intensities is denoted by r^2 , then it is possible to derive the following relationships, via the Fresnel equations:

$$n = \frac{1 - r^2}{1 + r^2 - 2r \cos \theta} \quad (1)$$

$$k = \frac{2r}{1 + r^2 - 2r \cos \theta} \quad (2)$$

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The determination of θ , the phase change on reflection, is achieved by use of a Kramers-Kronig integral transformation of the reflectance data. A detailed discussion of this technique has been given elsewhere (1, 2 and references therein). In practice, the determination of the phase angle involves an approximation procedure which thereby introduces an uncertainty in the computed values of n and k . The errors, from this cause, can become important only near the end-points of the experimental data energy range (2). Since the optical behavior at the long-wavelength end is known (because the crystal is transparent here), only the data beyond 26 eV is likely to be in error from the computation procedure.

The experimental measurements of the reflectance are accurate to about 5%, as estimated from the scatter of the original data points and the reproducibility of the spectrum. In any reflectance measurements however, only the surface layers of the material are examined and it is difficult to assess how nearly even a freshly cleaved surface resembles the bulk crystal in its optical properties. Since any defects or surface contamination tend to decrease the sharpness and intensity of ultraviolet reflectance structure, only data from surfaces exhibiting the highest reflectance at the 7.58 eV peak (about 27.5% at 300°K) were used in the final computation. In practice, the variations in peak reflectance from different freshly cleaved surfaces were less than 5%. It is doubtful if the true reflectance, intrinsic to the bulk crystal, is more than 5% different from that measured, because of the above and also because the low energy tail of the first reflectance band could be smoothly matched onto the near ultraviolet

reflectance as computed from known values of the refractive index in this region (3).

The spectral dependence of both n and k is shown in figure 1. Since there is some variation in the literature in the use of symbols for absorption, it should be noted that the absorption index, denoted here by k , is related to the absorption coefficient, α , through the expression $\alpha = 4\pi k/\lambda$. A discussion of the temperature dependence of the optical properties, particularly near the first band, has been described previously (4). The electronic transitions responsible for the observed spectral structure will be discussed elsewhere.

The values of n and k at given photon energies are presented in table 1, where the choice of photon energies was determined by the need to define the original reflectance spectrum sufficiently for a reliable Kramers-Kronig analysis.

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TABLE CAPTIONS

Table 1. Values of the refractive and absorption indices, n and k , for magnesium oxide at photon energies in the range 5 - 28 eV.

TABLE I

| $\hbar\omega$ (eV) | n | k | $\hbar\omega$ (eV) | n | k |
|--------------------|----------|----------|--------------------|----------|----------|
| 5.00 | 1.86 | 0.00 | 7.68 | 2.29 | 0.88 (5) |
| 5.50 | 1.91 | 0.00 | 7.70 | 2.24 | 0.84 |
| 6.00 | 1.97 | 0.00 | 7.75 | 2.16 | 0.75 |
| 6.50 | 2.07 | 0.00 | 7.80 | 2.11 | 0.67 (5) |
| 7.00 | 2.20 | 0.01 | 7.83 | 2.11 | 0.63 |
| 7.20 | 2.31 | 0.02 | 7.85 | 2.11 | 0.61 |
| 7.30 | 2.41 | 0.03 | 7.90 | 2.12 | 0.58 |
| 7.35 | 2.47 | 0.04 | 7.95 | 2.13 | 0.56 |
| 7.40 | 2.54 | 0.05 (5) | 8.00 | 2.14 | 0.55 |
| 7.45 | 2.65 | 0.09 | 8.10 | 2.15 (5) | 0.55 |
| 7.48 | 2.73 | 0.13 | 8.20 | 2.16 | 0.56 |
| 7.50 | 2.79 | 0.17 | 8.50 | 2.15 | 0.60 |
| 7.52 | 2.89 | 0.22 | 9.00 | 2.12 | 0.69 |
| 7.53 | 2.94 | 0.27 | 9.30 | 2.09 | 0.74 |
| 7.54 | 3.01 | 0.33 | 9.50 | 2.08 | 0.77 |
| 7.55 | 3.06 (5) | 0.45 | 9.70 | 2.06 (5) | 0.81 |
| 7.56 | 3.06 (5) | 0.58 | 9.80 | 2.06 | 0.83 |
| 7.57 | 3.03 | 0.70 | 10.20 | 2.03 | 0.93 |
| 7.58 | 2.97 | 0.80 | 10.50 | 1.98 | 1.05 |
| 7.59 | 2.89 | 0.89 | 10.80 | 1.86 | 1.17 |
| 7.60 | 2.81 | 0.95 (5) | 10.90 | 1.79 (5) | 1.20 (5) |
| 7.61 | 2.70 | 1.00 | 11.00 | 1.72 | 1.23 |
| 7.62 | 2.60 | 1.01 | 11.10 | 1.63 | 1.23 |
| 7.63 | 2.52 | 1.00 | 11.15 | 1.59 | 1.22 |
| 7.64 | 2.45 (5) | 0.97 (5) | 11.20 | 1.54 | 1.21 |
| 7.66 | 2.35 | 0.92 | 11.30 | 1.46 | 1.16 |

| $\hbar\omega$ (eV) | n | k | $\hbar\omega$ (eV) | n | k |
|--------------------|---------|---------|--------------------|---------|---------|
| 11.40 | 1.40 | 1.08 | 15.10 | 1.13 | 0.82 |
| 11.50 | 1.36 | 1.00 | 15.30 | 1.13 | 0.80 |
| 11.65 | 1.39 | 0.84 | 15.50 | 1.15 | 0.77 |
| 11.80 | 1.46 | 0.79 | 15.70 | 1.17 | 0.75 |
| 11.90 | 1.51 | 0.77 | 15.80 | 1.19 | 0.75 |
| 12.00 | 1.55 | 0.77 | 15.90 | 1.21 | 0.76 |
| 12.10 | 1.59 | 0.77(5) | 16.00 | 1.23 | 0.77 |
| 12.40 | 1.68 | 0.83 | 16.20 | 1.25(5) | 0.79(5) |
| 12.60 | 1.73 | 0.90 | 16.40 | 1.28 | 0.83 |
| 12.80 | 1.77 | 1.00 | 16.60 | 1.30 | 0.88 |
| 12.95 | 1.78 | 1.11 | 16.80 | 1.27 | 0.98 |
| 13.00 | 1.78 | 1.16 | 16.90 | 1.23 | 1.01 |
| 13.25 | 1.58 | 1.44 | 17.00 | 1.20 | 1.01 |
| 13.30 | 1.50 | 1.47 | 17.20 | 1.17 | 1.04 |
| 13.40 | 1.34 | 1.49 | 17.40 | 1.09(5) | 1.10 |
| 13.45 | 1.25 | 1.48(5) | 17.50 | 1.04 | 1.10(5) |
| 13.50 | 1.16 | 1.45(5) | 17.60 | 0.99 | 1.10 |
| 13.55 | 1.08 | 1.40 | 17.65 | 0.97 | 1.09 |
| 13.60 | 1.02 | 1.32 | 17.70 | 0.95 | 1.07 |
| 13.75 | 0.98 | 1.13 | 17.80 | 0.93 | 1.04 |
| 13.80 | 0.98(5) | 1.07 | 17.90 | 0.91(5) | 1.02 |
| 13.90 | 1.02 | 0.99 | 18.00 | 0.90 | 1.02 |
| 14.00 | 1.05 | 0.95 | 18.20 | 0.87 | 1.00 |
| 14.10 | 1.08 | 0.92 | 18.50 | 0.81 | 0.98 |
| 14.30 | 1.11 | 0.89 | 18.60 | 0.79 | 0.97 |
| 14.80 | 1.13 | 0.84 | 18.70 | 0.78 | 0.95 |

| $\hbar\omega(\text{eV})$ | n | k | $\hbar\omega(\text{eV})$ | n | k |
|--------------------------|----------|----------|--------------------------|----------|----------|
| 18.90 | 0.75 | 0.93 | 21.70 | 0.46 | 0.50 |
| 19.00 | 0.73 | 0.92 | 22.00 | 0.47 | 0.42 |
| 19.20 | 0.71 | 0.89 | 22.50 | 0.52 | 0.33 |
| 19.30 | 0.69 | 0.88 (5) | 22.90 | 0.58 | 0.29 |
| 19.60 | 0.64 | 0.85 | 23.00 | 0.59 | 0.28 (5) |
| 19.70 | 0.62 | 0.83 | 23.10 | 0.60 | 0.29 |
| 19.80 | 0.60 (5) | 0.81 | 23.20 | 0.61 | 0.29 |
| 19.90 | 0.59 | 0.79 | 23.60 | 0.62 | 0.27 |
| 20.00 | 0.58 | 0.76 | 23.80 | 0.62 | 0.26 |
| 20.10 | 0.58 | 0.73 | 24.00 | 0.62 | 0.25 |
| 20.20 | 0.59 (5) | 0.71 | 24.20 | 0.63 | 0.24 |
| 20.30 | 0.61 | 0.70 | 24.30 | 0.63 (5) | 0.24 |
| 20.40 | 0.61 | 0.70 | 24.40 | 0.63 | 0.24 |
| 20.50 | 0.61 | 0.70 | 24.60 | 0.62 | 0.23 (5) |
| 20.60 | 0.60 | 0.70 (5) | 24.70 | 0.61 | 0.22 |
| 20.80 | 0.56 | 0.70 | 24.80 | 0.61 | 0.21 |
| 20.90 | 0.54 | 0.69 | 24.90 | 0.62 | 0.20 |
| 21.00 | 0.52 | 0.67 | 25.50 | 0.64 | 0.14 |
| 21.10 | 0.50 | 0.65 | 26.00 | 0.67 | 0.11 |
| 21.20 | 0.49 | 0.62 (5) | 26.50 | 0.70 | 0.08 |
| 21.30 | 0.48 | 0.60 | 27.00 | 0.73 | 0.06 |
| 21.40 | 0.47 | 0.57 (5) | 27.50 | 0.75 (5) | 0.04 |
| 21.50 | 0.46 | 0.55 | 28.00 | 0.78 | 0.03 |

FIGURE CAPTIONS

Figure 1. The spectral dependence of n and k , at room temperature, for single-crystal magnesium oxide.

