5-1973

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Absorptivity of Single-Crystal Yttrium at 4.2 K

Abstract
Measurements of the absorptivity of single crystals of Y were made between 0.15 and 4.4 eV at 4.2 K. Polarized radiation was used with the electric vector parallel or perpendicular to the c^ axis of the crystal. The observed structures in the absorptivity were interpreted on the basis of band calculations for Sc, Re, and Gd and qualitative agreement was found between the band structures and the observed spectra.

Keywords
Polarized radiation, electric vector, Ames Laboratory

Disciplines
Atomic, Molecular and Optical Physics | Condensed Matter Physics | Physics

Comments
Absorptivity of Single-Crystal Yttrium at 4.2 K

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(Received 5 January 1973)

Measurements of the absorptivity of single crystals of Y were made between 0.15 and 4.4 eV at 4.2 K. Polarized radiation was used with the electric vector parallel or perpendicular to the c axis of the crystal. The observed structures in the absorptivity were interpreted on the basis of band calculations for Sc, Re, and Gd and qualitative agreement was found between the band structures and the observed spectra.

In the present paper the absorption spectra of single crystals of hcp yttrium are discussed. In earlier papers, we have considered the optical properties of the bcc transition metals Cr, Nb, Ta, V, and Mo over a wide energy range, typically 0.1–35 eV, as calculated from the measured absorptivity or reflectivity. For these metals, the oxide layer was to increase the magnitude of the absorptivity A. At 4.18 eV, A rose from 0.719 (0.783) to 0.753 (0.826) for \( E \parallel \bar{c} \) \( (E \perp \bar{c}) \). It appears, then, that the spectra below 3 eV are reliable and that between 3 and 4.4 eV, the oxide might be weakly affecting the absorptivity.

The anisotropy is quite pronounced below about 1 eV; above 1.5 eV, both curves display the same structure, with maxima occurring at about 1.5 and 2.1 eV. Above about 2.6 eV, the absorptivities rise smoothly to the limit of the data (4.42 eV). At low energies, the absorptivities rise very dramatically from 0.0229 \( (E \parallel \bar{c}) \) and 0.0430 \( (E \perp \bar{c}) \) at 0.15 eV, indicating that interband transitions persist to very low energy.

To account for the structure in the dielectric function (and the reflectivity) one usually compares the optical spectra with existing band structures. While Loucks has considered the Fermi-surface topology of Y, there have been no band calculations per se. However, it has been pointed out that Y is very similar in atomic configuration \( (4d5s^2) \) to the hexagonal rare-earth metals with atomic configurations \( 5d6s^6 \). Further, augmented-plane-wave calculations have shown that the band density-of-states curves for Re, Gd, Y, and Dy are quite similar. On the basis of the rigid-band model, one might further expect the bands of Y to be quite similar to those of Sc. Photomission results have shown that Y and Sc possess similar optical densities of states. The occupied portion of the d bands is approximately equal for the two metals. The bands for Sc calculated by Fleming and Loucks are shown in Fig. 2. While a certain similarity will exist, the bands near the Fermi level can be expected to show some appreciable differences as one goes from Sc to Y to, say, Gd. In particular, we have noted that the shape of the band \( \Gamma_{6s}-\Sigma_1-M_{-1}-K_1 \) is nearly the same for Gd and Re (it is basically a pure 5d state) but for Sc it is quite different (it never crosses above \( E_p \) at \( M \)). Presumably, in Sc the state is a 3d state and the difference between 3d and 5d states might account for the different shape of the band. Nevertheless,
while we expect certain differences, it is possible to make certain conservative identifications for some of the observed optical structure.

From the absorptivity, we see a slight shoulder at about 0.45 eV for $\mathbf{E} \parallel \mathbf{c}$. For Sc, parallel bands cross the Fermi surface along $T$ and are separated by about 0.25 eV (see Fig. 2). These $T_1$ and $T_3$ bands probably persist in Y and would give rise to the observed anisotropic structure which occurs at low energy for $\mathbf{E} \parallel \mathbf{c}$ only. Such transitions are forbidden by electric dipole selection rules for $\mathbf{E} \parallel \mathbf{c}$. Further, selection rules allow transitions $\Sigma_3 - \Sigma_1$ for $\mathbf{E} \parallel \mathbf{c}$ which should appear in Y, and are separated in Sc by ~0.6 eV; since the bands are not parallel, the absorption would be relatively weak. Transitions at $H$ and nearby regions of $k$ space would likewise contribute to the structure in Fig. 1.

For Sc, $H_4 - H_3$ (~0.9 eV, both polarizations) and near $H_1 - H_2$ (~0.5 eV, $\mathbf{E} \parallel \mathbf{c}$ only) transitions are apparent and would probably persist in Y. Finally,
transitions like \( L_1 \) to \( L_1 \) (1.4 eV in Sc, not calculated for Gd and suppressed more deeply below \( E_f \) in Re) might account for further absorption. In all cases large volumes of reciprocal space may be involved, not just regions along symmetry lines. It is quite impossible to make even qualitative estimates of the origins of the higher-energy structures in \( A \) for both polarizations.

Thus, the data presented here not only allow tentative information concerning the bands of \( Y \) itself, but also provide support for the existing bands of Sc and Gd. Likewise, these data represent the only existing data on oriented crystals of \( Y \). It is hoped that a more detailed calculation of the bands of \( Y \) will follow as more experimental information becomes available for \( Y \). More positive identifications than those presented here must await these bands and measurements in the vacuum ultraviolet of (probably) ultrahigh-vacuum-evaporated films of \( Y \), which, when used in conjunction with our data, will make it possible to determine the optical constants.

The authors thank B. Beaudry and P. E. Palmer for providing the starting material and F. A. Schmidt for strain annealing the material to obtain the single crystal.

\[ \text{INTRODUCTION} \]

5. Transparent films of \( Y \) have been investigated over the range of \( \approx 1.5-6 \) eV and minima in the transmission have been noted at \( \approx 2.5 \) and 5.6 eV (J. P. Petrkian, J. P. Palmari, and G. Rasing, Appl. Opt. 9, 2115 (1970)).

**PHYSICAL REVIEW B**

**VOLUME 7, NUMBER 10**

**15 MAY 1973**

**Hot-Electron Hall Transport in \( n \)-Type Germanium**

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(Received 11 October 1972)

The hot-electron Hall coefficient in \( n \)-Ge is theoretically estimated incorporating the band nonparabolicity, the electron transfer to the \( (100) \) minima, and the effect of the magnetic field on the distribution function. A better agreement with the nature of the experimental curve at 200°K is obtained when the nonparabolicity is considered than when it is ignored. A close fit with experiment requires the value of the deformation-potential constants for the optical and for the nonequivalent intervalley scattering to be \( 0.66 \times 10^6 \) and \( 0.5 \times 10^6 \) eV cm\(^{-1}\), respectively.

**I. INTRODUCTION**

In an earlier paper, \(^1\) calculations of the Hall factor in \( n \)-type germanium at high electric fields were reported taking into account the influence of the electron population in the \((100)\) minima and that of the magnetic field on the valley distribution function. The nonparabolicity of the \((111)\) bands was, however, not included in these calculations and the value of the optical-phonon deformation-potential constant \( D_0 \) required for an agreement with the experimental results at 200°K was found to be unusually high. It may be mentioned that when parabolic bands are considered, there remain discrepancies in the values of \( D_0 \) obtained from various studies. \(^1\) Incorporation of nonparabol-