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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

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Absorptivity of Single-Crystal Yttrium at 4.2 K

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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 $\hat{c}$ 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,[1,2] Nb,[3] Ta,[4] V,[4] and Mo[4] over a wide energy range, typically 0.1–35 eV, as calculated from the measured absorptivity or reflectivity. For these metals, the oxide formed slowly and/or had known optical properties and the dielectric function could be determined reliably in the vacuum ultraviolet. For Y, however, it is not clear that the oxide forms slowly; since the oxide dielectric function is not known, we have measured the absorptivity only below 4.4 eV, where it has been assumed that the oxide is transparent; i.e., the absorption coefficient of the oxide is zero. Since no vacuum-ultraviolet data are available,[5] and since any extrapolation of the absorptivity to high energy appears artificial, we have not calculated the dielectric function. Qualitative information can be obtained, nevertheless, from the absorption spectra.

High-purity Y was obtained within the Ames Laboratory and single crystals were grown by a strain-anneal method. The samples used were spark cut from one of two single-crystal ingots (approximately 50×12 mm diameter) that had been oriented by Laue back-reflection x-ray diffraction. The crystals were polished mechanically and electropolished in a solution of 6% perchloric acid in methanol (cooled by a bath of dry ice and acetone). They were exposed to the atmosphere for only about 3–5 min before being placed in the vacuum chamber, which was flushed with high-purity N_2 as it was being sealed. Within about 15 min the vacuum was about 10^{-4} Torr. The calorimeter was then cooled to 4.2 K and the measurements performed. The absorption spectra shown in Fig. 1 were obtained in this manner. Details of the method are given in Ref. 1. To determine the effect of an oxide, one of the samples was run as outlined above, then stored in an atmosphere of high-purity oxygen at room temperature for 14 days; it was then run a second time. The absorptivity below about 3 eV was practically identical; above 3 eV the effect of

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 $\vec{E} \parallel \hat{c}$ ($\vec{E} \perp \hat{c}$). 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 ($\vec{E} \parallel \hat{c}$) and 0.0430 ($\vec{E} \perp \hat{c}$) 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[6] has considered the Fermi-surface topology of Y, there have been no band calculations *per se*. However, it has been pointed out[6] that Y is very similar in atomic configuration ($4d\,5s^2$) to the hexagonal rare-earth metals with atomic configurations $5d\,6s^2$. Further, augmented-plane-wave calculations have shown[7] that the band density-of-states curves for Re,[8] Gd,[9] Y,[6] and Dy[10] 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.[11] Photoemission results[12] 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[11] 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 $\Gamma_6^- - \Sigma_1 - M_1^+ - K_1$ 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_F 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,

FIG. 1. Absorptivity of single crystals of Y at 4.2 K.

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 $\vec{E} \parallel \hat{c}$. 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_2 bands probably persist in Y and would give rise to the observed anisotropic structure which occurs at low energy for $\vec{E} \parallel \hat{c}$ only. Such transitions are for-

bidden by electric dipole selection rules for $\vec{E} \perp \hat{c}$.[13] Further, selection rules allow transitions $\Sigma_3 \rightarrow \Sigma_1$ for $\vec{E} \parallel \hat{c}$ 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 $\vec{k}$ space would likewise contribute to the structure in Fig. 1. For Sc, $H_3 - H_2$ (~ 0.9 eV, both polarizations) and near $H_1 - H_2$ (~ 0.5 eV, $\vec{E} \perp \hat{c}$ only) transitions are apparent and would probably persist in Y. Finally,

FIG. 2. Electronic energy bands for Sc from Ref. 11.

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.

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Hot-Electron Hall Transport in n-Type Germanium

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The hot-electron Hall coefficient in n-Ge is theoretically estimated incorporating the band nonparabolicity, the electron transfer to the $\langle 100 \rangle$ 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 0.66×10^9 and 0.5×10^9 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 $\langle 100 \rangle$ minima and that of the magnetic field on the valley distribution function. The nonparabolicity of the $\langle 111 \rangle$ 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-

icity has recently been found to reduce to a large extent the disparity in the D_0 values obtained from the conductivity results at high and low electric fields.[2,3] It would be of interest to examine whether the hot-electron Hall-coefficient characteristic can also be explained with the same value of D_0 as that obtained from the conductivity data when the nonparabolic nature of the band structure is taken into account in addition to the carrier transfer to the $\langle 100 \rangle$ minima and the influence of the magnetic field on the carrier distribution function. In this paper we present the results of such calculations. We have also studied the effect of a change in the coupling constant for nonequivalent intervalley scattering D_{ni} and have determined the value required for a fit with the experimental results.