PHYSICAL REVIEW VOLUME 172, NUMBER 3 15 AUGUST 1968

Effect of Uniaxial and Hydrostatic Strain on the Optical Constants and the Electronic Structure of Copper*

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(Received 27 December 1967)

The linear response of the optical constants of Cu to a general strain is presented for the range $1.5 \leq \hbar\omega \leq 5.5$ eV. The transitions $X_5 \rightarrow X_4'$ at 4.0 eV and $E_F \rightarrow L_1$ at 4.15 eV are identified. The deformation potentials $\partial(E_F - L_3^{\text{upper}})/\partial e = -(1.1 \pm 0.1)$ eV and $\partial(L_1 - E_F)/\partial e = -(9.6 \pm 1.5)$ eV with $e = \Delta V/V$, and $\partial L_1/\partial e_{yz} = -(72 \pm 12)$ eV with $e_{xy} = e_{yz} = e_{zx}$, $e_{xx} = e_{yy} = e_{zz} = 0$ for $\mathbf{k} \| [111]$ are evaluated from the measurements. They are used to derive the volume coefficients of the Fermi energy, $\partial(\ln E_F)/\partial e = -1.1 \pm 0.3$, and of the position of the d bands, $\partial(\ln E_d)/\partial e = -1.2 \pm 0.5$, with respect to Γ_1. The measurements are consistent with the assumption that direct interband transitions dominate the absorption above 2 eV.

INTRODUCTION

APPLYING a shear strain to a single crystal reduces its symmetry and may split formerly degenerate levels. In optical experiments, the first such splitting was observed accidentally in the investigation of the excitonic absorption of germanium.[1–3] The power of the method was soon recognized; it was used to study the excitonic absorption of other crystals, e.g., CdTe[4] and Cu_2O.[5] The method was first applied to the continuous interband absorption by studying the strain-induced change of the reflectance of Ge and Si.[6,7] Modulation techniques were also used successfully.[8–10] Polycrystalline films of the noble metals were investigated.[11] A preliminary version of the present paper was published elsewhere.[12]

According to the band-structure calculations of Cu,[13,14] direct, k-conserving interband transitions are possible for $\hbar\omega > 2$ eV. These lead to a continuous absorption in contrast to the sharp excitonic structure of solids mentioned above. However, the topology and the symmetry of the problem give rise to singularities in the joint density of states,[15–17] which dominate the behavior of semiconductors and insulators in the region of the interband transitions. In metals, the modifications of this structure due to the overlap of the Fermi energy with the electron bands might give even sharper singularities in the absorption.[18]

The basic virtue of the measurements to be discussed here is their ability to distinguish between singularities of different symmetry. The main difficulty in the analysis is that the "symmetry of a singularity" is quite frequently not well defined. For example, a structure in the absorption caused by an M_1 or an M_2 type singularity in the joint density of states is composed of transitions with k vectors terminating on the optical energy surfaces $E(\mathbf{k}) = E(M_1)$ and $E(\mathbf{k}) = E(M_2)$, respectively. These surfaces stretch through the Brillouin zone, i.e., there is a whole range of transitions with different k vectors which contribute to the observed structure in the absorption. However, if the structure in the absorption is made up of transitions with wave vectors confined to a region close to a symmetry point $\mathbf{k}_s$ in k space, the structure will approximately respond to a perturbation as if it were composed of transitions with $\mathbf{k}_s$ only. We will refer to transitions of this kind as strongly localized transitions. Transitions arising from the M_1 and M_2 type singularities mentioned above are only moderately localized around the corresponding saddlepoints, and some transitions connected with singularities caused by the Fermi energy are not localized at all.

The experiments reported here were done with a technique similar to the one used for the alkali halides.[10] They give the linear response of the optical constants to an arbitrary strain for photon energies between 1.5 and 5.5 eV. This information is used to determine the symmetry of strongly and moderately localized transitions; it also reveals which structure in the absorption

* Work supported by the U. S. Air Force Office of Scientific Research, Contract No. AF 49(638)-1653.

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