

measured relative change of optical constants Q_{ij} .

from	Stress axis	Points Fig. 7
	[111]	Circles
	[001]	Squares
	[111]	Circles
and $Q_{11}+2Q_{12}$	[110]	Squares
	[001]	Circles
Q_{12}	[110]	Squares

the zero line for $\hbar\omega > 5.5$ eV. The error introduced by the Kramers-Kronig transform at the time the function was calculated was $Q_{11}+2Q_{12} = -2$ at 6 eV and zero line above 6.5 eV. The two extrapolations have the maximum value (81.5%) in the Kramers-Kronig error due to the extrapolation energy. The error bars near the origin are due to the extrapolation as the ones at 3.5 eV give the error signal in ΔR .

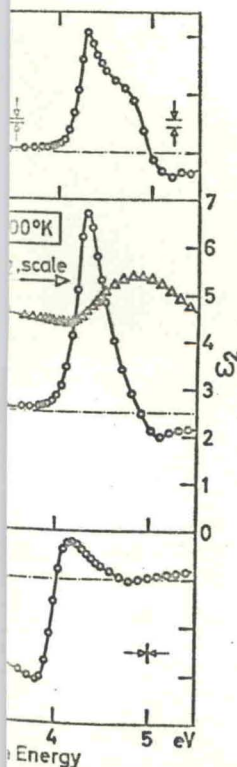


FIG. 8. The experimental function $(W_{11}-W_{12})/(\hbar\omega)^2$ is plotted.

TABLE III. Symmetry rules for the optical transitions, considering the splitting of the k degeneracy only.

$W_{11} \neq 0; W_{11}-W_{12}=0$	Δ or L transitions
$W_{11} = 0; W_{11}-W_{12} \neq 0$	Δ or X transitions
$W_{11} \neq 0; W_{11}-W_{12} \neq 0$	All transitions except Δ, L, Δ, X

The spectral resolution given in Figs. 6-8 is the half-width of atomic mercury lines, as recorded with our optical system.

THEORETICAL ANALYSIS

Symmetry Rules for Optical Transitions

Throughout the theoretical analysis we assume that we are dealing with direct, k-conserving interband transitions, i.e., that ϵ_2 is dominated by this process. We exclude the region below 2 eV where free carrier absorption is important.

There are two types of degeneracies in a solid, namely, the orbital degeneracy (e.g., L_3 , twofold neglecting spin) and the k degeneracy (e.g., the star of k_L contains four equivalent vectors; any L level will be fourfold degenerate with respect to k). Most of the orbital degeneracy is lifted already by spin-orbit interaction. If we include the effect of strain and assume that the center of gravity of the levels under consideration is not changed by the strain, the total splitting will be given by²⁵

$$\Delta = (\Delta_{spin\ orbit}^2 + \Delta_{strain}^2)^{1/2} \quad (5)$$

In Cu, the spin-orbit splitting is about ten times the splitting produced by strain (the strain applied was about 5×10^{-4}). This means that the change of Δ is

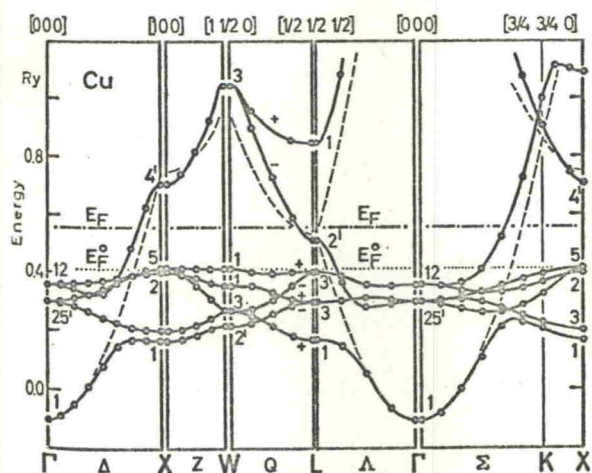


FIG. 9. The band structure of Cu as calculated by Segall (see Ref. 13) and Burdick (see Ref. 14) using Chodorow's potential (see Ref. 26). The dashed curves are the free-electron eigenvalues. E_F is the Fermi energy as calculated by Segall and Burdick and E_F^0 the Fermi energy calculated for the free-electron eigenvalues of the sp bands.

²⁵ J. Goroff and L. Kleinman, Phys. Rev. 132, 1080 (1963).

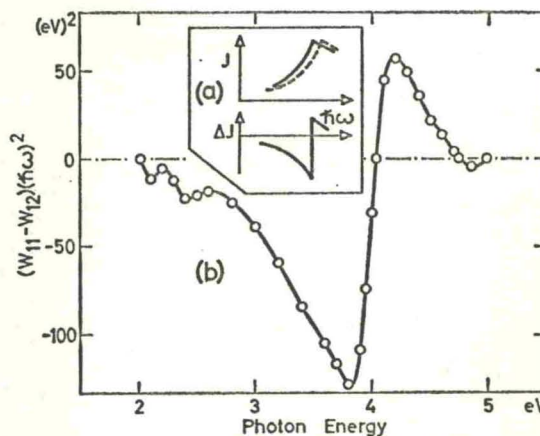


FIG. 10. The insert (a) shows the change of the joint density of states in the neighborhood of an M_1 singularity produced by a rigid energy shift of the joint density of states; in part (b) of the figure the experimental function $(W_{11}-W_{12})/(\hbar\omega)^2$ is plotted.

second order in the strain and thus not detected in our measurements. We therefore must exclude the effect of a change of the spin-orbit splitting from our considerations.

Four effects may contribute to the observed $\Delta\epsilon_2$ in Cu, namely, the lifting of the k degeneracy, changes in the oscillator strength, changes in the joint density of states, and the splitting of the orbital degeneracy not lifted by spin-orbit interaction. The lifting of the k degeneracy normally is the most important effect. We confine the discussion to this effect for the time being. The symmetry rules which follow are summarized in Table III. They were derived by considering the effect of trigonal and tetragonal shear strain on the set of originally equivalent k vectors (the star of k). These rules depend only on the symmetry of the crystal for zero strain and on the symmetry of the distortion. Exceptions from these rules can arise only from accidental degeneracy, e.g., an L and an X transition at the same energy will produce a nonzero change in ϵ_2 for both trigonal and tetragonal shear strain. It is largely due to these simple symmetry rules that the effect of shear strain on the optical constants is so powerful a method in analyzing the electronic structure of crystals.

Using Table III and the experimental results given in Fig. 8, we expect the edge at 2.1 eV to be caused by nonlocalized transitions, because shear strain gives only very small $\Delta\epsilon_2$ without pronounced symmetry behavior. Going from 2 to 4 eV, a Δ or X transition must become increasingly important. A singularity in the joint density of states connected with these transitions is likely to occur at about 4.0 eV corresponding to the minimum in $W_{11}-W_{12}$ (see Fig. 8). Finally, there must be a pronounced singularity connected with Δ or L transitions at 4.3 eV, which is responsible for the large maximum in W_{44} .