in some metals prior to melting[12,13] might be explained in terms of the thermal generation of point defects and the above postulated affinity of positrons to reside at vacancy sites.

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PIEZO-OPTICAL CONSTANTS, DEFORMATION POTENTIALS, AND THE ELECTRONIC STRUCTURE OF COPPER*

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From the strain-induced change of the reflectance, the change of ϵ_2 is derived. The measurements are used to identify electronic transitions and to evaluate three deformation potentials. Two of the deformation potentials are compared with the result of a theoretical model.

The piezo-optical measurements given in this paper are used to identify electronic transitions in copper, which could not be identified using the relatively less detailed structure of the optical constants alone. In fact, most of our experimental knowledge on the electronic structure of metals has originated from Fermi-surface studies. Piezo-optical studies, however, may well be competitive in this respect.

The strain-induced change of the reflectivity is measured at room temperature between 1.5 and 5.5 eV, using freshly electropolished single crystals of three different orientations and plane-polarized light. The strain is produced by a low-frequency (200 Hz) bending of the crystals. From the six measurements (polarizer parallel and perpendicular to each of the three axes), the relative change of the reflectivity for a change in volume and for pure trigonal and tetragonal shear strain is evaluated. The result is shown in Fig. 1, together with the reflectivity itself (definition of Q_{ij} equivalent to that of stiffness constants). The Q_{ij} evaluated from samples with different orientations are in excellent agreement. The zero line is not adjusted, in contrast to similar experiments previously reported.[1-3] Using a Kramers-Kronig analysis, the change of ϵ_2 is derived. It is given in terms of W_{ij}, Fig. 2, together with ϵ_2.

In the analysis of W_{ij} we neglect the change of the oscillator strength and of the joint density of states. In this case, a pure shear strain can produce a change in ϵ_2 only by lifting the $\vec{k}$ degeneracy (e.g., sixfold for Δ). From Fig. 2, we find a maximum of $|W_{11}-W_{12}|$ at 3.9 eV. At this energy, trigonal shear produces no effect. Thus, we are dealing with Δ or X transitions, since these are the only ones whose $\vec{k}$ degeneracy is not lifted by a trigonal shear strain. Examination of the energy bands of

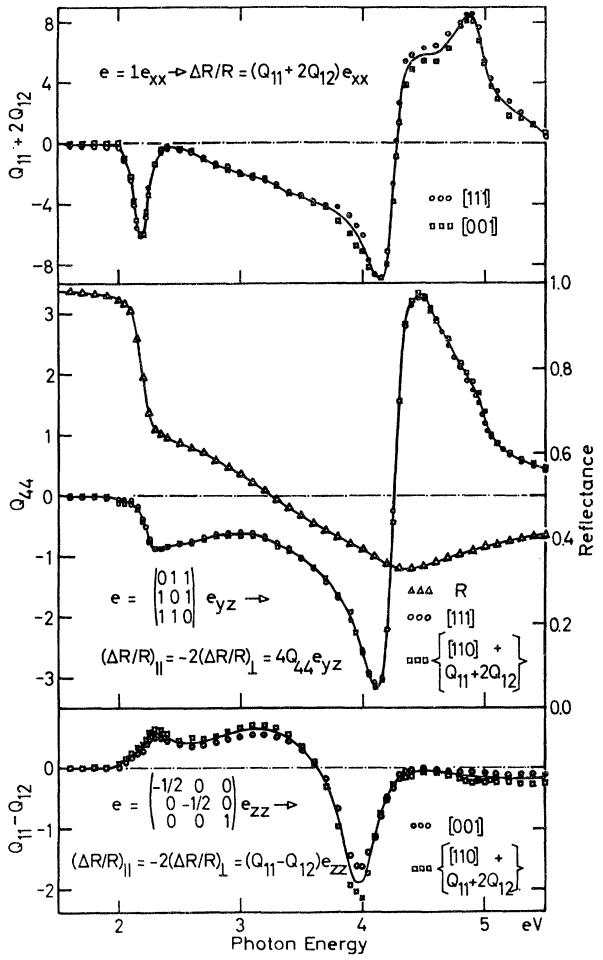

FIG. 1. The reflectance R of copper (scale on the right-hand side) and the relative change of R, caused by the strain $\vec{e}$ (scale on left-hand side). The definitions of Q_{ij} for the three independent distortions are given in the left half of the figure. Measurements on crystals with different orientations have been used to calculate Q_{ij}; their orientations are indicated in the right half of the figure. The strain along the stress axis has been about 3×10^{-4} rms.

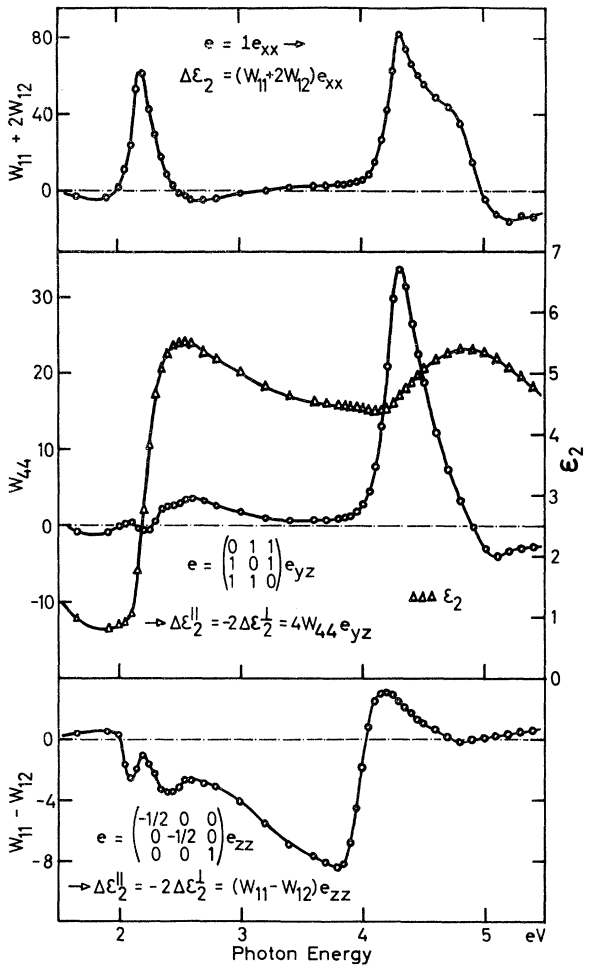

FIG. 2. The imaginary part of the dielectric constant, ϵ_2, of copper (scale on right-hand side) and the change of ϵ_2 caused by the strain $\vec{e}$ (scale on left-hand side). The points shown indicate the spacing of the input data, taken from the average values (solid lines) of Fig. 1.

copper[4,5] yields as the only possibility the transition $X_5 \rightarrow X_4'$ (M_1 saddle point); all other singularities are well removed from the observed energy. Going from 2 to 3.9 eV, $|W_{11}-W_{12}|$ increases in accordance with the expected behavior for an M_1 saddle point at 3.9 eV. There are no contributions below 2 eV, because the Δ_1 band is below E_F (Fermi energy) in this region. The sign of $W_{11}-W_{12}$ is also consistent with the above assignment. Because of the localization of the d functions in the unit cell, the change of X_5 with shear strain will be small. The X_4' level is roughly equal to the free electron energy (neglecting a small pseudopotential form factor), the change of which is easily calculated. Together with the selection rule for $X_5 \rightarrow X_4'$, this yields $W_{11}-W_{12}<0$ as observed. The magnitude of the strain-induced energy shift ΔE for the $X_5 \rightarrow X_4'$ transition could not be obtained from our results because this transition contributes too little to ϵ_2 to convert $\Delta\epsilon_2$ into ΔE using the slope of the ϵ_2 curve.

A quantitative analysis is possible for the observed structure in $W_{11}+2W_{12}$ and W_{44} around 4.3 eV, which clearly is connected with the edge of ϵ_2 at the same energy. Since $W_{11}-W_{12}$ is small here, we conclude that the structure must be caused by a singularity at L or Λ. Comparing with the band structure,[5] we find

$E_F(L_2') - L_1$ closest to the observed energy. This assignment is also consistent with the positive slope in ϵ_2 and the large oscillator strength,[6] and it has also been derived from photoemission studies.[7] Furthermore, these transitions are strongly affected by trigonal shear, because their $\vec{k}$ vectors terminate in the region enclosed by the neck around L. Transitions from the d states to states above E_F are not strongly localized. Finally, the observed changes of $L_2'-E_F$ with volume and trigonal shear strain agree well with the ones calculated using the simple model discussed below. The experimental values were derived from $\Delta\epsilon_2$ assuming a small negative slope (−0.3/eV) of the background in ϵ_2. The neglect of changes in the oscillator strength and in the density of states is justified because $\Delta\epsilon_2$ has its maximum where the contribution to the total ϵ_2 is still small.

Our model yields the L_1 level as eigenvalue of a pseudo-Schrödinger equation. The eigenfunction to L_1 is an orthogonalized plane wave, orthogonalized to the d state L_1^d, and the eigenfunction of L_1^d, $|d\rangle$, is approximated by the LCAO of atomic d functions, the effective Bohr radius of which is adjusted to give the augmented-plane-wave eigenvalues.[5] The plane-wave admixture to L_1^d is neglected. The L_2' level does not interact with the d levels; it is given by $k_L^2 - W_{111}$. The strain coefficient of L_1 requires knowledge of the strain dependence of the free electron-d overlap $(2/\Omega)^{1/2}\langle \vec{k}_L \cdot \vec{r}\,|d\rangle$ (calculated using the assumed $|d\rangle$ functions) and of the form factor W_{111} (calculated using Ashcroft's potential).[8] For the volume coefficient, we need in addition the deformation potentials for $E_F - L_3^{\text{upper}}$ (taken from the shift of the 2-eV edge, see below), $E_F - L_2'$ (Templeton[9]), and $L_3^{\text{upper}} - L_1^d$ (calculated using d-d overlap). The deformation potentials derived from the experiments and from the theoretical model are (theoretical coefficients in brackets) $\Delta(L_1 - E_F)/(\Delta V/V) = -10.4$ eV ± 1.5 eV (−16.4 eV); $\Delta(L_1 - E_F)/e_{yz} = -78$ eV ± 12 eV (−97 eV) ($e_{xx} = e_{yy} = e_{zz} = 0$; $e_{xy} = e_{yz} = e_{zx}$). The experimental volume coefficient agrees well with the one determined from hydrostatic experiments.[10]

The 2-eV edge in ϵ_2 has long been recognized as due to transitions from the top of the d bands to the Fermi surface, which probably starts near L. The experimental volume coefficient, derived from $W_{11} + 2W_{12}$, is (−1.1 ± 0.1) eV. The lack of response to shear strain is consistent with the fact that the contributions come mostly from general points in the Brillouin zone.

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