12 ging matrix elements ore closely the actual f. Figure 10(b) gives nich is to be compared g. 10(a). The agree ependence of W11-11 by the above assignt ructure in W44, we the because the structure egion. The main differen .) and the FS  $\rightarrow L_1$  transformed to the transformed state of the tran e original contributions e truncated by the Fa energy are shown for ce  $L_1 - L_2'$  in a plane c density of states around wn in Fig. 11. The ency nall compared to  $L_{1-1}$  $L_1$  are also used to de: es for typographical ariation of J in the reg n by

1:2

 $m_1(\hbar\omega - L_1 + E_F)^{1/2}$ .

ie neck was approximat J as given by Eq. (6) than  $L_1 - E_F$ . The sl cause of lifetime broad ij will thus occur at rovided Wij is caused  $\epsilon_2$ . Figure 11 and Eq. ions are strongly locali ors terminate in a regi

ons  $L^d \rightarrow FS$  termin nsitions are not localiz xpect a change in  $\epsilon_2$ ear strain, and we exp experiments show a ve 12 at the same energy X<sub>4</sub>' transitions near racy mentioned abov is most probably due 1 transitions.

the momentum matr ons of interest here, given in Table IV. T  $\rightarrow L_1$  transition is mu originating from d ba illips29 found that ab 5 eV is due to the c transitions. The act r due to lifetime broz the height of the sha a these transitions (F

(1958).

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TABLE IV. Transition matrix elements in (Ry) for selected transitions.
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Transitiona	$L_2' \rightarrow L_1$	$L_1^d \rightarrow L_2'$	$L_3^l \rightarrow L_2'$	$X_5 \rightarrow X_4'$
2P::2/m	3.17	0.533	0.015	0.250

The matrix elements are calculated using the eigenvalues given in t-14 [F. M. Mueller (private communication)].

1). From the experimental  $\epsilon_2$  we estimate a total atribution of about 30%, extrapolating the contribuon of the background below 4.1 eV to about 4.65 eV. the high percentage of  $L_2' \rightarrow L_1$  transitions as calcuated from theory is consistent with the pronounced due in the experimental  $\epsilon_2$  and with the large  $W_{44}$  as ell. This leads again to the conclusion that the oberved structure in  $\epsilon^2$  and  $\Delta \epsilon_2$  at 4.3 eV is caused by the  $FS \rightarrow L_1$  transition.

Another striking feature of the functions  $W_{ij}$  is the astly different magnitude of  $W_{44}$  and  $W_{11} - W_{12}$ . The aximum  $\Delta \epsilon_2$  observed for trigonal shear strain is nine times the corresponding value for tetragonal shear train (the amount of the strain being the same). This is partly due to the different degree of localization in k pace discussed above and partly to the difference in he oscillator strength (Table IV). The small oscillator trength for  $X_5 \rightarrow X_4'$  as compared with the one for  $L_1' \rightarrow L_1$  suggests that there is no pronounced structure  $a \epsilon_2$  around 4.0 eV, and indeed the experimental curve s nearly flat in this region. However, we believe to have resolved a tiny hump in our room-temperature measurements of  $\epsilon_2$ , as shown in Fig. 12. The reflectance at quid He temperatures<sup>30</sup> shows a well-resolved structure it about the same energy. The transition does show up dearly as a minimum in  $W_{11} - W_{12}$  at room temperature. The hydrostatic change  $(W_{11}+2W_{12})$  and the change with trigonal shear strain  $(W_{44})$  have the same shape tetween 4 and 4.5 eV. The position of the maximum is 1.3 eV in both cases. This suggests that both effects the due to the FS  $\rightarrow L_1$  transition. The two functions differ between 4.5 and 5 eV, where  $W_{11}+2W_{12}$  exhibits an additional shoulder around 4.8 eV, whereas  $W_{44}$ approaches zero rapidly. This behavior can be explained assuming transitions from the bottom of the dbands to the FS. As in the case of the 2.1-eV edge (where the top of the d bands provides the initial states), these transitions originate from general points of the BZ. This explains the lack of response to shear strain. The transitions will of course change under hydrostatic strain. The situation is equivalent to the one at the <sup>2.1</sup>-eV edge, where only hydrostatic strain produces a significant change in  $\epsilon_2$ .

## **Experimental Deformation Potentials**

The assignment of the structure observed in  $W_{ij}$ and  $\epsilon_2$  has been established in the preceding sections. This information can be used to calculate the deforma-

<sup>40</sup> M. A. Biondi and J. A. Rayne, Phys. Rev. 115, 1522 (1959).



FIG. 12. A blow-up of the imaginary part of the dielectric constant of Cu at room temperature around 4 eV, showing weak structure slightly below 4 eV. The slope of the edge at 4.3 eV and the slope of the background which were used to calculate the deformation potentials of the  $E_F \rightarrow L_1$  transition are also included.

tion potentials of the corresponding transitions from the experiments, i.e., the difference in the deformation potentials of the final and the initial state. Additional knowledge is required to do so, namely, the slope  $d\epsilon_2/d(h\omega)$  of that part of  $\epsilon_2$  which is responsible for the observed structure in  $W_{ij}$  and the selection rules (required for the shear-strain coefficients only). Furthermore, it must be possible to separate that part of  $W_{ij}$ which is due to a change of the energy levels from the ones due to modifications of the transition matrix elements M and of the density of states J.

The slope of the edge at 2.1 eV is large; modifications due to a background of transitions other than  $L_3^u \rightarrow FS$ (e.g., free carrier absorption) will be small. The selection rules are not needed because only hydrostatic strain produces a pronounced change in  $\epsilon_2$ . The changes in M and J produced by a hydrostatic strain will be much smaller than the ones produced by shear strain, in which case they are required by symmetry.7 Only  $W_{11}+2W_{12}$  is large at this edge, which shows that changes of M and J contribute very little to  $W_{11}+2W_{12}$ . The deformation potential will be given quite accurately by the maximum value of  $W_{11}+2W_{12}$  and by the uncorrected slope of  $\epsilon_2$ .

As discussed above, the 2.1-eV edge is due to nonlocalized transitions; the transitions with lowest energy have k vectors terminating just outside the neck, but at slightly higher energies transitions with k vectors located in other parts of the BZ will contribute. The deformation potential determined from the energy shift of the edge will be an average over the deformation potentials of all transitions which contribute. However, the top of the d bands is rather flat, particularly the portion  $L_3^u - Q_+$ , and it will remain flat if the volume of the crystal is changed. Thus the deformation potentials of transitions contributing to the edge differ only slightly from each other. We therefore no

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