Density of states above the Fermi level in copper*

C. C. Chu and P. E. Best
Department of Physics and Institute of Materials Science, University of Connecticut, Storrs, Connecticut 06268
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We report new measurements of the bremsstrahlung isochromat of copper which corroborate the results of Turtle and Liefeld. Overall agreement between the experimental and calculated density-of-states curves is very good. A suggestion on how to improve agreement between the curves is made.

The importance of copper as a testing ground for our understanding of the electronic structure of nonsimple metals is well recognized.[1] In this paper we report a new measurement of the bremsstrahlung isochromat (BI) from copper, and compare this with earlier experimental results, and with the calculated density of states above the Fermi level in copper.

The BI is essentially a measurement of structure near the short-wavelength limit of the bremsstrahlung spectra.[2,3] In a direct measurement of this structure, the electron beam voltage remains fixed, and the intensity of the resulting x-ray spectrum is recorded as a function of wavelength. In the BI method, a fixed x-ray wavelength is passed by a monochromator, and the electron beam voltage is scanned from just below the Duane-Hunt limit to higher values, while recording the x-ray intensity as a function of beam energy. No significant differences have been observed in structure recorded by the two methods.[4]

For a monochromatic beam of electrons passing through a sample, at an energy well removed from ionization thresholds of atoms present, the BI spectrum reflects the density of vacant states spectrum.[2,3,5] In practice, the energy spectrum of electrons in a thick sample consists of characteristic loss peaks,[6] as well as the elastic component. These loss peaks give rise to their own "echoes" of the BI, displaced in energy from the main BI by the value of the energy loss.[7] A comparison between the energy loss[8] and BI indicates no significant component from that source in the BI spectra of copper.

In this work the sample was prepared by evaporation of high-purity copper within an ultra-high-vacuum chamber.[9] A 100-μA beam from an electron gun strikes the sample at close to normal incidence. The precisely controllable energy of the beam is about 5414 eV, the energy of the chromium $K\alpha_1$ line. This line was used in the alignment of the bent-mica-crystal monochromator, and sets the pass wavelength of the monochromator in fifth order.[10] The take-off angle of the x rays from the sample is about 87° from the surface normal. The x rays pass from the sample chamber, through a 0.025-cm-thick beryllium window, to the monochromator and detector which are in air.

Curve *B* of Fig. 1 is our BI, while curve *C* is the raw data of Turtle and Liefeld. Curve *A* is their data corrected for the instrumental window and for a plateau region of the energy-loss spectrum, although not for discrete losses.[8] Our overall instrumental window width is estimated to be 0.5 eV, with the largest effect occurring at the threshold. Considering the state of art of BI measurements, agreement between the experimental results shown in Fig. 1 is remarkable. Taking in account the many differences in technique between the two measurements, it can be claimed that this BI is better established than any other, except that of tungsten.[7] In particular, both measurements show peaks at energies of 2.0 ± 0.5,

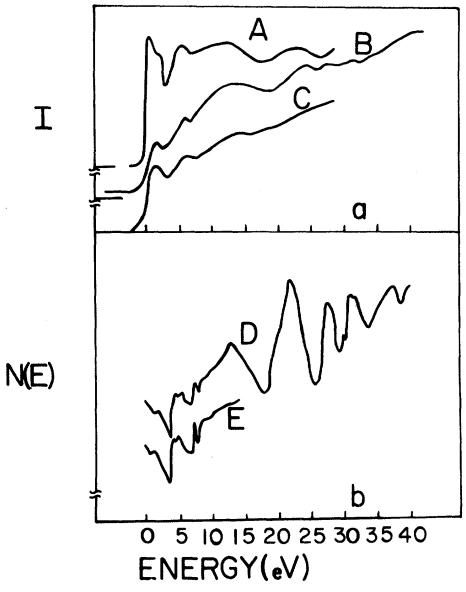

FIG. 1. (a) Bremsstrahlung isochromat from copper: *B*, present work, *A* and *C* are the corrected and raw data curves, respectively, reported by Turtle and Liefeld (Ref. 2). (b) Calculated density of states above the Fermi level for copper: *D*, calculated with a Chodorow potential (Ref. 11); *E*, reported by Janak, Williams, and Moruzzi, (Ref. 1).

5.5 ± 0.5, and 13.0 ± 0.5 eV. The spectra differ mostly in the shape and location of the broad maximum at about 23 eV. All the features shown in our raw-experimental-data curve are reproducible, with statistical noise limited to about two linewidths on the graph in Fig. 1.

Figure 1(b) shows the calculated density-of-states spectrum for copper; curve *D* is that calculated with a Chodorow potential,[11] and curve *E* is the result reported by Janak *et al.*[1] Comparison between the experimental and calculated density-of-states curves brings out the following points. The correlation from the edge to the minimum at 3.5 ± 0.5 eV is good. There are two features in the region from 3.5 to 7.0 eV. In the calculated structure, a peak at about 5.5 eV "sits" on an apparently larger structure with a threshold at 4 eV. The experimental curves indicate that the 5.5 eV structure is the major one, with the increase from 4.0 eV being more gradual. This suggests that the bands at and near the *L* and *K* points in *k* space have a greater slope than indicated by the band-structure calculation.[1] This specific information is one of the advantages of the BI method: States at only one energy contribute to each spectral point, and there are no uncertainties introduced by matrix elements. The sharp feature at 7.5 eV in the calculated structure does not appear in the experimental curves. However, hot-electron broadening and the instrumental width could smear out such a narrow feature.

For higher energies there is again good correlation between theory and experiment for peaks at 13, 22, 27, and 31 eV. With increasing energy above the Fermi level, lifetime broadening effects become greater[12] and should be folded into the calculated density-of-states curve to make comparison at these higher energies really significant.

Overall, the experimental results reported here corroborate the results reported previously by Turtle and Liefeld, in a field in which such concurrence has been relatively rare. Agreement between the experimental results and the calculated density-of-states curves is remarkably good with the experimental data suggesting one way in which agreement could be improved.

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