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A HIGH RESOLUTION STUDY OF THE $\text{CuK}\alpha$ SATELLITE SPECTRUM

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ABSTRACT The $\text{CuK}\alpha$ x-ray satellite spectrum was measured using a silicon monolithic double crystal spectrometer. The intensity relative to that of the $\text{K}\alpha_1$ line was found to be $6.2 \cdot 10^{-3}$ and the width 12.7 eV, both in good agreement with previous measurements and theoretical predictions. The spectrum was resolved into four component lines, which are downshifted by ~1 eV relative to previous measurements but otherwise are in good agreement with them. The uncertainties in the widths positions and relative intensities of the component lines are also discussed.

INTRODUCTION Electronic transitions in multiply-ionized atoms provide insight into intra-atomic electron correlations and excitation dynamics [1]. This is the motivation behind the recent increased research activity in the field of multielectronic transitions in general and x-ray satellites in particular [2]-[4]. Nonetheless, the $\text{K}\alpha$ satellite spectra of transition metals, a favourite testing ground for atomic structure studies, were not measured since the pioneering work of Parratt [5] over 50 years ago. We have therefore undertaken to remeasure the KL satellite spectrum of copper, using the high resolution monolithic double crystal spectrometer (MDCS) developed recently [6].

EXPERIMENTAL The MDCS is a spectrometer cut entirely from a single block of dislocation-free perfect silicon crystal. Two sets of Bragg planes play the role of the separate crystals in a conventional two-crystal spectrometer, and energy-scanning is done by rotating the spectrometer by some angle α about the normal to the first set of reflecting planes, thereby changing the effective angle of incidence of the beam emerging from the first set of planes onto the second one. The compact, monolithic structure of the MDCS greatly enhances stability by providing high immunity to vibrations, temperature changes, etc. This is of crucial importance for the long data collection runs required by the low-intensity satellite lines. Its high resolution, <1 eV, and inherent absolute wavelength accuracy, of order 1 ppm, also contribute towards rendering the MDCS the device of choice for the type of measurement reported here. For further details see [6].

Our MDCS employs two consecutive reflections in each of the 135 and $\bar{1}\bar{3}5$ planes. Absolute energy scale was established to 1.5 ppm accuracy by scanning the $\text{K}\alpha_1$ line at $\alpha = 12.69^\circ$. The radiation source employed was a commercial sealed x-ray tube with Cu anode run at 30 kV and 16 mA. The data was collected under microcomputer control, using the repeated scan technique.

DATA ANALYSIS, RESULTS AND DISCUSSION The intensity due to the flanks of the $\text{K}\alpha_1$ line in the satellite region was represented by a Lorentzian plus energy independent term representing background. These were fitted to the data at energies both below and above the satellite spectrum and subsequently subtracted from it. The resultant spectrum is shown in fig. 1. Subsequent analysis was carried out on this data set.

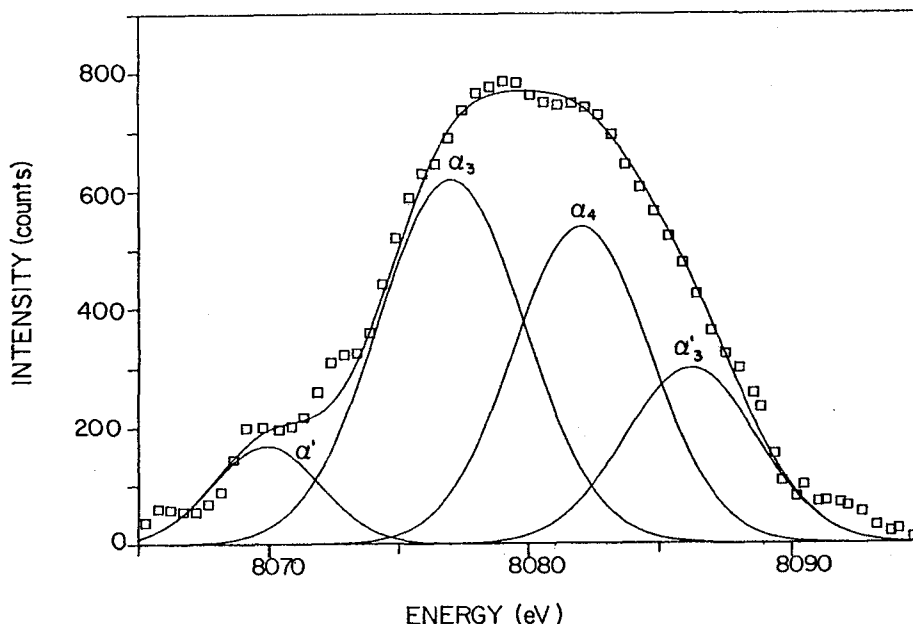


FIGURE 1 Measured ($\square$) and fitted (—) $K\alpha$ satellite spectrum of Cu. A resolution into the underlying component lines is also shown.

The intensity of the $K\alpha$ satellite spectrum relative to the $K\alpha_1$ line is defined [5] as the ratio of areas under the corresponding curves. Our data yields $6.2 \cdot 10^{-3}$, in very good agreement with Parratt's [5] measured value of $6.0 \cdot 10^{-3}$ and the theoretical values of Aberg [8]: $5.8 \cdot 10^{-3}$, and Richtmyer [9]: $6.2 \cdot 10^{-3}$. The agreement with the last value is remarkable indeed in view of the fact that it is based on a simple hydrogenic Hartree calculation, and a single, z -independent screening constant. The full width at half maximum (FWHM) of our data is 12.7 eV, also in good agreement with the FWHM of 12.2 eV calculated by us from Parratt's [5] work.

As already pointed out by Parratt, the resolution of the satellite spectrum into individual components invariably yields large uncertainties in the widths, heights and positions of the lines, due to their large widths and degree of overlap. The shape of the spectrum in fig. 1 indicates four underlying component lines. The fast decrease in intensity at the edges clearly favours Gaussian rather than Lorentzian shapes for these components. This observation was borne out by a series of non-linear least-squares computer fits of four component lines to the data using both Lorentzian and Gaussian lineshapes. The last lineshape yielded invariably better fits. The best fit is shown in fig. 1, with the relevant parameters listed in Table 1 along with those of Parratt [5] Cauchois and Senemaud [10], and the nonrelativistic Hartree-Fock calculated energies of Nigam and Soni [3]. Based on numerous computer fits to different line combinations the uncertainties in our energies and widths are estimated to be ~ 1 eV, while those of the relative intensity are $\sim 20\%$. Note that the uncertainties in energy refer only to the position of the fitted individual lines and result exclusively from the difficulties discussed above in resolving the broad, featureless spectrum. The measurement accuracy in the energy of each point is 1.5 ppm only.

	α'			α_3			α_4			α'_3		
	E	I	W	E	I	W	E	I	W	E	I	W
Present work	8069.9	0.049	4.8	8077.0	0.25	6.6	8082.0	0.20	6.2	8086.2	0.11	6.0
Parratt [5]	8070.7	0.008	4.0	8078.3	0.22	5.7	8082.9	0.27	6.4	8087.3	0.10	6.6
Cauchois [10]	8070.75			8078.2			8082.4			8087.8		
Nigam [8]	8070.6			8079.2			8082.4			8087.6		

TABLE 1 Energy (E), width (W) and intensity (I) relative to that of the $K\alpha_1$ line for the resolved satellite lines of Cu. E and W in eV, I - in % units.

Considering our uncertainties and those of Parratt's data [5] the overall agreement between the four data sets in Table is quite satisfactory. The ~1 eV systematic shift towards lower energies of our results as compared to those of Parratt seem, however, to be significant as is the difference in the relative intensity of the α' line. By contrast, α_3 and α_4 seem to be equally intense within the quoted uncertainty, and no significance should be attached to the apparent reversal in $I(\alpha_3)/I(\alpha_4)$ between our results and Parratt's.

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