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ABSTRACT

Values are tabulated for the real and imaginary dispersion corrections for the x-ray scattering factors for elements 20 to 96 for K_α radiation of chromium, copper, and molybdenum.

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The atomic scattering factor $\underline{f}$ for x-rays is a complex number:

$$f = f_o + \Delta f' + i\Delta f''$$

where f_o is a real function of $\sin\theta/\lambda$ which has been tabulated for many atoms.[1] The dispersion corrections $\Delta f'$ and $\Delta f''$ are functions of λ and vanish for wave lengths which are very small compared with the K absorption edge of the atom. These corrections are nearly independent of θ because the tightly-bound electrons responsible for these effects are concentrated in a small volume close to the atomic nucleus.

For convenience in using these corrections, we have tabulated values for elements 20 to 96 for three wave lengths frequently used in crystal analysis, the K_α lines of chromium (λ 2.2909 Å), copper (λ 1.5418 Å), and molybdenum (λ 0.7107 Å). These values were calculated by the methods of Parratt and Hempstead[2] for the contributions of K, L, and M electrons. The absorption edges were obtained from the tables of Cauchois and Hulubei[3] or by Moseley interpolation or

extrapolation. The oscillator strengths were estimated in a highly arbitrary way from data from several sources.[4-10] The uncertainty in these values is the chief source of error in our results. The exponents p have been chosen according to the example given for tungsten by Parratt and Hempstead.[2] Damping effects have been neglected.

The corrections are listed in Table I. Those for Cu K_α radiation are plotted in Figures 1 and 2.

TABLE I

Dispersion Corrections

Atomic Number		Cr K_α X-Rays $\Delta f''$	Cr K_α X-Rays $-\Delta f'$	Cu K_α X-Rays $\Delta f''$	Cu K_α X-Rays $-\Delta f'$	Mo K_α X-Rays $\Delta f''$	Mo K_α X-Rays $-\Delta f'$
20	Ca	2.7	0.2	1.4	-0.2	0.2	-0.2
21	Sc	3.2	0.7	1.6	-0.2	0.3	-0.2
22	Ti	3.8	1.7	1.9	-0.2	0.4	-0.3
23	V	0.6	4.4*	2.3	-0.2	0.5	-0.3
24	Cr	0.7	2.2	2.6	0.1	0.6	-0.4
25	Mn	0.8	1.8	3.0	0.5	0.8	-0.4
26	Fe	0.9	1.6	3.4	1.1	1.0	-0.4
27	Co	1.0	1.4	3.9	2.2	1.1	-0.4
28	Ni	1.2	1.2	0.6	3.1*	1.2	-0.4
29	Cu	1.3	1.1	0.7	2.1	1.4	-0.4
30	Zn	1.5	1.0	0.8	1.7	1.6	-0.3
31	Ga	1.7	0.9	0.9	1.5	1.7	-0.2
32	Ge	1.9	0.8	1.1	1.3	1.9	-0.2
33	As	2.2	0.7	1.2	1.2	2.2	-0.1
34	Se	2.4	0.7	1.3	1.0	2.4	0.1
35	Br	2.7	0.6	1.5	0.9	2.6	0.3
36	Kr	3.0	0.6	1.7	0.9	2.9	0.6
37	Rb	3.4	0.6	1.9	0.8	3.2	0.9
38	Sr	3.8	0.6	2.1	0.7	3.6	1.4
39	Y	4.2	0.6	2.3	0.7	3.9	2.3
40	Zr	4.6	0.7	2.5	0.6	0.8	2.8
41	Nb	5.1	0.8	2.8	0.6	0.9	2.1
42	Mo	5.6	0.9	3.0	0.5	0.9	1.7
43	Tc	6.2	1.0	3.3	0.5	1.0	1.4
44	Ru	6.7	1.2	3.6	0.5	1.1	1.2

Atomic Number		Cr K_α X-Rays		Cu K_α X-Rays		Mo K_α X-Rays	
		$\Delta f''$	$-\Delta f'$	$\Delta f''$	$-\Delta f'$	$\Delta f''$	$-\Delta f'$
45	Rh	7.3	1.3	4.0	0.5	1.2	1.1
46	Pd	7.9	1.6	4.3	0.5	1.3	1.0
47	Ag	8.6	1.9	4.7	0.5	1.4	0.9
48	Cd	9.2	2.2	5.0	0.6	1.6	0.8
49	In	10	2.7	5.4	0.6	1.7	0.7
50	Sn	11	3.2	5.8	0.7	1.9	0.6
51	Sb	12	4.0	6.3	0.8	2.0	0.6
52	Te	12	5.0	6.7	0.9	2.2	0.5
53	I	14	7.2*	7.2	1.1	2.4	0.5
54	Xe	11	**	7.8	1.4	2.5	0.4
55	Cs	12	12*	8.3	1.7	2.7	0.4
56	Ba	8	11*	8.9	2.1	2.9	0.4
57	La	3	14*	9.6	2.5	3.1	0.3
58	Ce	3	10	10	3.0	3.3	0.3
59	Pr	4	9	11	3.5	3.6	0.3
60	Nd	4	8	12	4.3	3.8	0.3
61	Pm	4	7	12	5.2	4.0	0.3
62	Sm	5	7	13	6.7	4.2	0.3
63	Eu	5	6	11	**	4.5	0.3
64	Gd	5	6	12	12*	4.7	0.3
65	Tb	6	6	8	11*	5.0	0.4
66	Dy	6	6	8	10	5.2	0.4
67	Ho	7	6	4	13*	5.5	0.4
68	Er	7	5	4	9*	5.8	0.5
69	Tm	8	5	4	8	6.2	0.5
70	Yb	8	5	4	8	6.4	0.6
71	Lu	9	5	5	7	6.8	0.7
72	Hf	9	5	5	7	7.1	0.8
73	Ta	10	5	5	6	7.4	0.9

Atomic Number		Cr K_α X-Rays $\Delta f''$	Cr K_α X-Rays $-\Delta f'$	Cu K_α X-Rays $\Delta f''$	Cu K_α X-Rays $-\Delta f'$	Mo K_α X-Rays $\Delta f''$	Mo K_α X-Rays $-\Delta f'$
74	W	11	5	6	6	7.8	1.1
75	Re	11	5	6	6	8.1	1.3
76	Os	12	5	6	6	8.5	1.5
77	Ir	13	5	7	5	8.9	1.8
78	Pt	13	5	7	5	9.3	2.0
79	Au	14	6	8	5	9.8	2.4
80	Hg	15	6	8	5	10	2.8
81	Tl	16	6	8	5	11	3.4
82	Pb	16	7	9	5	11	4.0
83	Bi	17	7	9	5	12	4.8
84	Po	18	8	10	5	12	5.6
85	At	20	9	10	5	10	**
86	Rn	20	9	11	5	10	8*
87	Fr	21	10	11	5	7	8*
88	Ra	23	11	12	5	7	7
89	Ac	24	13	12	5	8	7
90	Th	25	15	13	5	8	7
91	Pa	26	17*	14	5	8	7
92	U	19	19*	15	5	8	8*
93	Np	--	--	15	5	5	--
94	Pu	--	--	16	5	5	--
95	Am	--	--	17	6	5	--
96	Cm	--	--	18	6	5	--

* These values are especially uncertain because of proximity to absorption edges.

** Not calculated.

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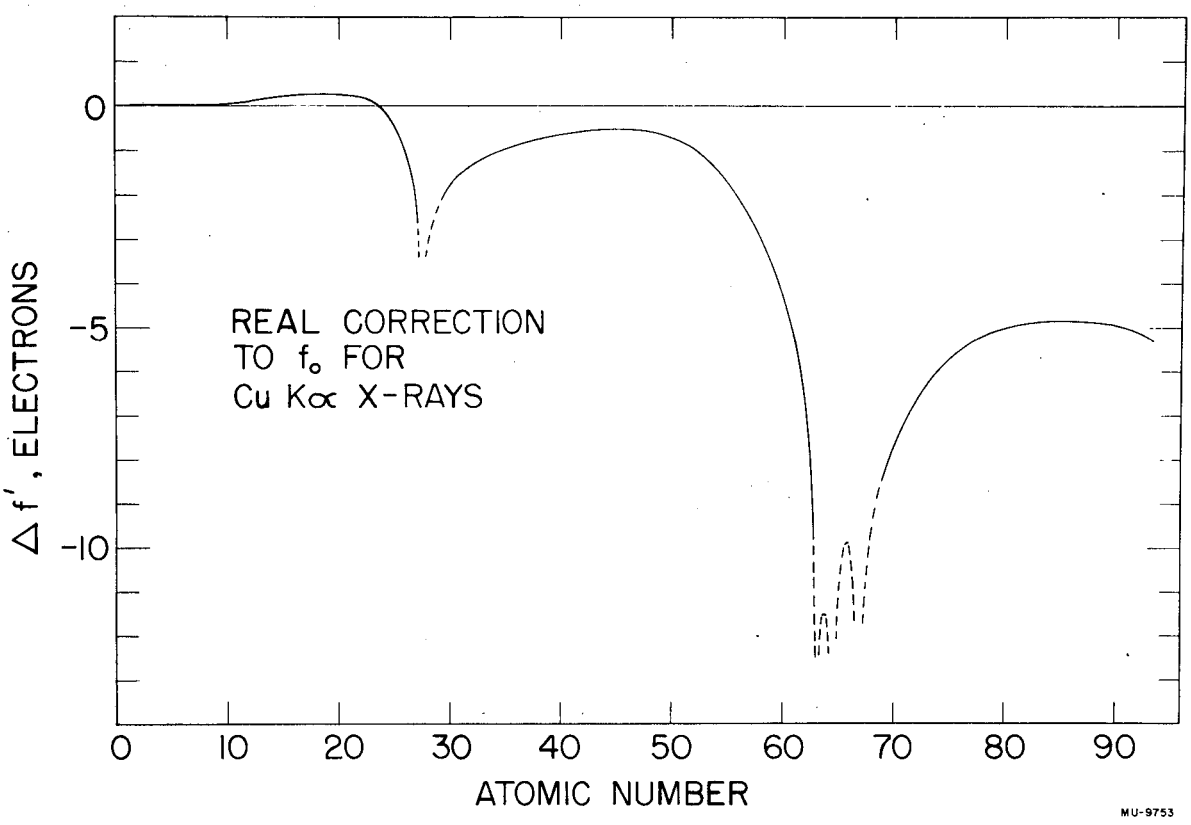

Fig. 1. Real correction to f_o for copper K_α x-rays.

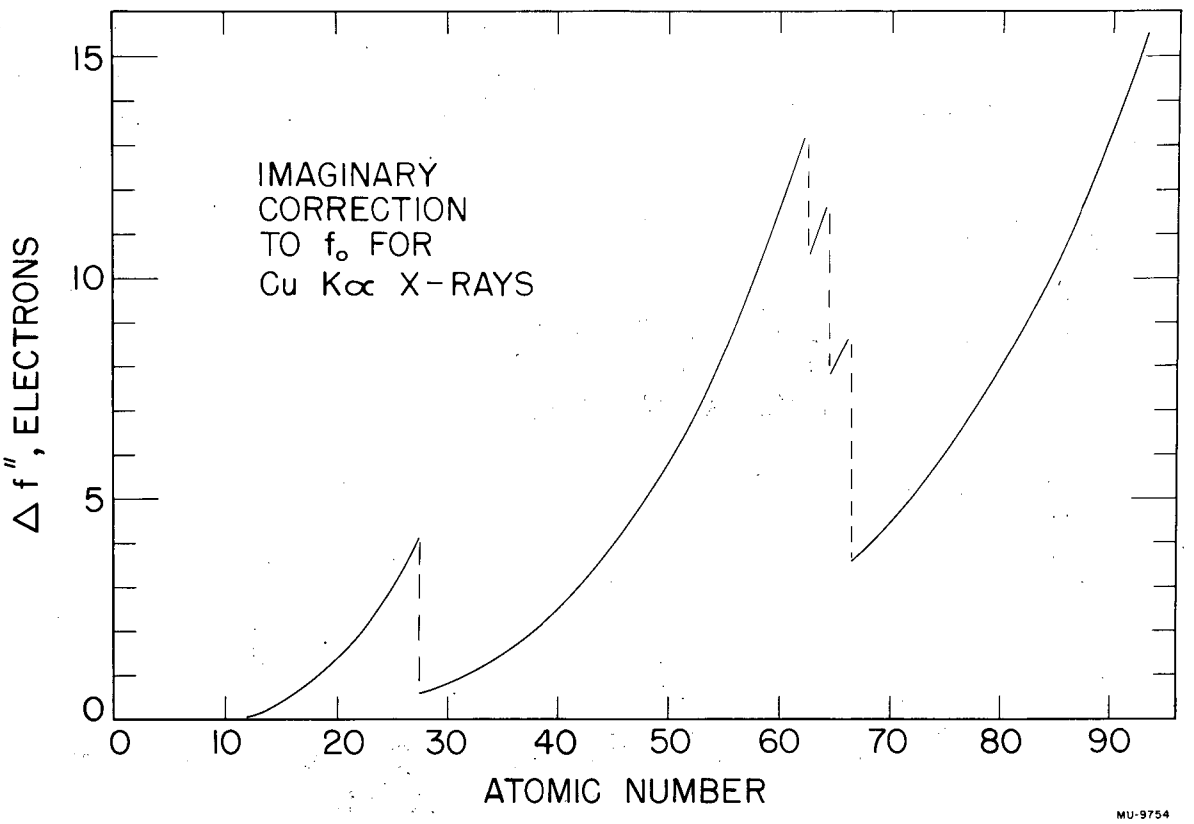

Fig. 2. Imaginary correction to f_o for copper K_α x-rays.