observed in addition to lines of the untransformed b.c.c. phase. The new lines corresponded to a heavily faulted close-packed hexagonal structure in alloys near the Cu–Ga binary axis, gradually changing into a faulted structure showing both the face-centered cubic and close-packed hexagonal characteristics near the Cu–Zn binary axis (Massalski & Barrett, 1957).

In Table 1 are shown lattice parameters of the transformation structure calculated from the 311 reflections of Debye–Scherrer patterns, indexed as f.c.c.

Deformation faulting causes shifts of certain reflections in the f.c.c. Debye–Scherrer pattern (Paterson, 1952) but it was found that in the case of binary Cu–Zn alloys (Massalski & Barrett, 1957) lattice-parameter values could be estimated with reasonable precision using the assumption that the 311 reflection remained practically unshifted by the presence of faults.

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Atomic scattering factors for Mo^+.*

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For the heavier elements the earliest scattering curves were approximated by James & Brindley (1931) with an interpolation method based upon the Thomas–Fermi treatment in which the atomic electron cloud is considered in terms of a degenerate gas. The scattering curves for molybdenum have not been corrected since; however in 1955 accurate self-consistent wave-field data for the molybdenum monovalent positive ion became available through the work of the Hartree school in Cambridge. The present computation of the new scattering curve (Table 1 and Fig. 1) is based upon the self-consistent field data, calculated by Ridley (1955) on the Cambridge E.D.S.A.C. computer.

It was decided to undertake the programming of the calculation of scattering curves from wave-field data in general form, so that other elements could be computed also. The digital computer at C.I.T., an ElectroData Datatron, was utilized for this purpose. The numerical integration of expressions of the form

$$\int_0^\infty \frac{P_j^2(r).\sin 4\pi\sigma r}{4\pi\sigma r}.dr$$

(where $P_j(r)$ is the radially dependent part of the wave function for shell j at distance r (in Bohr units) from the nucleus, and $\sigma = \sin\theta/\lambda$) is carried out by a curve-fitting procedure, the accuracy of which is of the same order as

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Table 1. *Atomic scattering factors for* Mo^+

$\frac{\sin\theta}{\lambda}\times 10^{-8}$ (cm.)	$f(Mo^+)$	$\frac{\sin\theta}{\lambda}\times 10^{-8}$ (cm.)	$f(Mo^+)$	$\frac{\sin\theta}{\lambda}\times 10^{-8}$ (cm.)	$f(Mo^+)$	$\frac{\sin\theta}{\lambda}\times 10^{-8}$ (cm.)	$f(Mo^+)$
0·00	41·00	0·46	22·48	0·92	13·78	1·38	8·43
0·02	40·85	0·48	21·96	0·94	13·48	1·40	8·26
0·04	40·44	0·50	21·47	0·96	13·17	1·42	8·13
0·06	39·77	0·52	21·01	0·98	12·89	1·44	7·98
0·08	38·93	0·54	20·56	1·00	12·59	1·46	7·86
0·10	37·95	0·56	20·14	1·02	12·32	1·48	7·73
0·12	36·90	0·58	19·71	1·04	12·04	1·50	7·62
0·14	35·81	0·60	19·32	1·06	11·76	1·52	7·48
0·16	34·71	0·62	18·92	1·08	11·51	1·54	7·38
0·18	33·62	0·64	18·54	1·10	11·25	1·56	7·26
0·20	32·53	0·66	18·16	1·12	11·01	1·58	7·16
0·22	31·51	0·68	17·80	1·14	10·75	1·60	7·06
0·24	30·52	0·70	17·43	1·16	10·53	1·62	6·98
0·26	29·58	0·72	17·07	1·18	10·30	1·64	6·88
0·28	28·68	0·74	16·73	1·20	10·09	1·66	6·80
0·30	27·83	0·76	16·38	1·22	9·87	1·68	6·71
0·32	27·01	0·78	16·04	1·24	9·67	1·70	6·63
0·34	26·25	0·80	15·70	1·26	9·46	1·72	6·55
0·36	25·55	0·82	15·38	1·28	9·28	1·74	6·47
0·38	24·84	0·84	15·04	1·30	9·10	1·76	6·41
0·40	24·21	0·86	14·71	1·32	8·93	1·78	6·33
0·42	23·59	0·88	14·39	1·34	8·75	1·80	6·26
0·44	23·03	0·90	14·09	1·36	8·59		

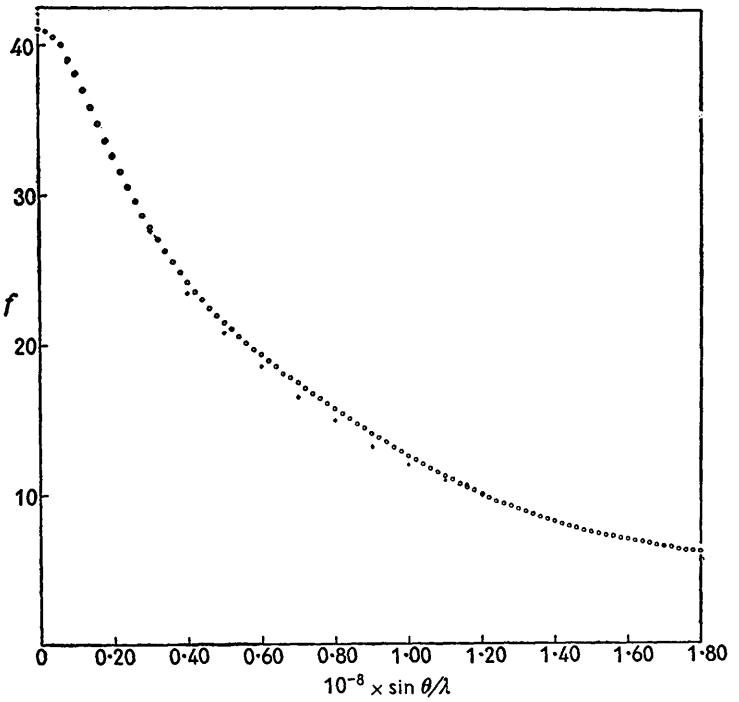

Fig. 1. Atomic scattering factors for Mo^+. Circles: present work; crosses: James & Brindley.

that obtained with Simpson's Rule. This approach has the advantage of better adaptation to computer operation in that it is independent of the use of equal integration intervals. The program developed by us will also take care of difficulties mentioned in the footnote to the paper by Berghuis *et al.* (1955), i.e. the conversion of radial distances given on a logarithmic scale and the conversion of dependent variables of the type $Q(r) = P(r).f(r)$, where $f(r)$ is an exponential function of r. This is achieved by the overlay of a special sub-routine.

In the present case the atomic scattering factors were calculated for Mo^+ at intervals of 0·02 in σ up to $\sigma = 1{\cdot}80$ corresponding approximately to the radius of the Ag K-radiation limiting sphere. In essence the same checking methods were applied as described by Berghuis *et al.* (1955) in their paper.

The total scattering factor was compounded from the different shells, by first calculating the contributions per electron per shell, and then multiplying the value found by the number of electrons in the shell. Since the electron contribution is computed to four decimal places, multiplication with the shell multiplicity factor, reduces the accuracy one decimal place. In summing the contributions of the nine shells, rounding-off errors take care of another decimal place, so that the final f-curve is given to two decimal places. Mo^+ has the following distribution of electrons over the shells:

$$(1s)^2\ (2s)^2\ (2p)^6\ (3s)^2\ (3p)^6\ (3d)^{10}\ (4s)^2\ (4p)^6\ (4d)^5.$$

It has been pointed out by various authors that at larger values of σ the difference in scattering value is insignificant between the element in the ground state and the monovalent ion. It is expected that the influence of the $(5s)^1$ electron would die away near $\sigma = 0{\cdot}35$ and we may therefore safely compare the present values of Mo^+ scattering factors above $\sigma = 0{\cdot}4$ to those of James & Brindley. It can be seen from Fig. 1 that the difference is considerable, and of the general order of 5%, the James–Brindley curve being consistently lower in the region above $\sigma = 0{\cdot}4$.

The self-consistent field data computed by Ridley do not take into account spin-exchange energy or relativistic corrections. It is not expected that such corrections would greatly alter the scattering curve, but they have nevertheless been scheduled for computation and will be reported on at a later date.

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