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Atomic scattering factor for O^{2-}.

By T. SUZUKI, *Institute of Physics, College of General Education, University of Tokyo, Komaba, Meguro-ku, Tokyo, Japan*

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It is well known that the existence of the doubly charged negative oxygen ion in some oxide crystals is a useful working hypothesis, although the free O^{2-} ion is not confirmed experimentally. With the aid of the variational method Yamashita & Kojima (1952) first obtained the $2p$ wave function of the O^{2-} ion in the crystalline state of MgO. They found it possible that the O^{2-} ion can exist there by the stabilizing effects of the mutual interaction of ions. Recently Watson (1958) has calculated the wave functions of the O^{2-} ion in the additive potential wells of +1 and +2 charge by means of the self-consistent method.

Table 1. *f values for* O^{2-}

	f (total)		*f*(2*p*)		
sin θ/λ	+1 well	+2 well	+1 well	+2 well	MgO
0·00	10·000	10·000	1·000	1·000	1·000
0·05	9·491	9·551	0·926	0·937	0·932
0·10	8·357	8·475	0·769	0·789	0·768
0·15	7·027	7·159	0·592	0·616	0·580
0·20	5·802	5·908	0·439	0·459	0·418
0·25	4·789	4·857	0·321	0·334	0·296
0·30	3·994	4·028	0·234	0·241	0·208
0·35	3·383	3·394	0·170	0·173	0·145
0·40	2·918	2·916	0·123	0·124	0·100
0·50	2·298	2·287	0·063	0·062	0·044
0·60	1·938	1·929	0·029	0·028	0·016
0·70	1·721	1·714	0·012	0·010	0·002
0·80	1·578	1·574	0·002	0·001	−0·003
0·90	1·472	1·469	−0·002	−0·003	−0·005
1·00	1·382	1·381	−0·004	−0·004	−0·005
1·10	1·300	1·299	−0·004	−0·005	−0·005
1·20	1·221	1·220	−0·004	−0·004	−0·004
1·30	1·144	1·143	−0·004	−0·004	−0·003

Since the above wave functions are represented in analytical forms and the electron distribution of the O^{2-} ion can be safely assumed to be spherical, the atomic scattering factor of the O^{2-} ion can also be expressed by an analytical formulae. We have thus computed the *f* values of the O^{2-} ion in the +1 and +2 wells using the results of Watson. The scattering factor of a $2p$ electron in MgO has also been calculated on the basis of the wave function of Yamashita & Kojima. The results are summarized in Table 1. The difference in *f* values for the two models of the +1 and +2 wells in our procedure seems to be insignificant. The *f*(2*p*) values of MgO deviate a little from that of the general models of Watson. The values of *f*(total) are reasonable in comparison with the *f* values of the other states of oxygen calculated by Freeman (1959).

The numerical computations were performed by the P–C–1 in the University of Tokyo. The author wishes to express his thanks to Mr M. Tokonami for his kindly help in this computation.

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Notes and News

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International Union of Crystallography

World Directory of Crystallographers

As announced earlier in this journal (see *Acta Cryst.* (1959), **12**, 826) a second edition of the *World Directory of Crystallographers* will be published before the forthcoming Fifth International Congress of the Union in August 1960. Questionnaires were distributed to crystallographers throughout the world, and national lists are now being prepared by Sub-Editors in the various countries.

The *Directory* will contain the names, addresses, and further biographical information concerning crystallographers and all other scientists who in their research make to a great extent use of crystallographic methods. This means that the booklet will also contain the names of a great number of solid-state physicists and chemists who are applying crystallographic and diffraction methods, of many mineralogists and geologists who are studying crystal minerals, *etc.*

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