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**Atomic scattering factor for O<sup>2-</sup>** By MASAYASU TOKONAMI, *Institute for Solid State Physics, University of Tokyo, Azabu, Minato-ku, Tokyo, Japan*

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An isolated O<sup>2-</sup> ion, which is unstable by itself, can be stabilized by a suitable boundary condition. Using the self-consistent field method, Watson (1958) calculated the wave function for O<sup>2-</sup> in a hypothetical potential well due to a spherical distribution of +1 or +2 charge. Suzuki (1960) gave a table of the atomic scattering factor of O<sup>2-</sup> based on Watson's calculation.

On the other hand, Yamashita & Kojima (1952) dealt with the atomic state of oxygen atoms in magnesium oxide crystals. By taking account of exchange energy and electrostatic overlapping energy between the nearest neighbour ions, as well as Madelung energy, it was concluded that the oxygen atoms are in the ionic state O<sup>2-</sup>. On the assumption of spherical symmetry, they calculated the wave function  $\psi_{2p}$  for O<sup>2-</sup> by the variational method, using the  $\psi_{1s}$  and  $\psi_{2s}$  wave functions appropriate to the O<sup>1-</sup> state. Yamashita (1964) has recently refined his calculation on  $\psi_{2p}$ , by adopting the wave functions of  $\psi_{1s}$  and  $\psi_{2s}$  calculated by Watson for O<sup>2-</sup> in the +1 well.

In the present study, a new scattering factor of O<sup>2-</sup> was calculated as a function of  $s = \sin \theta / \lambda$ , using the new wave function of Yamashita. The result obtained is compared with that by Suzuki in Table 1. Values of the former are a little larger than those of the latter in the low angle region. This trend may imply that the oxygen atom shrinks because of repulsion by neighbouring atoms. The new scattering factor may also be used for the state of O<sup>2-</sup> in other crystals.

The values of the new scattering factor shown in Table 1 can be approximated by

$$f(s) = 4.758 \exp(-7.831s^2) + 3.637 \exp(-30.05s^2) + 1.594$$

for Cu  $K\alpha$  range,

$$f(s) = 2.755 \exp(-3.949s^2) + 5.907 \exp(-20.64s^2) + 1.269$$

for Mo  $K\alpha$  range,

as shown in the structure factor tables by Hosoya & Satake (1964).

Recently, Togawa (1965) carried out an absolute intensity measurement of X-ray reflexions from magnesium oxide powders, and found that the observed scattering factor of oxygen showed a better agreement with the new scattering factor. This fact seems to suggest that, for atoms in a crystal, especially for large negative ions, the use of wave functions calculated in the crystalline field or at least under the influence of neighbouring atoms gives better approximation than the wave functions calculated in an isolated state.

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Table 1.  $f$  values for O<sup>2-</sup>

sin $\theta/\lambda$	$f$		sin $\theta/\lambda$	$f$	
	(present work)	(Suzuki*)		(present work)	(Suzuki*)
0.00	10.000	10.000	0.70	1.676	1.721
0.05	9.633	9.491	0.80	1.543	1.578
0.10	8.671	8.357	0.90	1.447	1.472
0.15	7.423	7.027	1.00	1.367	1.382
0.20	6.174	5.802	1.10	1.291	1.300
0.25	5.081	4.789	1.20	1.216	1.221
0.30	4.192	3.994	1.30	1.142	1.144
0.35	3.498	3.383	1.50	0.995	
0.40	2.968	2.918	1.70	0.856	
0.50	2.274	2.298	1.90	0.729	
0.60	1.891	1.938			

\* Values calculated for the +1 well.