SOME PROPERTIES OF CRYSTALLINE ALUMINIUM;
ITS DEBYE TEMPERATURE AND THE PROBABILITY
DENSITY DISTRIBUTION OF THE VALENCE
ELECTRONS, AS DETERMINED BY
X-RAY DIFFRACTION

by


A thesis submitted for the degree of
Doctor of Philosophy in the University of Adelaide

The work described in this thesis was carried out in the Department of Physics between January 1964 and December 1968; except where stated otherwise it is the personal work of the author.

No material contained in this thesis has been submitted for the award of another degree or diploma in this or any other university.

P. E. Dingle
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**Acknowledgements**

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SUMMARY

This thesis describes an accurate X-ray study of crystalline aluminium, and the results obtained from this. A detailed review of the results and the limitations of previous work on aluminium is given.

Single crystals of 4N purity aluminium were grown and several sets of Weissenberg photographic intensities for different crystals were obtained. It was most important for this project that the greatest possible accuracy of measurement was obtained. Accordingly, the intensities were carefully collected and corrected, and similar sets of structure factors are given for the two different crystals. An overall error of 2° is obtained for each set of structure factors.

The effects of extinction in aluminium single crystals are investigated and evaluated. A very accurate value of the Debye temperature for aluminium is obtained from the results, and this is used to find the variation of the Debye temperature with temperature to a precisely known accuracy.
Fourier synthesis for the best experimental structure factors show the ten core electrons to be within the Hartree-Fock L-shell. The small amount of core electron anisotropy which is also shown is claimed to be due to the slight homopolar character of the bonding in solid aluminium.

The valence electron distribution around an atom in the solid is accurately determined for the first time, using the measured structure factors in combination with the Hartree-Fock values in the Fourier integral for an atom. The valence electron density distribution shows that the valence electrons are not free, either in the classical or wave mechanical sense. Although the valence electrons are distributed throughout the volume of the solid, the bulk of the valence electron distribution is confined to a narrower "shell" than in the free atom case.

The valence electron distribution, by its departure from that postulated by the Hartree-Fock free atom model, shows experimentally that Harrison's pseudopotential model has some merit for solid aluminium. A radial wave function which corresponds to the measurements for the valence electron distribution is given.
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