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A new method of determining the atom form factor by high voltage electron diffraction. An application of the effect of vanishing of the second order reflexion.

By D. WATANABE* and R. UYEDA, *Department of Physics, Nagoya University, Nagoya, Japan* and A. FUKUHARA, *Hitachi Central Research Laboratory, Kokubunji, Tokyo, Japan*

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The accelerating voltage E_c at which a second order Kikuchi line vanishes was measured for 220 of iron (305 kV), and 222 of nickel (295 kV) and aluminum (430 kV). A measured value of E_c made it possible to determine accurately the X-ray atom form factor f^X for the first order reflexion assuming those for the second and higher order reflections.

Watanabe, Uyeda & Kogiso (1968) showed that the second order reflexion in electron diffraction vanishes at a certain accelerating voltage E_c owing to dynamical interaction. They observed this effect on Kikuchi lines with a 500 kV electron microscope and predicted that the experimental value of E_c could be used for determining the Fourier coefficient V_1 of the potential for the first order, and thus the corresponding value of the X-ray atom form factor f^X.

The principle of the method is as follows. According to the dynamical theory, the intensity I_2 of the second order reflexion depends not only on the coefficient V_2 of the second order but also on V_1 and V_3, *etc.* I_2 depends, at the same time, on the accelerating voltage due to the relativistic effect. As a result of these effects, I_2 vanishes at a certain voltage E_c. We have, therefore, a relation

$$I_2 = f(V_1, V_2, V_3, \ldots; E_c) = 0 . \qquad (1)$$

In Bethe's second approximation (Bethe, 1928; Uyeda, 1968), for instance, equation (1) is reduced to

$$U_2 - Rd^2 \left\{ U_1^2 - \frac{2}{3} U_1 U_3 - \frac{2}{8} U_2 U_4 - \frac{2}{15} U_3 U_5 \ldots \right\} = 0 , \qquad (1')$$

where $R = 1 + eE_c/(m_0c^2)$, $U_i = 2m_0eV_i/h^2$ and d is the lattice spacing for the first order reflexion. Therefore, if E_c is determined, V_1 can be calculated assuming the values of V_2, V_3, *etc.* The value of V_1 gives the atom form factor for electrons f^e at the first order reflexion and thus also that for X-rays f^X. The error of f^X thus obtained can be roughly estimated by equation (1′) and it can be shown that contributions of δV_2 and δE_c to $\delta f^X/f^X$ are about one fifth of $\delta V_2/V_2$ and less than one fifth of $\delta E_c/E_c$ respectively. Those of δV_3, *etc.* are still less. Since V_2, V_3, *etc.* are known with sufficiently good accuracy, the measurement of E_c enables us to determine f^X very accurately.

In the present study, Kikuchi lines of iron, nickel and aluminum were examined. The values of E_c determined by observation of Kikuchi patterns (Uyeda, Nonoyama & Kogiso, 1965) are given in Table 1. The error of E_c was less than 10 kV. The values of V_i's ($i = 2, \ldots, 6$) were calculated from the theoretical Hartree–Fock values of f^X for the free atoms (Freeman & Watson, 1961; *International Tables for X-ray Crystallography*, 1962). The errors of V_2 estimated from reliable data [Bensch, Witte & Wölfel, 1955; Hosoya & Fukamachi, 1968; Inkinen & Suortti, 1964; Paakari & Suortti, 1967; Sachs, 1967; Wakoh, 1968 (theoretical calculation)] are less than 1% for iron and nickel and less than 2% for aluminum. The values of V_1 were calculated from the measured values of E_c with the use of theoretical V_2, *etc.* by Bethe's second approximation, equation (1′), taking account of eleven beams ($i = -4, -3, \ldots, +6$), and by many-beam theory (Fukuhara, 1966) covering nine beams ($i = -3, -2, \ldots, +5$). The results of both calculations agreed almost exactly. Table 1 shows the results for f^X at the first order reflexion calculated by the many-beam theory, together with other available data for comparison. The estimated errors of f^X are about 0·6% for iron and nickel and 0·9% for aluminum (Table 1), including those arising from the temperature factors assumed

* On leave from the Department of Physics, Tohoku University, Sendai, Japan.

Table 1. *Experimental and theoretical X-ray atom form factors for iron, nickel and aluminum at the first order reflexion*

	Fe	Ni	Al
E_c	305 kV (for 220)	295 kV (for 222)	430 kV (for 222)
Debye temperature Θ (°K)	425	390	395
Temperature factor, B (Å^2)	0·36	0·40	0·85
f^X (present result)	(for 110) 18·34 ± 0·11	(for 111) 20·48 ± 0·12	(for 111) 8·87 ± 0·08
f^X			
Freeman & Watson (1961)	18·51	20·57	8·95
Bensch, Witte & Wölfel (1955)			8·55
Batterman, Chipman & DeMarco (1961)	17·63 ± 0·20		8·63 ± 0·14
Inkinen & Suortti (1964)		20·46 ± 0·13	
Paakari & Suortti (1967)	18·19 ± 0·20		
Hosoya & Fukamachi (1968)	18·44 ± 0·15	20·78 ± 0·26	

(see below). The present values of f^X are smaller than those of Freeman & Watson by 0·9% for iron and aluminum and by 0·5% for nickel.

It should be mentioned here that in equation (1) or (1′) only the systematic interactions are taken into consideration. In the present experiment, great care was taken to avoid the effect of simultaneous reflexions. The effect of weak accidental interactions seems to be negligible, although this effect should be studied in more detail.

The value of f^X determined from the observed value of E_c depends upon the temperature factor, B. In the present analysis, the Debye temperature Θ and the estimated B value at room temperature were assumed as shown in Table 1. The contribution to the error of f^X from that of the assumed B values was estimated to be 0·2%.

The temperature rise of the specimen due to the electron irradiation must be taken into consideration in the analysis. In the present experiment, the temperature rise was proved to be less than 40 °C by changing the intensity of irradiation. The final values of f^X given in Table 1 were corrected for the temperature rise.

Details of analysis and discussion will be published in the near future.

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Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (M. M. Woolfson, Physics Department, University of York, Heslington, York, England). As far as practicable books will be reviewed in a country different from that of publication.

Theory of crystal dislocations. Von F. R. N. NABARRO. 821 Seiten. Oxford: Clarendon Press, 1967. Preis £9·9*s*.

Versetzungen sind einerseits abstrakte Gebilde innerhalb der Elastizitätstheorie, deren mathematischen 'Strukturen' unabhängig von einer unmittelbar praktischen Anwendung studiert werden. Versetzungen sind andererseits inzwischen, z.B. durch Elektronenmikroskopie und Ätzgrübchenverfahren, zu 'anschaulichen' Realitäten geworden, die zum täglichen Handwerkszeug von Physikern, Metallkundlern und Kristallographen gehören. Professor Nabarro hat in langjähriger Arbeit den schier aussichtslos erscheinenden Versuch unternommen, sowohl die abstrakt-mathematischen als auch die physikalischen Aspekte einer allgemeinen Theorie der Versetzungen nach dem derzeitigen Kenntnisstand in einem Buch zusammenzufassen. Nach Meinung des Rezensenten ist dieser Versuch voll geglückt.

Etwa die Hälfte des Buches behandelt die geometrischen Strukturen, die elastischen Spannungen und Energien ruhender und bewegter Versetzungen in verschiedenen mathematischen Näherungen. Die andere Hälfte des Buches befasst sich mit dem Einfluss von Versetzungen auf physikalische Eigenschaften von Kristallen wie z.B. elektrischer Widerstand, Wärmewiderstand, Magnetismus sowie Wechselwirkung mit Punktdefekten. Ein Kapitel referiert speziell über die Beugung von Röntgen-, Elektronen- und Neutronenwellen an Kristallen mit Versetzungen.

Versetzungen haben sich längst von ihren 'physikalischen Eltern', der Plastizität und Verfestigung von Kristallen, emanzipiert. Man erkennt das deutlich daran, dass von diesen beiden, in der Festkörperphysik nach wie vor wichtigen Themen, nur am Rande die Rede ist.

Die Fülle des verarbeiteten Materials, die sehr ausführlich referierte Literatur, sowie die notwendigerweise knappe, aber immer auf das Wesentliche drängende Darstellung lassen erwarten, dass das vorliegende Buch für viele Jahre zu einem Standardbuch für Theoretiker und Experimentatoren werden wird.

M. WILKENS

Max-Planck Institut für Metallforschung
7 *Stuttgart* 1
Azenbergstrasse 12
Deutschland

Structure and properties of solids. By L. SODONKA. Pp. 176. London: Physics Paperbacks (Iliffe Books Ltd.) Price 15 *s*. (U.K. only).

This modestly priced paperback, published in conjunction with the Czechoslovakian Publishers SNTL, covers a wide variety of solid state topics at a brisk pace. An empirical approach at around the level of Dekker's *Solid State Physics* is adopted, though many formulae are merely quoted. There are good descriptive passages, but the cursory references to recent techniques, such as inelastic neutron scattering and the Mössbauer effect, can scarcely illuminate the uninitiated. The book provides fair value for money, but must be regarded as complementary to the orthodox undergraduate Solid State Physics texts rather than as a replacement for them.

J. A. D. MATTHEW

University of York
Heslington
York
England