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Some definitions and units in electron diffraction. By B. DAWSON, P. GOODMAN, A. W. S. JOHNSON, D. F. LYNCH and A. F. MOODIE, *Division of Chemical Physics, CSIRO, P.O. Box* 160, *Clayton, Victoria* 3168, *Australia*

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Changes are advocated in some of the definitions, units and notation current in electron diffraction. The purpose of those changes is to separate descriptions of properties of materials from the experiments intended to measure them, and to exhibit as clearly as possible the relationship between the differing properties of a material accessible in X-ray and electron work.

The purpose of this note is to advocate certain definitions and units in electron diffraction different from those current in *International Tables for X-ray Crystallography* (1962) (I.T.C.). There is no innate novelty in the approach we propose here; indeed we maintain that it is simply the direct one, whereas that in the I.T.C. reflects a series of historical accidents in which (i) structure amplitude is equated to scattering amplitude in the first Born approximation, and (ii) the grouping of the constants deriving from Schrödinger's equation is chosen largely for manipulative convenience. This can tend to confuse a basically straightforward situation. For instance, with these conventions the expression for the expansion of classical potential into a Fourier series includes Planck's constant.

We have been guided by the following considerations: (*a*) Properties of a material should refer directly to the material itself rather than being described in terms of an experiment intended to measure those properties or in terms of an approximation to theory associated with the experiment. (*b*) The relationship between those properties of a material which are accessible respectively to X-ray and electron work should be exhibited as directly as possible. (*c*) Units should be those in general use in such related fields as solid-state physics and chemistry.

In the light of (*a*) our suggestions extend only to the description of N-beam elastic scattering of electrons in the one-body approximation, wherein the wavefunction satisfies a constant-energy one-body Schrödinger equation with relativistically corrected mass and wavelength. This approximation is quite adequate for all current work involving elastic scattering however, or, for that matter, inelastic scattering within the framework of a one-body phenomenological description. The property then of direct interest to us is a potential ϕ, naturally expressed in volts.

This potential is next related to a charge density by Poisson's equation, $\nabla^2\phi = -4\pi(\varrho_{\text{nucl.}} - \varrho_{\text{el.}})$, and the electronic part of this charge density constitutes that property of the material associated with the one-body (though possibly N-beam) X-ray scattering equation.

Consider the electron-diffraction case first. If the material is perfectly crystalline, the potential (*cf.* Fig. 1) can be expanded in the Fourier series,

$$\phi(\mathbf{r}) = \sum_{h} V(\mathbf{h}) \exp\{-2\pi i \mathbf{h} \cdot \mathbf{r}\}, \qquad (1)$$

with the coefficients $V(\mathbf{h})$, the structure amplitudes, having the same units as $\phi(\mathbf{r})$. If the material is in the form of an atom, an atomic scattering factor denoted by script f_p can be defined as the Fourier transform of the potential appropriate to the atom. Ions can be incorporated directly in this definition. If the unit of length is chosen as the Ångström, the units of the atomic scattering factor will then be V Å^3. To the approximation that the potential in the repeat unit of the crystal is the sum of individual atom potentials, we also have

$$V(\mathbf{h}) = \frac{1}{\Omega} \sum_{p} f_p \exp\{2\pi i \mathbf{h} \cdot \mathbf{r}_p\}, \qquad (2)$$

where Ω is the volume of the unit cell and $(\mathbf{r}_p)$ the coordinate of the pth atom. That the volume of the unit cell appears in equation (2) rather than in equation (1), which direct analogy with X-ray work might have suggested, acknowledges firstly the relationship between potential and charge *density*. Further we then avoid the situation where slight differences in composition (which might result in large differences in unit-cell size) would give widely different values for the leading term of equation (1), $V(0,0,0)$. Clearly, we need this constant [as well as the $V(h,k,l)$ values] to relate to a physical property, namely the refractive index, which bears no relation to unit-cell size.

In the X-ray case where the atomic scattering factor f_p is the Fourier transform of the electron density appropriate to the atom, the units for this quantity will be those given in the I.T.C., *viz.* electrons. Further, since chemical formula alone is sufficient to establish the number of electrons in the repeat unit, it is then proper to express the X-ray amplitudes $F(h,k,l)$ in electrons as well. The position is quite different in electron diffraction, however, since chemical formula does not determine inner potential $V(0,0,0)$.

Fig. 1 constitutes a summary of our suggestions, but a few supplementary remarks may clarify the situation. The current I.T.C. basically describes properties of the atom and of the crystal in terms of the first Born approximation. Not only is this at variance with consideration (*a*), but it suggests, quite erroneously, that this approximation has a wide range of validity in the scattering of electrons by solids. If the scattering amplitude in the first Born approximation should be required, it is only necessary to multiply $V(\mathbf{h})$ by $i\sigma H$ (where H is the thickness of the crystal,

Table 1. *Variation of* σ *with accelerating voltage*

W (kV)	σ (V Å)$^{-1}$
20	0·001864
50	0·001228
75	0·001035
80	0·001009
100	0·000924
200	0·000729
500	0·000587
1000	0·000539
2000	0·000518

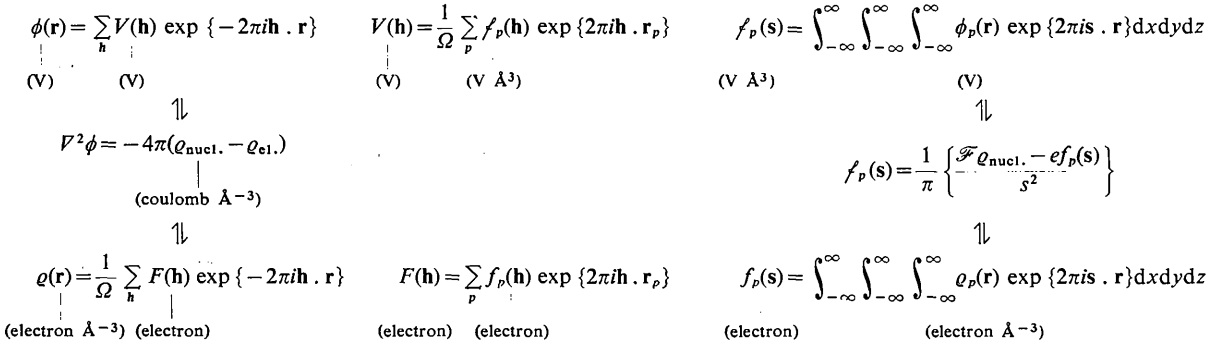

Fig. 1. Relationship between X-ray and electron structure amplitudes and atomic scattering factors. $\varrho_{\text{el.}}$ and $\varrho_{\text{nucl.}}$ are charge densities with units coulomb Å^{-3}, while ϱ_p and $\varrho(\mathbf{r})$ are electron densities with units electron Å^{-3}.

$$\sigma = \frac{\pi}{W\lambda} \cdot \frac{2}{1 + \left(1 - \frac{v^2}{c^2}\right)^{1/2}},$$

W is the accelerating voltage, and the other symbols have their conventional meaning.) Since the dimensionless quantity $\sigma V(\mathbf{h})H$ is important in all scattering calculations, some typical values for σ are given in Table 1.

The direct relationship between the atomic scattering factors for electrons and X-rays is obtained by taking Fourier transforms of both sides of Poisson's equation and applying standard boundary conditions at infinity to give

$$\mathscr{F}\phi = f_p(\mathbf{s}) = \frac{1}{\pi}\left\{\frac{\mathscr{F}\varrho_{\text{nucl.}} - e f_p(\mathbf{s})}{s^2}\right\},$$

where $s = 2 \sin\theta/\lambda$, e is the electronic charge, and $f_p(\mathbf{s})$ the X-ray atomic scattering factor.

Reference

International Tables for X-ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press.

Acta Cryst. (1973). A**29**, 298

Erratum to: *n*-Beam lattice images. I. Experimental and computed images from $W_4Nb_{26}O_{77}$.

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Corrections are given to Allpress, Hewatt, Moodie & Sanders [*Acta Cryst.* (1972). A**28**, 528–536].

The following corrections to Allpress, Hewatt, Moodie & Sanders (1972) are given.

1. Page 529, equation (2) and next line should read:

$$U_{n+1} = U_n \exp[+i2\pi\zeta(h,k)\Delta z] * Q_{n+1} \qquad (2)$$

where $\zeta(h,k) = -(u^2+v^2)\lambda/2$ is the excitation error for

2. Page 530, column one, fifth line from the bottom should read:

tude of the diffraction pattern with $\exp\{-i\pi\lambda\varepsilon(u^2+v^2)\}$, (u,v) being the reciprocal lattice coordinates of the appropriate reflexions.

3. Page 531, column two, line one should read:

$C * \mathscr{S}$ and $\overline{C\varrho_p} = C\varrho_p * \mathscr{S}$, where $\mathscr{S}$ is the shape transform of

4. Page 535, column one line 13 should read:

$I_0 = (\bar{C}^2 + \bar{S}^2)$; *i.e.* at the Gaussian focus, the contrast

Reference

ALLPRESS, J. G., HEWATT, E. A., MOODIE, A. F. & SANDERS, J. V. (1972). *Acta Cryst.* A**28**, 528–536.

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