

$$\begin{array}{ccccc}
 \phi(\mathbf{r}) = \sum_{\mathbf{h}} V(\mathbf{h}) \exp \{-2\pi i \mathbf{h} \cdot \mathbf{r}\} & V(\mathbf{h}) = \frac{1}{\Omega} \sum_{\mathbf{p}} f_p(\mathbf{h}) \exp \{2\pi i \mathbf{h} \cdot \mathbf{r}_p\} & f_p(\mathbf{s}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi_p(\mathbf{r}) \exp \{2\pi i \mathbf{s} \cdot \mathbf{r}\} dx dy dz \\
 \text{(V)} & \text{(V)} & \text{(V } \text{\AA}^3) & & \text{(V)} \\
 & \Downarrow & & & \Downarrow \\
 \nabla^2 \phi = -4\pi(\rho_{\text{nuc1.}} - \rho_{\text{el.}}) & & & & f_p(\mathbf{s}) = \frac{1}{\pi} \left\{ \frac{\mathcal{F} \rho_{\text{nuc1.}} - e f_p(\mathbf{s})}{s^2} \right\} \\
 & \text{(coulomb } \text{\AA}^{-3}) & & & \Downarrow \\
 \rho(\mathbf{r}) = \frac{1}{\Omega} \sum_{\mathbf{h}} F(\mathbf{h}) \exp \{-2\pi i \mathbf{h} \cdot \mathbf{r}\} & F(\mathbf{h}) = \sum_{\mathbf{p}} f_p(\mathbf{h}) \exp \{2\pi i \mathbf{h} \cdot \mathbf{r}_p\} & f_p(\mathbf{s}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho_p(\mathbf{r}) \exp \{2\pi i \mathbf{s} \cdot \mathbf{r}\} dx dy dz \\
 \text{(electron } \text{\AA}^{-3}) & \text{(electron)} & \text{(electron)} & & \text{(electron } \text{\AA}^{-3})
 \end{array}$$

Fig. 1. Relationship between X-ray and electron structure amplitudes and atomic scattering factors. $\rho_{\text{el.}}$ and $\rho_{\text{nuc1.}}$ are charge densities with units coulomb \AA^{-3} , while ρ_p and $\rho(\mathbf{r})$ are electron densities with units electron \AA^{-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

$$\mathcal{F} \phi = f_p(\mathbf{s}) = \frac{1}{\pi} \left\{ \frac{\mathcal{F} \rho_{\text{nuc1.}} - e f_p(\mathbf{s})}{s^2} \right\},$$

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 $W_4\text{Nb}_{26}\text{O}_{77}$. By J. G. ALLPRESS, ELIZABETH A. HEWATT, A. F. MOODIE and J. V. SANDERS, *Division of Chemical Physics, CSIRO, P.O. Box 160, Clayton, Victoria, Australia 3168**

(Received 7 August 1973; accepted 8 August 1973)

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:

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

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:

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

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

$I_0 = (\overline{C}^2 + \overline{S}^2)$; 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.

* All correspondence to be addressed to The Chief at this address.