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4.3. Electron diffraction

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4.3.1. Scattering factors for the diffraction of electrons by crystalline solids (By J. M. Cowley)

4.3.1.1. *Elastic scattering from a perfect crystal*

The most important interaction of electrons with crystalline matter is the interaction with the electrostatic potential field. The scattering into sharp, Bragg reflections is considered in terms of the interaction of an incident plane wave with a time-independent, averaged, periodic potential field which may be written

$$\varphi(\mathbf{r}) = \frac{1}{\Omega}\sum_{\mathbf{h}} V(\mathbf{h})\exp\{-2\pi i\mathbf{h}\cdot\mathbf{r}\}, \qquad (4.3.1.1)$$

where Ω is the unit-cell volume and the Fourier coefficients, $V(\mathbf{h})$, may be referred to as the structure amplitudes corresponding to the reciprocal-lattice vectors $\mathbf{h}$. In conformity with the crystallographic sign convention used thoughout this volume [see also Volume B (*IT* B, 1992)], we choose a free-electron approximation for the incident electron beam of the form $\exp(-i\mathbf{k}\cdot\mathbf{r})$ and the interaction is represented by inserting the potential (4.3.1.1) in the Schrödinger wave equation

$$\nabla^2\psi(r) + 2k\sigma\{E + \varphi(r)\}\psi(r) = 0, \qquad (4.3.1.2)$$

where eE is the kinetic energy of the incident beam, $k\,(= 2\pi/\lambda)$ is the magnitude of the wavevector for the incident electrons, and σ is an 'interaction constant' defined by

$$\sigma = 2\pi me\lambda/h^2, \qquad (4.3.1.3)$$

where h is Planck's constant. Relativistic values of m and λ are assumed (see Subsection 4.3.1.4).

The solution of equation (4.3.1.2), subject to the boundary conditions imposed by the need to fit the waves in the crystal with the incoming and outgoing waves in vacuum at the crystal surfaces, then allows the directions and amplitudes of the diffracted beams to be obtained in terms of the crystal periodicities and the Fourier coefficients, $V(\mathbf{h})$, of $\varphi(\mathbf{r})$ by the eigenvalue or Bloch-wave method (Bethe, 1928).

Alternatively, the scattered amplitudes may be obtained from the integral form of (4.3.1.2),

$$\psi(\mathbf{r}) = \exp\{-i\mathbf{k}_0\cdot\mathbf{r}\} + K\int \frac{\exp\{-ik|\mathbf{r}-\mathbf{r}'|\}}{|\mathbf{r}-\mathbf{r}'|}\varphi(\mathbf{r}')\psi(\mathbf{r}')\,\mathrm{d}\tau_{\mathbf{r}'}, \qquad (4.3.1.4)$$

where $\exp\{-i\mathbf{k}_0\cdot\mathbf{r}\}$ represents the incident beam, $K = \sigma/\lambda$, and the integral is taken over the space of the variable, $\mathbf{r}'$. An iterative solution of (4.3.1.4) leads to the Born series,

$$\psi = \psi_0 + \psi_1 + \psi_2 + \ldots,$$

where

$$\psi_0 = \exp\{-i\mathbf{k}_0\cdot\mathbf{r}\}$$

and

$$\psi_n(\mathbf{r}) = K\int \frac{\exp\{-ik|\mathbf{r}-\mathbf{r}'|\}}{|\mathbf{r}-\mathbf{r}'|}\varphi(\mathbf{r}')\psi_{n-1}(\mathbf{r}')\,\mathrm{d}\tau_{\mathbf{r}'}, \qquad (4.3.1.5)$$

for $n \geq 1$. Terms of the series for $n = 1, 2, \ldots$ may be considered to represent the contributions from single, double and multiple scattering of the incident electron beam. This method has been applied to the diffraction from crystals by Fujiwara (1959).

A further formulation of the scattering problem in integral form is that due to Cowley & Moodie (1957) who considered the progressive modification of an incident plane wave as it passed through successive thin slices of a crystal. The effect of the nth slice on the incident electron wave is that of a phase-grating so that the wavefunction is modified by multiplication by a transmission function,

$$q_n(xy) = \exp\{-i\sigma\varphi_n(xy)\}, \qquad (4.3.1.6)$$

where $\varphi_n(xy)$ is the projection of the potential distribution within the slice in the direction of the incident beam, taken to be the z axis;

$$\varphi_n(x, y) = \int\limits_{z_n}^{z_n+\Delta z} \varphi(x, y, z)\,\mathrm{d}z. \qquad (4.3.1.7)$$

Propagation of the wave between the centres of slices is represented by convolution with a propagation function, $p(xy)$, so that the wave entering the $(n+1)$th slice may be written

$$\psi_{n+1}(xy) = [\psi_n(xy)\cdot q_n(xy)] * p_n(xy). \qquad (4.3.1.8)$$

In the small-angle approximation, the function $p_n(xy)$ is given by the usual Fresnel diffraction theory as

$$p(xy) = (i/\lambda\Delta z)\exp\{-ik(x^2 + y^2)/2\Delta z\}. \qquad (4.3.1.9)$$

In the limit that the slice thickness, Δz, tends to zero, the iteration of (4.3.1.8) gives an exact account of the diffraction by the crystal.

On the basis of the above-mentioned and other related formulations of the diffraction problem, several computing methods have been devised for calculation of the amplitudes and intensities of the many diffracted beams of appreciable intensity that may emerge simultaneously from a crystal (see Section 4.3.6). In this way, a degree of accuracy may be achieved in the calculation of the intensities of spots in diffraction patterns or of the contrast in electron-microscope images of crystals (Section 4.3.8).

4.3.1.2. *Atomic scattering factors*

All such calculations require a knowledge of the potential distribution, $\varphi(\mathbf{r})$, or its Fourier coefficients, $V(\mathbf{h})$. It is usually convenient to express the potential distribution in terms of the sum of contributions of individual atoms centred at the positions $\mathbf{r} = \mathbf{r}_i$. Thus:

$$\varphi(\mathbf{r}) = \sum_i \varphi_i(\mathbf{r} - \mathbf{r}_i) \qquad (4.3.1.10)$$

or, in terms of the Fourier transforms, V_i, of the $\varphi_i(\mathbf{r})$

$$V(\mathbf{h}) = \sum_i V_i(\mathbf{h})\exp\{+2\pi i\mathbf{h}\cdot\mathbf{r}_i\}. \qquad (4.3.1.11)$$

As a first approximation, the functions $\varphi_i(\mathbf{r})$ may be identified with the potential distributions for individual, isolated atoms or ions, with the usual spreading due to thermal motion. The interatomic binding and the interactions of ions that are thereby neglected may have important effects on diffraction intensities in some cases.

In this approximation, the Fourier transforms for individual atoms may be written

$$V_i(s) = f_i^B(s)/K, \tag{4.3.1.12}$$

where $s = 4\pi\lambda^{-1}\sin\theta = |\mathbf{k} - \mathbf{k}_0|$ and the f^B are the Born electron scattering amplitudes, as conventionally defined, in units of Å. Here θ is half the scattering angle and, again, $K = \sigma/\lambda$. Some values of $f^B(s)$ listed in the accompanying Tables 4.3.1.1 and 4.3.1.2 are obtained from the atomic potentials $\varphi_0(\mathbf{r})$ for isolated, spherically symmetrical atoms or ions by the relation

$$f^B(s) = 4\pi K \int\limits_0^\infty r^2\varphi(r)\frac{\sin sr}{sr}\,\mathrm{d}r. \tag{4.3.1.13}$$

By the use of Poisson's equation relating the potential and charge-density distributions, it is possible to derive the Mott–Bethe formula for $f^B(s)$ in terms of the atomic scattering factors for X-rays, $f_x(s)$:

$$f^B(s) = 2\pi\frac{me^2}{h^2\varepsilon_0}\{Z - f_x(s)\}/s^2, \tag{4.3.1.14}$$

where ε_0 is the permittivity of vacuum, or

$$f^B(s) = 0.023934\,\lambda^2\{Z - f_x(s)\}/\sin^2\theta \tag{4.3.1.15}$$

[for λ in Å, $f^B(s)$ in Å, and $f_x(s)$ in electron units]. This was used for the other listed $f^B(s)$ values.

4.3.1.3. *Approximations of restricted validity*

(*a*) *Kinematical approximation.* In the limiting case of a vanishingly weak interaction of the incident electrons with the scattering potential of the crystal, the Born series (4.3.1.5) may be terminated at the term ψ_1, corresponding to single scattering. Then the diffracted wave is given for a potential $\varphi(r)$ as $\psi(\mathbf{s})(\exp -ikR)/R$, with

$$\psi(\mathbf{s}) = K\int\varphi(\mathbf{r})\exp\{i[\mathbf{r}\cdot\mathbf{s}]\}\,\mathrm{d}\tau_{\mathbf{r}}, \tag{4.3.1.16}$$

where R is the distance to the point of observation. For a periodic potential, $\varphi(\mathbf{r})$, the scattering amplitude for the $\mathbf{h}$ beam is

$$\psi(\mathbf{h}) = NK\int\varphi(\mathbf{r})\exp\{2\pi i\mathbf{h}\cdot\mathbf{r}\}\,\mathrm{d}\tau_{\mathbf{r}}, \tag{4.3.1.17}$$

where the integral is taken over one unit cell and N is the number of unit cells. From (4.3.1.16), it then follows that the scattering amplitude $\psi(\mathbf{h})$ is proportional to the structure amplitude, $V(\mathbf{h})$;

$$\psi(\mathbf{h}) = NKV(h) \tag{4.3.1.18}$$

$$= NK\sum_i f_{\mathrm{el},i}(\mathbf{h})\exp\{2\pi i\mathbf{h}\cdot\mathbf{r}_i\}. \tag{4.3.1.19}$$

The intensity of the $\mathbf{h}$ diffracted beam is then proportional to $\psi(\mathbf{h})\psi^*(\mathbf{h})$, and so to $|V(\mathbf{h})|^2$.

Similarly, we may write the differential scattering cross section for the scattering from a single isolated atom as

$$|f^B(s)|^2 = K^2|V_i(s)|^2. \tag{4.3.1.20}$$

(*b*) *Two-beam approximation.* For some specific orientations of a crystal of relatively simple structure, the incident beam may be close to the Bragg angle for a strong, inner reflection but not for any other reflection. Then the approximation may be made that only those beams with indices $\mathbf{0}$ and $\mathbf{h}$ have appreciable intensity. The intensities of these beams for a parallel-sided, plate-shaped, centrosymmetric crystal are given in MacGillary's (1940) development of the theory of Bethe (1928) as

$$I(\mathbf{h}) = I_0\{\sigma V(\mathbf{h})\}^2\frac{\sin^2\{\pi t(\zeta_{\mathbf{h}}^2 + \xi_{\mathbf{h}}^{-2})^{1/2}\}}{\pi^2(\zeta_{\mathbf{h}}^2 + \xi_{\mathbf{h}}^{-2})} \tag{4.3.1.21}$$

and $I(\mathbf{0}) = I_0 - I(\mathbf{h})$, where I_0 is the incident-beam intensity, t is the crystal thickness, $\xi_{\mathbf{h}}$ is the extinction distance given by $\xi_{\mathbf{h}} = \pi/\sigma V(\mathbf{h})$, and $\zeta_{\mathbf{h}}$ is the excitation error which measures the distance of the reciprocal-lattice point $\mathbf{h}$ from the Ewald sphere.

A formula due to Blackman (1939), obtained by integrating (4.3.1.21) over $\xi_{\mathbf{h}}$, provides a useful first approximation for the intensities of ring or arc patterns given by polycrystalline material (see Section 2.5.2).

(*c*) *Phase-grating approximations.* For extremely thin crystals, the scattering can be approximated by that of a two-dimensional potential distribution given by projection of the three-dimensional distribution in the beam direction. Then, by analogy with (4.3.1.6), the emerging wave is

$$\psi(xy) = \exp\{-i\sigma\varphi(xy)\} \tag{4.3.1.22}$$

when

$$\varphi(xy) = \int\limits_0^H \varphi(xyz)\,\mathrm{d}z \tag{4.3.1.23}$$

and the diffraction amplitudes are given by the Fourier transform of this expression.

For thicker crystals, this approximation applies in the limit of very high electron-accelerating voltage, with the value of σ appropriate for the Compton wavelength, $\lambda = 0.024262$ Å, *viz* $\sigma = 0.0005068$.

It may be noted that for the special case of a single layer of atoms the solution of the wave equations (4.3.1.2) or (4.3.1.4), with the real potential (4.3.1.1) inserted, leads to a form equivalent to the Moliere high-energy approximation for the scattering by single atoms, namely

$$KV(s) = -\frac{i}{\lambda}\int\limits_{-\infty}^{\infty}\{\exp[-i\sigma\varphi(\boldsymbol{\rho})] - 1\}\exp\{i\boldsymbol{\rho}\cdot\mathbf{s}\}\,\mathrm{d}^2\boldsymbol{\rho}, \tag{4.3.1.24}$$

where $\boldsymbol{\rho}$ is a two-dimensional vector with components x, y, and

$$\varphi(\boldsymbol{\rho}) = \int\limits_{-\infty}^{\infty}\varphi(\boldsymbol{\rho}, z)\,\mathrm{d}z, \tag{4.3.1.25}$$

and this, in the low-angle approximation, is the same as (4.3.1.23). Then the scattered amplitude can be considered as made up from contributions from individual atoms that are equal (apart from bonding effects) to the complex atomic scattering amplitudes tabulated in connection with the diffraction of electrons by gases.

4.3.1.4. *Relativistic effects*

It has been shown by Fujiwara (1961) that, at least for electron energies up to 1 MeV or so, the relativistic effects on diffraction amplitudes and geometry are adequately described by the use of relativisitically corrected values for the mass and wavelength of the electrons;

$$m = m_0(1 - \beta^2)^{-1/2} \tag{4.3.1.26}$$

$$\lambda = h\bigg/\left[2em_0E\left(1 + \frac{eE}{2m_0c^2}\right)\right]^{1/2} = \lambda_c\frac{(1 - \beta^2)^{1/2}}{\beta}$$

$$= 12.2639/(E + 0.97845\times10^{-6}E^2)^{1/2}, \tag{4.3.1.27}$$

where m_0 is the rest mass, λ_c is the Compton wavelength $\beta = v/c$, and λ is given in Å if E is in volts. Consequently, σ varies with the incident electron energy as $[1 + h^2/m_0^2c^2\lambda^2)]^{1/2}$, or

$$\sigma = 2\pi/\{\lambda E[1 + (1 - \beta^2)^{1/2}]\}.$$

Values of $\lambda, \lambda^{-1}, m/m_0, \beta = v/c$, and σ are listed for various values of the accelerating voltage, E, in Table 4.3.2.1 with λ in Å and E in volts.

4.3.1.5. *Absorption effects*

Any scattering process, whether elastic or inelastic, which removes energy from the set of diffracted beams being considered, may be said to constitute an absorption process. For example, for a measurement of the intensities of the elastically scattered, sharp Bragg reflections from a crystal, any process which gives diffuse background scattering or results in a detectable loss of energy gives rise to absorption.

The diffracted amplitudes in such cases may be calculated, at least as a first approximation, in terms of a complex potential, $\varphi_c(\mathbf{r})$, containing an imaginary part $\varphi_i(r)$ due to an 'absorption function' and a small added real part $\Delta\varphi(r)$. Then under the crystallographic sign convention, $\varphi_c(r) = \varphi(r) - i\varphi_i(r) + \Delta\varphi(r)$. Correspondingly, for a centrosymmetric crystal, the structure amplitude becomes complex and may be written

$$V(\mathbf{h}) = V_0(\mathbf{h}) - iV'(\mathbf{h}) + V''(\mathbf{h}). \qquad (4.3.1.28)$$

Under the appropriate conditions of observation, important contributions to the imaginary and real additions to the structure amplitudes may be given by the excitation of phonons, plasmons, or electron transitions, or by diffuse scattering due to crystal defects or disorder.

The additional terms $iV'(\mathbf{h})$ and $V''(\mathbf{h})$, however, are not invariant properties of the crystal structure but depend on the conditions of the diffraction experiment, such as the accelerating voltage and orientation of the incident beam, the aperture or resolution of the recording system, and the use of energy filtering or discrimination. In spite of this, it may often be convenient to treat them as being produced by phenomenological complex potentials, defined for a limited range of experimental conditions.

4.3.1.6. *Tables of atomic scattering amplitudes for electrons*

Tables 4.3.1.1 and 4.3.1.2 list values of $f^B(s)$ in Å for all neutral atoms and most chemically significant ions, respectively. The values have been given by Doyle & Turner (1968) for several cases, denoted by RHF using the relativistic Hartree–Fock atomic potentials of Coulthard (1967). For all other atoms and ions, $f^B(s)$ has been found using the Mott–Bethe formula [equation (4.3.1.15)] for $s \neq 0$, and the X-ray scattering factors of Table 2.2A of *IT* IV (1974). Thus all other neutral atoms except hydrogen are based on the relativistic Hartree–Fock wavefunctions of Mann (1968). These are designated by *RHF. For H and for ions below Rb, denoted by HF, $f^B(s)$ is ultimately based on the nonrelativistic Hartree–Fock wavefunctions of Mann (1968). For ions above Rb, denoted by *DS, modified relativistic Dirac–Slater wavefunctions calculated by Cromer & Waber (1974) are used.

For low values of s, the Mott formula becomes less accurate, since $[Z - f_x(s)]$ tends to zero with s for neutral atoms. Except for the RHF atoms, $f^B(s)$ for s from 0.01 to 0.03 are omitted in Table 4.3.1.1 and for s from 0.04 to 0.11, only two decimal places are given. $f^B(s)$ is then accurate to the figure quoted. For these atoms, $f^B(0)$ was found using the formula given by Ibers (1958):

$$f^B(0) = \frac{4\pi me^2}{3h^2} Z\langle r^2\rangle, \qquad (4.3.1.29)$$

where $\langle r^2\rangle$ is the mean-square atomic radius.

For ionized atoms, $f_{\rm el}(0) = \pm\infty$. The values listed at $s = 0$ in Table 4.3.1.2 for RHF atoms were calculated by Doyle & Turner (1968) with $\varphi(r)$ in equation (4.3.1.13) replaced by $\varphi'(\mathbf{r})$, where

$$\varphi'(\mathbf{r}) = \varphi(\mathbf{r}) - e\Delta Z/r. \qquad (4.3.1.30)$$

Here, ΔZ is the ionic charge. This approach omits the Coulomb field due to the excess or deficiency of charge on the nucleus. With the use of these values, the structure factor for forward scattering by a neutral unit cell containing ions may be found in the conventional way. Similar values are not available for other ions because the atomic potential data are lacking.

For computer applications, numerical approximations to the $f(s)$ of these tables have been given by Doyle & Turner (1968) as sums of Gaussians for the range $s = 0$ to 2 Å^{-1}. An alternative is to make Gaussian fits to X-ray scattering factors, then use the Mott formula to derive electron scattering factors. As discussed by Peng & Cowley (1988), this practice may lead to problems for small values of s. An additional problem occurs in high-resolution electron-microscopy (HREM) image-simulation programs, where it is usually necessary to have electron scattering factors for the range 0 to 6 Å^{-1}. Fox, O'Keefe & Tabbernor (1989) point out that extrapolation of the Gaussian fits of Doyle & Turner (1968) to values past 2 Å^{-1} can be highly inaccurate. For the range of s from 2 to 6 Å^{-1}, Fox *et al.* have used sums of polynomials to make accurate fits to the X-ray scattering factors of Doyle & Turner (1968) for many elements (Section 6.1.1), and electron scattering factors can be generated from these data by use of the Mott formula.

Recently, Rez, Rez & Grant (1994) have published new tables of X-ray scattering factors obtained using a multiconfiguration Dirac–Fock code and two parameterizations in terms of four Gaussians, one of higher accuracy over the range of about 2 Å^{-1} and the other of lower accuracy over the extended range of about 6 Å^{-1}. These authors suggest that electron scattering factors may best be obtained from these X-ray scattering factors by using the Mott formula. They provide a table of values for the electron scattering factor values for zero scattering angle, $f_{\rm el}(0)$, for many elements and ions, which may be of value for the calculation of mean inner potentials.

4.3.1.7. *Use of Tables 4.3.1.1 and 4.3.1.2*

In order to calculate the Fourier coefficients $V(\mathbf{h})$ of the potential distribution $\varphi(\mathbf{r})$, for insertion in the formulae used to calculate intensities [such as (4.3.1.6), (4.3.1.20), (4.3.1.21)], or in the numerical methods for dynamical diffraction calculations, use

$$V(\mathbf{h})(\text{in volts}) = 47.87801\Phi(\mathbf{h})/\Omega, \qquad (4.3.1.31)$$

where

$$\Phi(\mathbf{h}) = \sum_i f_i \exp\{2\pi i\, \mathbf{h}\cdot\mathbf{r}_i\}. \qquad (4.3.1.32)$$

The f_i values are obtained from Tables 4.3.1.1 and 4.3.1.2, and Ω is the unit-cell volume in Å^3. The $V(\mathbf{h})$ and the f_i tabulated are properties of the crystal structure and the isolated atoms, respectively, and are independent of the particular scattering theory assumed.

Expressions for the calculation of intensities in the kinematical approximation are given for powder patterns and oblique texture patterns in Section 2.5.3, and for thin crystal plates in Section 2.5.1 of Volume B (*IT* B, 1992). Since the formulas for kinematical scattering, such as (4.3.1.19) and (4.3.1.20), include the parameter $K = \sigma/\lambda$, which varies with the energy of the electron beam through relativistic effects, it may be considered that the electron scattering factors for kinematical calculations should be multiplied by relativistic factors.

For high-energy electrons, the relativistic variations of the electron mass, the electron wavelength and the interaction constant, σ, become significant. The relations are

$$\begin{aligned} m &= m_0(1-\beta^2)^{-1/2}, \\ \lambda &= h\left[2em_0E\left(1+\frac{eE}{2m_0c^2}\right)\right]^{-1/2} \\ &= \lambda_c\frac{(1-\beta^2)^{1/2}}{\beta}, \end{aligned} \qquad (4.3.1.33)$$

where m_0 is the rest mass, λ_c is the Compton wavelength, h/m_0c, and $\beta = v/c$. Consequently, σ varies with the incident electron energy as

$$\begin{aligned} \sigma &= 2\pi/\{\lambda E[1+(1-\beta^2)^{1/2}]\} \\ &= 2\pi e/hc\beta. \end{aligned} \qquad (4.3.1.34)$$

For the calculation of intensities in the kinematical approximation, the values of $f^B(s)$ listed in Tables 4.3.1.1 and 4.3.1.2, which were calculated using m_0, must be multiplied by $m/m_0 = (1-\beta^2)^{-1/2}$ for electrons of velocity v. Values of λ, $1/\lambda$, m/m_0, $\beta = v/c$, and σ are listed for various values of the accelerating voltage, E, in Table 4.3.2.1.

4.3.2. Parameterizations of electron atomic scattering factors (By J. M. Cowley, L. M. Peng, G. Ren, S. L. Dudarev, and M. J. Whelan)

For computer applications, numerical approximations to the $f(s)$ of Tables 4.3.1.1 or 4.3.1.2 are usually preferred and various approximations as sums of Gaussians have been proposed. The initial Gaussian fits were given by Doyle & Turner (1968) for the range $s = 0$ to $2\,\text{Å}^{-1}$. However, for some purposes, as in the image-simulation programs for high-resolution electron microscopy, atomic scattering factors are needed for higher s values, up to $6\,\text{Å}^{-1}$, and, as pointed out by Fox, O'Keefe & Tabbernor (1989), extrapolation of the Gaussian fits of Doyle & Turner to values above $2\,\text{Å}^{-1}$ can be highly inaccurate.

An alternative approach to obtaining numerical values for the electron scattering factors is to make use of the polynomial fits to X-ray scattering factors of Fox *et al.* or the more recent tables of X-ray scattering factors produced by Rez, Rez & Grant (1994), who used a multiconfiguration Dirac–Fock code and two parameterizations in terms of four Gaussians, one of higher accuracy over the range of about $2\,\text{Å}^{-1}$ and the other of lower accuracy over the extended range of about $6\,\text{Å}^{-1}$. The electron scattering factors may then be derived from the X-ray scattering factors by use of the Mott formula (4.3.1.14). For small angles of scattering, the determination of electron scattering factors in this way may give problems, since the X-ray scattering factor tends to the atomic number, and both the numerator and denominator of (4.3.1.14) tend to zero. However, the electron scattering factor may be determined for zero scattering angle using equation (4.3.1.29) and Rez, Rez & Grant (1994) listed values of $f_{\rm el}(0)$ for many elements and ions.

Recently, Peng, Ren, Dudarev & Whelan (1996) have developed a new algorithm, based on a combined modified simulated-annealing and least-squares method, to parameterize both the elastic and absorptive scattering factors as sums of five Gaussians of the form

$$f_{\rm el}(s) = \sum_{i=1}^{n} a_i \exp\left(-b_i s^2\right), \qquad (4.3.2.1)$$

where a_i and b_i are fitting parameters. The values of their fitting parameters for the range of s values from 0 to 2.0 for elastic electron scattering factors for all neutral atoms with atomic numbers up to 98 are given in Table 4.3.2.2 and the values obtained separately for these atoms for the range of s from 0 to $6.0\,\text{Å}^{-1}$ are given in Table 4.3.2.3. For Table 4.3.2.2, the fitting was made to the values of f given in Table 4.3.1.1. For Table 4.3.2.3, the f values in the range of s from 2.0 to $6.0\,\text{Å}^{-1}$ were those obtained by using the Mott formula to convert the X-ray scattering factors derived from the Dirac–Fock calculations of Rez, Rez & Grant (1994). Similar tables for atomic scattering factors of ions can be found in Peng (1998).

As an indication of the accuracy with which the parameterized f values of (4.3.2.1) reproduce the numerical values of the reference f values, Peng *et al.* (1996) computed values of $\varepsilon = 100\,\sigma/f(0)$, where σ is the square root of the mean square deviation, σ^2, between the numerical and fitted scattering factors. The values of ε are typically in the range 0.02 to 0.05, and are consistently smaller (with a few exceptions) than the corresponding values given for the parameterizations of previous workers (Weickenmeier & Kohl, 1991; Bird & King, 1990; Doyle & Turner, 1968).

For the absorptive scattering factors, corresponding to the imaginary parts added to the real elastic scattering factors as a consequence of inelastic scattering processes, Peng *et al.* (1996) have tabulated values for particular elemental crystals and a selection of crystals of compounds having the zinc-blend structure. The main contribution to the absorptive scattering factors arises from the thermal vibrations of the atoms in the crystals so that the numerical values are not characteristic of the individual atom types but depend on the type of bonding of the atoms in the crystal, as indicated by the Debye–Waller factor, and must be calculated separately for each temperature. The authors offer copies of their computer programs, freely available *via* electronic mail, from which the parameterization of the absorptive scattering factors can be derived for other materials and temperatures, given the values of the atomic numbers of the elements, the Debye–Waller factor and the electron accelerating voltage.

4.3.3. Complex scattering factors for the diffraction of electrons by gases (By A. W. Ross, M. Fink, R. Hilderbrandt, J. Wang, and V. H. Smith Jr)

4.3.3.1. *Introduction*

This section includes tables of scattering factors of interest for gas-phase electron diffraction from atoms and molecules in the keV energy region. In addition to the tables and a description of their uses, a discussion of the theoretical uncertainties related to the material in the tables is also provided. The tables give scattering factors for elastic and inelastic scattering from free atoms. The theory of molecular scattering based on these atomic quantities is also discussed.

4.3.3.2. *Complex atomic scattering factors for electrons*

4.3.3.2.1. *Elastic scattering factors for atoms*

It has long been known that the first Born approximation provides an inadequate description at the 4% accuracy level for elastic and total differential cross sections in the 40 keV energy range for atoms heavier than Ne (Schomaker & Glauber, 1952; Glauber & Schomaker, 1953). Results of early experimental work have been confirmed for both atomic and molecular

(*continued on page* 388)

references