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

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

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

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

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

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

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