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

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

$$f^B(s) = 4\pi K \int_0^\infty r^2\varphi(r)\frac{\sin sr}{sr}\,\mathrm{d}r. \tag{4.3.1.13}$$

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

$$\varphi(xy) = \int_0^H\varphi(xyz)\,\mathrm{d}z \tag{4.3.1.23}$$

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

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

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

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

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;

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

$$\lambda = h\Big/\left[2em_0E\left(1 + \frac{eE}{2m_0c^2}\right)\right]^{1/2} = \lambda_c\frac{(1-\beta^2)^{1/2}}{\beta}$$
$$= 12.2639/(E + 0.97845\times10^{-6}E^2)^{1/2}, \tag{4.3.1.27}$$

where m_0 is the rest mass, λ_c is the Compton wavelength $\beta = \nu/c$, 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

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

references