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Letters to the Editor

Plural electron scattering and the inclusion of phase factors

Abstract. A method is given for the calculation of the angular distributions of plurally scattered electrons for the case where the scattered wave is a complex quantity. An expression is given for the resultant scattered wave; the modulus of this quantity is then available for comparison with experiment.

The scattered electron wave $\phi_s(\boldsymbol{\theta})$ is in general a complex quantity $f_1(\boldsymbol{\theta}) \exp\{i\eta_1(\boldsymbol{\theta})\}$ (e.g. Schomaker and Glauber 1952, Ibers and Hoerni 1954), where $f_1(\boldsymbol{\theta})$ and $\eta_1(\boldsymbol{\theta})$ are the amplitude and phase of the scattered electron; $\boldsymbol{\theta}$ is a vector representing the polar (θ) and azimuthal (ϕ) angles of scattering. In most electron scattering experiments $f_1(\boldsymbol{\theta})$ and $\eta_1(\boldsymbol{\theta})$ exhibit cylindrical symmetry. Under single scattering conditions (or in the kinematical approximation) the measured intensity distribution is proportional to $|\phi_s(\boldsymbol{\theta})|^2$ and the phase factor $\eta_1(\boldsymbol{\theta})$ is not directly relevant to the experimental results. However, for plural electron scattering of medium energy electrons (5–100 keV) in thin films (100–1000 Å), these phase terms must be included in the calculations of angular distributions. In the first Born approximation for electron scattering by an atom, $\eta_1(\boldsymbol{\theta})$ is approximated to zero and the angular redistribution due to plural electron scattering may be calculated by a two-dimensional folding of $f_1{}^{B}(\boldsymbol{\theta})$ or $f_1{}^{B}(\boldsymbol{\theta})^2$ (Misell and Burge 1969). Schomaker and Glauber (1952) point out that, for the lower incident electron energies or with specimens containing atoms of high atomic number, the first Born approximation fails and $f_1{}^{B}(\boldsymbol{\theta})$ must be replaced by a complex scattering factor. These atomic phase shifts have been computed for a number of elements by the partial wave method and are tabulated by, for example, Ibers and Hoerni (1954), Karle and Bonham (1964), Kimura *et al.* (1967), Cox and Bonham (1967), and Haase (1968).

It is the purpose of this note to outline a method for the calculation of the complex scattering factor, and hence the scattered intensity, including the effects of plural electron scattering. It is assumed that the single scattering amplitude and phase factors are given, i.e. $f_1(\boldsymbol{\theta})$ and $\eta_1(\boldsymbol{\theta})$ are known.

For n scattering events in the specimen film, the scattered wave is given by

$$f_n(\boldsymbol{\theta}) \exp\{i\eta_n(\boldsymbol{\theta})\} = \int_{\boldsymbol{\theta}'} f_{n-1}(\boldsymbol{\theta}') \exp\{i\eta_{n-1}(\boldsymbol{\theta}')\} f_1(\boldsymbol{\theta}-\boldsymbol{\theta}') \times \exp\{i\eta_1(\boldsymbol{\theta}-\boldsymbol{\theta}')\}\, d\boldsymbol{\theta}' \quad (1)$$

where $d\boldsymbol{\theta}$ is the element of solid angle $d\Omega \simeq \sin\theta\, d\theta\, d\phi$.

If the incident electron wave is of unit intensity (or unit amplitude) then the resultant scattered wave $\phi_s(\boldsymbol{\theta})$, for a specimen of thickness t, is given by

$$\phi_s(\boldsymbol{\theta}) = \left\{\exp\left(-\frac{t}{\lambda}\right)\right\}^{1/2} \sum_{n=1}^{\infty} \left(\frac{t}{\lambda I_f}\right)^{n/2} \frac{f_n(\boldsymbol{\theta}) \exp\{i\eta_n(\boldsymbol{\theta})\}}{(n!)^{1/2}}. \tag{2}$$

Hence $\phi_s(\boldsymbol{\theta})$ is normalized such that

$$\int_{\boldsymbol{\theta}} |\phi_s(\boldsymbol{\theta})|^2 \, d\boldsymbol{\theta} = 1 - \exp\left(\frac{-t}{\lambda}\right).$$

λ is the mean free path for electron scattering into all angles and is related to the cross section σ by $\lambda = A/(N_0\rho\sigma)$ in the free-atom theory. It has been assumed that the scattering processes obey Poisson statistics (see, e.g. Misell and Burge 1969).

Further

$$\sigma = I_f = \int_{\boldsymbol{\theta}} |f_1(\boldsymbol{\theta})|^2 \, d\boldsymbol{\theta}$$

and

$$\int_{\boldsymbol{\theta}} |f_n(\boldsymbol{\theta})|^2 \, d\boldsymbol{\theta} = (I_f)^n.$$

In order to calculate the $f_n(\boldsymbol{\theta}) \exp\{i\eta_n(\boldsymbol{\theta})\}$, equation (1) is separated out into real and imaginary parts, i.e.

$$\begin{aligned} f_n(\boldsymbol{\theta}) \cos\{\eta_n(\boldsymbol{\theta})\} = & \int_{\boldsymbol{\theta}'} f_{n-1}(\boldsymbol{\theta}') \cos\{\eta_{n-1}(\boldsymbol{\theta}')\} f_1(\boldsymbol{\theta}-\boldsymbol{\theta}') \cos\{\eta_1(\boldsymbol{\theta}-\boldsymbol{\theta}')\} \, d\boldsymbol{\theta}' \\ & - \int_{\boldsymbol{\theta}'} f_{n-1}(\boldsymbol{\theta}') \sin\{\eta_{n-1}(\boldsymbol{\theta}')\} f_1(\boldsymbol{\theta}-\boldsymbol{\theta}') \sin\{\eta_1(\boldsymbol{\theta}-\boldsymbol{\theta}')\} \, d\boldsymbol{\theta}' \end{aligned} \tag{3}$$

and

$$\begin{aligned} f_n(\boldsymbol{\theta}) \sin\{\eta_n(\boldsymbol{\theta})\} = & \int_{\boldsymbol{\theta}'} f_{n-1}(\boldsymbol{\theta}') \sin\{\eta_{n-1}(\boldsymbol{\theta}')\} f_1(\boldsymbol{\theta}-\boldsymbol{\theta}') \cos\{\eta_1(\boldsymbol{\theta}-\boldsymbol{\theta}')\} \, d\boldsymbol{\theta}' \\ & + \int_{\boldsymbol{\theta}'} f_{n-1}(\boldsymbol{\theta}') \cos\{\eta_{n-1}(\boldsymbol{\theta}')\} f_1(\boldsymbol{\theta}-\boldsymbol{\theta}') \sin\{\eta_1(\boldsymbol{\theta}-\boldsymbol{\theta}')\} \, d\boldsymbol{\theta}'. \end{aligned} \tag{4}$$

From these equations it is seen that the scattered intensity $|\phi_s(\boldsymbol{\theta})|^2$ is dependent on the phase factor $\eta_1(\boldsymbol{\theta})$. Using the technique of projected scattering functions, previously given by Misell and Burge (1969) for the evaluation of angular folding integrals (in the first Born approximation), we define the projected scattering functions $g_n(\alpha)$ and $h_n(\alpha)$ by:

$$g_n(\alpha) = \int_{-\infty}^{+\infty} f_n\{(\alpha^2+\beta^2)^{1/2}\} \cos \eta_n\{(\alpha^2+\beta^2)^{1/2}\} \, d\beta \tag{5}$$

$$h_n(\alpha) = \int_{-\infty}^{+\infty} f_n\{(\alpha^2+\beta^2)^{1/2}\} \sin \eta_n\{(\alpha^2+\beta^2)^{1/2}\} \, d\beta \tag{6}$$

in the small-angle approximation (i.e. $\sin\theta \simeq \theta$) and assuming that $f_n(\boldsymbol{\theta})$ falls rapidly to zero for large arguments, so that finite limits for the integrations may be replaced by infinite limits.

The substitution of relations (5) and (6) into equations (3) and (4) respectively gives the following one-dimensional integrals:

$$g_n(\alpha) = \int_{-\infty}^{+\infty} \{g_{n-1}(\alpha')\, g_1(\alpha-\alpha') - h_{n-1}(\alpha')\, h_1(\alpha-\alpha')\}\, \mathrm{d}\alpha' \tag{7}$$

and

$$h_n(\alpha) = \int_{-\infty}^{+\infty} \{g_{n-1}(\alpha')\, h_1(\alpha-\alpha') + h_{n-1}(\alpha')\, g_1(\alpha-\alpha')\}\, \mathrm{d}\alpha' \tag{8}$$

with $g_n(\alpha) = g_n(-\alpha)$ and $h_n(\alpha) = h_n(-\alpha)$ for cylindrically symmetric functions. The evaluation of integrals of the type (7) and (8) has been given by Misell and Burge (1969).

The actual scattering factors are given by

$$f_n(\boldsymbol{\theta}) \cos\{\eta_n(\boldsymbol{\theta})\} = -\frac{1}{\pi}\int_0^{\infty} \frac{g_n'\{(\alpha^2+\theta^2)^{1/2}\}}{(\theta^2+\alpha^2)^{1/2}}\, \mathrm{d}\alpha \tag{9}$$

where $g_n'(\alpha) = \mathrm{d}g_n/\mathrm{d}\alpha$. A similar equation to (9) may be written for $f_n(\boldsymbol{\theta}) \sin\{\eta_n(\boldsymbol{\theta})\}$ and $h_n(\alpha)$.

Hence the summation (2) may be evaluated and $|\phi_s(\boldsymbol{\theta})|^2$ computed for a direct comparison with the experimentally determined scattering profiles. Although the specific problem considered here is the evaluation of angular folding integrals in the free-atom formulation (readily available from the literature) the analysis applies to electron scattering by amorphous specimens. The extension of this work to a consideration of diffraction effects is in progress.

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Department of Physics,
Queen Elizabeth College,
Campden Hill Road, London W8.

D. L. Misell
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Correlation functions for classical systems in the van der Waals limit

Abstract. A ν-dimensional system of particles with two-body potential $q(\boldsymbol{r})+\gamma^{\nu}K(\gamma\boldsymbol{r})$ is considered. Various correlation functions are defined and evaluated in the limit $\gamma \rightarrow 0$. Some of the results describe two-phase states, and others are closely related to the Ornstein–Zernike theory.