

Effects of Diffraction on the (e, 2e) Reaction in Crystals*

L. J. Allen,^A I. E. McCarthy,^B V. W. Maslen^C and C. J. Rossouw^C

^A School of Science and Mathematics Education, University of Melbourne, Parkville, Vic. 3052, Australia.

^B Electronic Structure of Materials Centre, Flinders University of South Australia, Bedford Park, S.A. 5042, Australia.

^C Division of Materials Science and Technology, CSIRO, Locked Bag 33, Clayton, Vic. 3168, Australia.

Abstract

An expression is derived for the (e, 2e) differential cross section of a crystal, with allowance for dynamic diffraction of both the incident and outgoing electrons, all of which are assumed to be fast. Conditions for unique momentum determination on the one hand or for maximum enhancement of the (e, 2e) signal on the other are discussed.

1. Introduction

The successful use of (e, 2e) scattering to map atomic and molecular wave functions (McCarthy and Weigold 1988) has encouraged renewed efforts to apply it to solids. Experimental attempts to study details of solid structure by means of the (e, 2e) reaction were first reported by Amaldi *et al.* (1969). But their energy resolution of 150 eV did not enable them to obtain information on the valence states. The first (e, 2e) measurement of the spectral momentum density of the valence band of a solid was reported by Ritter *et al.* (1984), whose energy resolution was 6 eV. Though this work was a big advance, Ritter and his colleagues (Chao Gao *et al.* 1988) have recently expressed pessimism about the merits of applying (e, 2e) to crystalline solids, stating that '... in general, most information regarding the electronic structure of crystalline solids can be obtained more expeditiously and with higher resolution by other techniques. Where (e, 2e) spectroscopy provides fundamental insights is in the investigation of disordered solids.' Hayes *et al.* (1988) have substantially reduced the data collection time of an (e, 2e) experiment by using position-sensitive detectors.

On the theoretical side, Neudachin *et al.* (1969) provided the first description of the (e, 2e) reaction in a crystal. They represented the incident and outgoing electrons by plane waves, but took account of the periodic nature of the crystal when describing the precollision state of the target electron. It was on the basis of this theory that Chao Gao *et al.* interpreted their experimental results for graphite. Neudachin *et al.* (1981) expressed optimism about the

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merits of applying (e,2e) to crystalline solids, stating that: 'On the whole, solid targets offer the most promising possibilities for the (e,2e) method.'

The present work builds on that of Neudachin and his colleagues (Neudachin *et al.* 1969; Levin *et al.* 1972) by including diffraction of the incident and outgoing electrons. It may also be viewed as an extension of the inelastic scattering theory of Rossouw and Maslen (Maslen and Rossouw 1984; Rossouw and Maslen 1984; Maslen 1987) to the case where the ejected electron is fast and is detected. The theory of electron diffraction at the voltages of, say, 25 keV being used or contemplated for (e,2e) studies of solids is well developed (see for example Humphreys 1979), and with several groups preparing to carry out such experiments, it is an opportune time to study the implications of diffraction for (e,2e). We will show that, in the presence of diffraction, an (e,2e) experiment no longer provides a 'clean' measurement of the wave function being sought and we will discuss the question of how to extract this information.

The form of the (e,2e) scattering amplitude which we derive may be interpreted as a sum of amplitudes of many atom-like (e,2e) reactions. We therefore first outline the underlying atomic model, then consider the model of Neudachin *et al.* for an (e,2e) reaction in a crystal and finally derive the scattering cross section in the presence of diffraction.

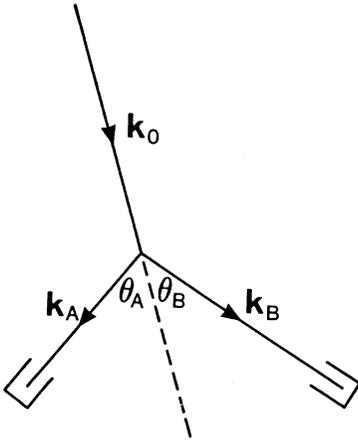


Fig. 1. Assumed scattering geometry of the (e,2e) reaction.

2. Basic Atomic Model

We assume throughout this paper that the incident and outgoing electrons may all be considered fast (Humphreys 1979), so that the collision involves a large transfer of momentum and large scattering angles as indicated in Fig. 1.

In atomic units, the differential scattering cross section for an (e,2e) reaction may be expressed, essentially without approximation, as

$$\frac{d^6\sigma}{d\Omega_A d\Omega_B dE_A dE_B} = (2\pi)^4 \frac{k_A k_B}{k_0} \sum |t_f(\mathbf{k}_A, \mathbf{k}_B \leftarrow \mathbf{k}_0)|^2 \delta(E_A + E_B - E_0 - \epsilon), \quad (1)$$

where \mathbf{k}_0 , \mathbf{k}_A and \mathbf{k}_B are the wave vectors, and E_0 , E_A and E_B the corresponding energies, of the incident and outgoing electrons, t_f is the amplitude of scattering to a final state and the summation extends over degenerate final states. The difference in energy between the precollision and postcollision states of the target is denoted by ϵ .

Our model of an atomic (e, 2e) event assumes that the incident and outgoing electrons can be described by plane waves and that atomic ionisation can be described by an independent particle model, so that ϵ becomes the energy of the precollision orbital occupied by the target electron. The expression for the differential scattering cross section then reduces to

$$\frac{d^5\sigma}{d\Omega_A d\Omega_B dE_A} \approx (2\pi)^4 \frac{k_A k_B}{k_0} f_{ee} |\phi(\boldsymbol{\kappa})|^2, \quad (2)$$

where

$$f_{ee} = \frac{1}{(2\pi^2)^2} \left(\frac{1}{|\mathbf{k}_0 - \mathbf{k}_A|^4} - \frac{1}{|\mathbf{k}_0 - \mathbf{k}_A|^2 |\mathbf{k}_0 - \mathbf{k}_B|^2} + \frac{1}{|\mathbf{k}_0 - \mathbf{k}_B|^4} \right), \quad (3)$$

$$\boldsymbol{\kappa} = \mathbf{k}_A + \mathbf{k}_B - \mathbf{k}_0, \quad (4)$$

and $\phi(\boldsymbol{\kappa})$ is the wave function of the precollision state of the target electron in the momentum, or wave vector, representation. The expression for f_{ee} takes into account the indistinguishability of the two outgoing electrons, and indefinite spin states are assumed in its derivation. The factorisation of the expression for the differential scattering cross section, which is evident in equation (2) and which also occurs for the more accurate distorted wave impulse approximation, enables a 'clean' measurement of $|\phi(\boldsymbol{\kappa})|^2$.

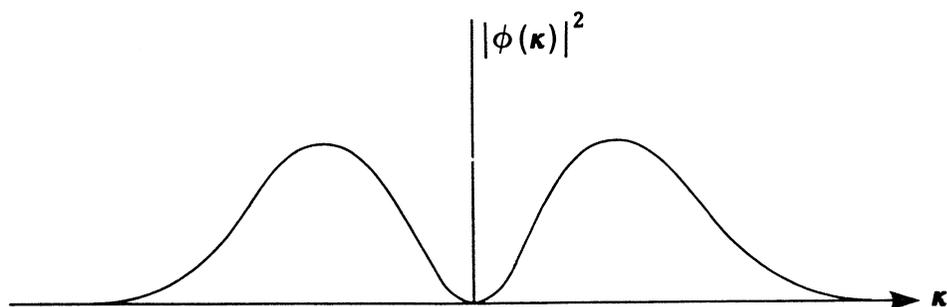


Fig. 2. Map of $|\phi(\boldsymbol{\kappa})|^2$ along one direction for a p-type orbital of energy ϵ , obtained by an atomic (e, 2e) experiment.

For an atom, ϵ is discrete and $|\phi(\boldsymbol{\kappa})|^2$ is a continuous function of $\boldsymbol{\kappa}$. Energy and momentum are conserved in the reaction. One can obtain $|\phi(\boldsymbol{\kappa})|^2$ by varying the scattering angles while keeping the energies fixed and Fig. 2 shows a plausible map of $|\phi(\boldsymbol{\kappa})|^2$ along one direction for a p-type orbital.

3. Crystal Model without Diffraction

Neudachin *et al.* (1969) used plane waves to describe the incident and outgoing electrons, and the precollision target orbital was represented by a tight binding wave function,

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_n \exp(i \mathbf{k} \cdot \mathbf{R}_n) \psi(\mathbf{r} - \mathbf{R}_n), \quad (5)$$

where \mathbf{R}_n denotes a crystal lattice vector, N is the number of unit cells in the crystal and $\psi(\mathbf{r} - \mathbf{R}_n)$ is an atomic orbital. The momentum representation of $\Psi_{\mathbf{k}}(\mathbf{r})$ is

$$\Phi_{\mathbf{k}}(\mathbf{q}) = \sqrt{N} \phi(\mathbf{q}) \delta_{\mathbf{q}, \mathbf{k} + \mathbf{g}}, \quad (6)$$

where \mathbf{g} is a vector of the reciprocal lattice.

The conditions under which an (e, 2e) reaction in a crystal will be observed are the conservation of energy,

$$E_A + E_B - E_0 = \epsilon(\mathbf{k}), \quad (7)$$

and the conservation of crystal momentum,

$$\mathbf{k}_A + \mathbf{k}_B - \mathbf{k}_0 \equiv \boldsymbol{\kappa} = \mathbf{k} + \mathbf{g}. \quad (8)$$

The continuous dependence of $\epsilon(\mathbf{k})$ on \mathbf{k} describes a crystal energy band and it leads to an additional factor, which we call the energy dispersion factor, in the expression for the differential scattering cross section. Thus we have

$$\begin{aligned} \frac{d^5\sigma}{d\Omega_A d\Omega_B dE_A} &\approx (2\pi)^4 N \frac{k_A k_B}{k_0} f_{ee} |\phi(\boldsymbol{\kappa})|^2 \\ &\times \left\{ 1 - \left(k_{Bx} \frac{\partial \epsilon}{\partial k_x} + k_{By} \frac{\partial \epsilon}{\partial k_y} + k_{Bz} \frac{\partial \epsilon}{\partial k_z} \right) / 2E_B \right\}^{-1} \delta_{\boldsymbol{\kappa}, \mathbf{k} + \mathbf{g}}. \end{aligned} \quad (9)$$

If in the (e, 2e) experiment the scattering angles are varied while the energies are held fixed, one would obtain $|\phi(\boldsymbol{\kappa})|^2$, but only for the discrete wave vectors \mathbf{k} , $\mathbf{k} + \mathbf{g}_1$, $\mathbf{k} + \mathbf{g}_2$, ..., as indicated in Fig. 3. One would have to vary both energies and angles to obtain $|\phi(\boldsymbol{\kappa})|^2$ for a continuous range of $\boldsymbol{\kappa}$. In the case of extreme tight binding, where ϵ is independent of \mathbf{k} , one would reproduce the atomic results of Fig. 2.

4. Crystal Model with Diffraction

The model of Neudachin *et al.* does not mention crystal surfaces. We assume the crystal to be a thin plate, with the x and y dimensions large and the z dimension small, with thickness d . The origin of coordinates and the xy -plane are chosen to lie in the entrance surface, and the z -axis points normally inwards (Fig. 4). We use the standard Bloch wave theory of dynamical

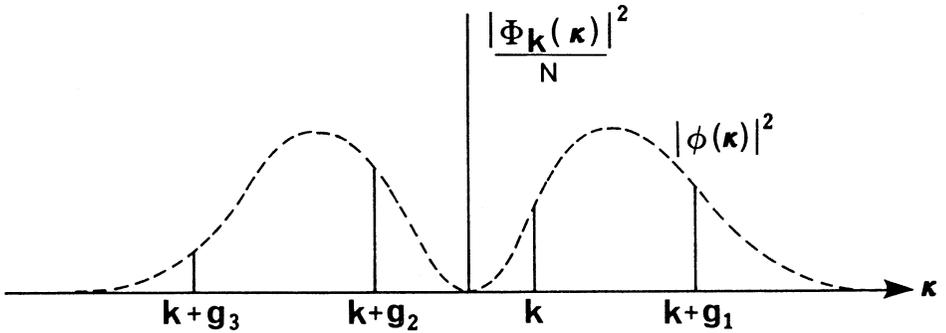


Fig. 3. Observed values of $|\Phi_k(\kappa)|^2$ along a fixed direction and at fixed energies. The dashed curve illustrates $|\phi(\kappa)|^2$.

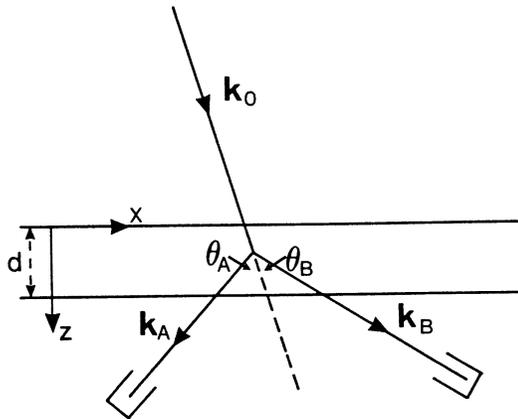


Fig. 4. Assumed scattering geometry of the (e, 2e) reaction in a crystal.

electron diffraction (Humphreys 1979; Metherell 1975) to describe the incident and outgoing electrons, which are assumed to be fast. This theory is mostly applied to situations of small momentum transfer, where the scattering cross sections are much higher, but we see no reason in principle why it should not hold for large momentum transfer as in (e, 2e) scattering.

The incident electron is represented by a plane wave before entering the crystal,

$$\chi^{(+)}(\mathbf{k}_0) = \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{k}_0 \cdot \mathbf{r}), \quad z < 0, \tag{10}$$

and by a sum of Bloch waves within the crystal,

$$\chi^{(+)}(\mathbf{k}_0) = \frac{1}{(2\pi)^{3/2}} \sum_{\lambda} \alpha_{\lambda}^0 \sum_{\mathbf{g}} C_{0\mathbf{g}}^{\lambda}(\mathbf{k}_0) \exp\{i(\mathbf{k}_0^{\lambda} + \mathbf{g}) \cdot \mathbf{r}\}, \quad 0 \leq z \leq d. \tag{11}$$

The quantities \mathbf{k}_0^λ and $C_{0\mathbf{g}}^\lambda(\mathbf{k}_0)$ are eigenvalues and eigenvector components of the dynamical diffraction eigenvalue problem determined by \mathbf{k}_0 and the crystal potential. The eigenvalue \mathbf{k}_0^λ has the special form

$$\mathbf{k}_0^\lambda = \mathbf{k}_0 + \gamma_0^\lambda \hat{\mathbf{z}} \quad (12)$$

and the values of the γ are typically of order 0.02 times a reciprocal lattice vector. The Bloch wave coefficients α_0^λ are determined by boundary conditions at the entrance surface and are proportional to elements of the inverse matrix C_0^{-1} (Allen and Rossouw 1989). In electron diffraction terminology, \mathbf{g} indexes a beam and λ indexes a branch of the dispersion surface associated with the incident vector \mathbf{k}_0 and electron energy $\frac{1}{2}k_0^2$. Common situations in electron diffraction are those of planar and axial diffraction where, to a good approximation, only vectors belonging, respectively, to a single row and to a single plane of reciprocal space need be included. The coefficients α_0^λ are well approximated by $(C_0^{\lambda*})$ except when the angle between \mathbf{k}_0 and the surface normal is large.

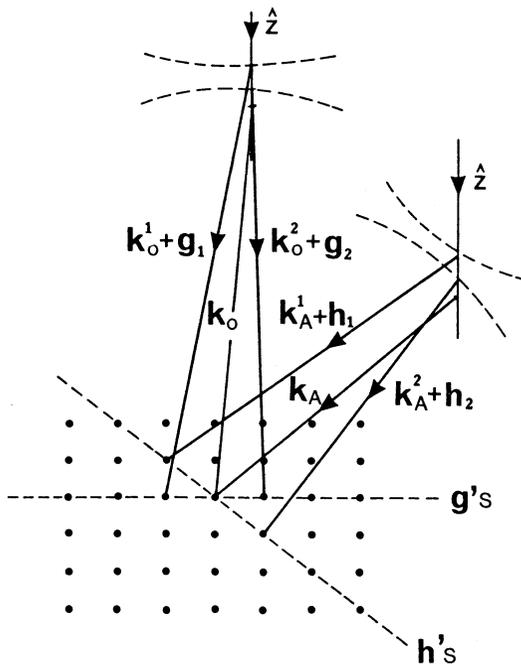


Fig. 5. Illustration of the dispersion surfaces (dashed curves) and reciprocal lattice vectors contributing to the diffraction of electrons 0 and A.

The outgoing electrons are similarly represented, except that matching at the exit surface, $z = d$, leads to an additional factor in the Bloch wave expressions.

Thus we have

$$\chi^{(-)}(\mathbf{k}_A) = \frac{1}{(2\pi)^{3/2}} \sum_{\mu} \alpha_A^{\mu} \exp(-i\gamma_A^{\mu} d) \sum_{\mathbf{h}} C_{A\mathbf{h}}^{\mu}(\mathbf{k}_A) \exp\{i(\mathbf{k}_A^{\mu} + \mathbf{h}) \cdot \mathbf{r}\}, \quad 0 \leq z \leq d, \quad (13)$$

$$= \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{k}_A \cdot \mathbf{r}), \quad z > d; \quad (14)$$

$$\chi^{(-)}(\mathbf{k}_B) = \frac{1}{(2\pi)^{3/2}} \sum_{\nu} \alpha_B^{\nu} \exp(-i\gamma_B^{\nu} d) \sum_{\mathbf{l}} C_{B\mathbf{l}}^{\nu}(\mathbf{k}_B) \exp\{i(\mathbf{k}_B^{\nu} + \mathbf{l}) \cdot \mathbf{r}\}, \quad 0 \leq z \leq d, \quad (15)$$

$$= \frac{1}{(2\pi)^{3/2}} \exp(i\mathbf{k}_B \cdot \mathbf{r}), \quad z > d. \quad (16)$$

The superscripts (+) and (-) refer to ingoing and outgoing electrons respectively. Fig. 5 depicts the different dispersion surfaces and reciprocal lattice vectors contributing to diffraction of the incident electron and of one of the outgoing electrons for the case where two beams are associated with each electron.

Since, in the Bloch wave theory, each of the fast electrons in the (e, 2e) reaction is represented by a double sum of plane waves the amplitude $t_f(\mathbf{k}_A, \mathbf{k}_B \leftarrow \mathbf{k}_0)$ becomes a six-fold sum of terms, each of which is a crystal (e, 2e) amplitude of the type considered by Neudachin *et al.* We write it as follows:

$$t_f(\mathbf{k}_A, \mathbf{k}_B \leftarrow \mathbf{k}_0) = \sum_{\mathbf{g}\mathbf{h}\mathbf{l}}^{\lambda\mu\nu} X^{\lambda\mu\nu} Y^{\mu\nu} Z_{\mathbf{g}\mathbf{h}\mathbf{l}}^{\lambda\mu\nu} W_{\mathbf{g}\mathbf{h}\mathbf{l}}^{\lambda\mu\nu}, \quad (17)$$

where $X^{\lambda\mu\nu} = \alpha_0^{\lambda} (\alpha_A^{\mu} \alpha_B^{\nu})^*$, (18)

$$Y^{\mu\nu} = \exp\{i(\gamma_A^{\mu} + \gamma_B^{\nu}) d\}, \quad (19)$$

$$Z_{\mathbf{g}\mathbf{h}\mathbf{l}}^{\lambda\mu\nu} = C_{0\mathbf{g}}^{\lambda} (C_{A\mathbf{h}}^{\mu} C_{B\mathbf{l}}^{\nu})^*, \quad (20)$$

and $W_{\mathbf{g}\mathbf{h}\mathbf{l}}^{\lambda\mu\nu}$ is the (e, 2e) amplitude associated with the vector triple $(\mathbf{k}_0^{\lambda} + \mathbf{g}, \mathbf{k}_A^{\mu} + \mathbf{h}, \mathbf{k}_B^{\nu} + \mathbf{l})$. It readily follows that

$$W_{\mathbf{g}\mathbf{h}\mathbf{l}}^{\lambda\mu\nu} = (f_{ee}^{\frac{1}{2}})_{\mathbf{g}\mathbf{h}\mathbf{l}}^{\lambda\mu\nu} \phi(\boldsymbol{\kappa} + \mathbf{h} + \mathbf{l} - \mathbf{g} + \gamma^{\lambda\mu\nu} \hat{\mathbf{z}}) S^{\lambda\mu\nu}, \quad (21)$$

where

$$\gamma^{\lambda\mu\nu} = \gamma_A^{\mu} + \gamma_B^{\nu} - \gamma_0^{\lambda}, \quad (22)$$

$$S^{\lambda\mu\nu} = \frac{1}{\sqrt{N}} \sum_{\mathbf{n}} \exp\{i(\mathbf{k} - \boldsymbol{\kappa} - \gamma^{\lambda\mu\nu} \hat{\mathbf{z}}) \cdot \mathbf{R}_n\}, \quad (23)$$

$$(f_{ee}^{\frac{1}{2}})_{\mathbf{g}\mathbf{h}\mathbf{l}}^{\lambda\mu\nu} = \frac{1}{2\pi^2} \left(\frac{1}{|\mathbf{k}_0^{\lambda} + \mathbf{g} - \mathbf{k}_A^{\mu} - \mathbf{h}|^2} \pm \frac{1}{|\mathbf{k}_0^{\lambda} + \mathbf{g} - \mathbf{k}_B^{\nu} - \mathbf{l}|^2} \right). \quad (24)$$

By regarding $\psi(\mathbf{r} - \mathbf{R}_n)$ in equation (5) as a non-overlapping unit cell wave function rather than an atomic orbital, equation (21) is then not limited to the valid range of tight binding theory. The \pm sign in equation (24) indicates an uncertainty in total spin of the outgoing electrons, which will be dealt with later by averaging the scattering cross section over various possibilities.

We now encounter a problem which did not arise in the theory of Neudachin *et al.* Equation (23) suggests that $S^{\lambda\mu\nu}$ will vanish unless

$$\boldsymbol{\kappa} = \mathbf{k} + \mathbf{G} - \gamma^{\lambda\mu\nu} \hat{\mathbf{z}}, \quad (25)$$

where \mathbf{G} is either zero or an arbitrary reciprocal lattice vector. The relation (25) depends on the branch indices of the dispersion surfaces. But one cannot generally satisfy simultaneously both this relation and the condition of energy conservation, which does not involve these indices. This problem, resulting from the boundary conditions imposed by the finite thickness of the crystal, was resolved by Young and Rez (1975). In the present case, their solution involves summing over a small range of k_z , the z component of the wave vector of the target orbital, which is not measured but only inferred in an (e,2e) experiment.

Now $S^{\lambda\mu\nu}$ can be reduced to a one dimensional integral as follows. Let \mathbf{G} be that reciprocal lattice vector such that the 'reduced' wave vector

$$\boldsymbol{\kappa}_R = \boldsymbol{\kappa} - \mathbf{G} \quad (26)$$

lies in the first Brillouin zone. Then, because $\gamma^{\lambda\mu\nu}$ is small, $S^{\lambda\mu\nu}$ should be very small unless $\boldsymbol{\kappa}_R$ is close to \mathbf{k} . Thus we can approximate $S^{\lambda\mu\nu}$ by the integral

$$S^{\lambda\mu\nu} \approx \frac{1}{\Omega\sqrt{N}} \iiint \exp\{i(\mathbf{k} - \boldsymbol{\kappa}_R - \gamma^{\lambda\mu\nu} \hat{\mathbf{z}}) \cdot \mathbf{R}\} d^3R, \quad (27)$$

where Ω is the volume of a unit cell. Because of the large x, y dimensions of the crystal, this reduces to the single integral

$$S^{\lambda\mu\nu} \approx \frac{(2\pi)^2}{\Omega\sqrt{N}} \delta_2(\mathbf{k}_s - \boldsymbol{\kappa}_{Rs}) \int_0^d \exp\{i(k_z - \kappa_{Rz} - \gamma^{\lambda\mu\nu} z)\} dz, \quad (28)$$

where the subscript s (surface) denotes projection onto the xy -plane. It is important to note that one cannot consider the z dimension of the crystal to be large and to make the corresponding approximation for it, thereby reducing $S^{\lambda\mu\nu}$ to a three dimensional delta function. Physically, this would imply that the detectors are inside the crystal and that we can resolve the individual $\gamma^{\lambda\mu\nu}$, which we cannot.

Evaluation of Differential Scattering Cross Section

To obtain the differential scattering cross section for the (e,2e) reaction, taking diffraction into account, we insert $t_f(\mathbf{k}_A, \mathbf{k}_B \leftarrow \mathbf{k}_0)$, given by equations (17)–(21), into equation (1) and then integrate over E_B and sum over \mathbf{k} . Using

expression (28) for $S^{\lambda\mu\nu}$ in $t_f(\mathbf{k}_A, \mathbf{k}_B \leftarrow \mathbf{k}_0)$ and expression (23), with primed superscripts, in t_f^* , we obtain

$$\begin{aligned} \frac{d^5\sigma}{d\Omega_A d\Omega_B dE_A} &= \frac{16\pi^2}{\Omega N} \frac{V}{(2\pi)^3} \frac{k_A k_B}{k_0} \iiint \delta(E_A + E_B - E_0 - \epsilon(\mathbf{k})) \delta(\mathbf{k}_S - \boldsymbol{\kappa}_{RS}) \\ &\times \sum_{\mathbf{ghl}}^{\lambda\mu\nu} X^{\lambda\mu\nu} Y^{\mu\nu} Z^{\lambda\mu\nu} (f_{ee}^{\frac{1}{2}})^{\lambda\mu\nu} \phi(\mathbf{k} + \mathbf{h} + \mathbf{l} - \mathbf{g} + \gamma^{\lambda\mu\nu} \hat{\mathbf{z}}) \\ &\times \int_0^d \exp\{i(k_z - \kappa_{Rz} - \gamma^{\lambda\mu\nu})z\} dz \\ &\times \sum_{\mathbf{g'h'l'}}^{\lambda'\mu'\nu'} X^{\lambda'\mu'\nu'} Y^{\mu'\nu'} Z^{\lambda'\mu'\nu'} (f_{ee}^{\frac{1}{2}})^{\lambda'\mu'\nu'} \phi(\mathbf{k} + \mathbf{h}' + \mathbf{l}' - \mathbf{g}' + \gamma^{\lambda'\mu'\nu'} \hat{\mathbf{z}}) \\ &\times \sum_n \exp\{i(\mathbf{k} - \boldsymbol{\kappa}_R - \gamma^{\lambda'\mu'\nu'} \hat{\mathbf{z}}) \cdot \mathbf{R}_n\} dE_B d^3k. \end{aligned} \tag{29}$$

Here V is the volume of the crystal and the factor $V/(2\pi)^3$ arises from replacement of the sum over \mathbf{k} by an integral.

Integrating firstly over \mathbf{k}_S , the second delta function in equation (29) disappears, $\epsilon(\mathbf{k})$ becomes $\epsilon(\boldsymbol{\kappa}_{RS}, k_z)$ and the lattice sum reduces to

$$\frac{N}{d} \int_0^d \exp\{i(k_z - \kappa_{Rz} - \gamma^{\lambda'\mu'\nu'})z'\} dz'. \tag{30}$$

Integration over E_B is carried out next, with \mathbf{k}_A and k_z held fixed. The first delta function in equation (29) disappears and the resulting expression is subject to the conservation of energy relation

$$\epsilon(\boldsymbol{\kappa}_{RS}, k_z) = E_A + E_B - E_0. \tag{31}$$

The integration also gives rise to an energy dispersion factor of the same form as in equation (9) except for the absence of the term $k_{Bz} \sigma\epsilon/\sigma k_z$. The final integration, that over k_z , has the form

$$I = \int \exp\{i(k_z - \kappa_{Rz})(z - z')\} M(k_z) dk_z, \tag{32}$$

where we assume that $M(k_z)$ is a slowly varying function of k_z . The dependence of κ_{Rz} on k_z implied by equation (31) allows us to approximate I by

$$I \approx \int \exp\{i(1 - b)(z - z')k_z\} M(k_z) dk_z, \tag{33}$$

where

$$b = \frac{1}{k_{Bz}} \frac{\partial \epsilon}{\partial k_z}. \tag{34}$$

Provided the range of integration is sufficient, I can be further approximated by

$$I \approx \frac{2\pi}{1-b} \delta(z-z') M(\kappa_{Rz}). \tag{35}$$

As pointed out by Young and Rez, the presence of $\delta(z-z')$ in equation (35) implies that crystal layers of different z contribute incoherently to the cross section. It also enables the two outstanding integrals over z and z' to be reduced to the single integral

$$\int_0^d \exp \{i(\gamma^{\lambda\mu\nu} - \gamma^{\lambda\mu\nu})z\} dz, \tag{36}$$

whose form is elementary.

The final expression for the differential scattering cross section, which results from carrying out the integrations indicated in equation (29) and averaging over spins, is

$$\begin{aligned} \frac{d^5\sigma}{d\Omega_A d\Omega_B dE_A} = & \frac{4N}{(1-a)(1-b)} \frac{k_A k_B}{k_0} [\sum_{ghl}^{\lambda\mu\nu} X^{\lambda\mu\nu} Z^{\lambda\mu\nu} \phi(\mathbf{k} + \mathbf{h} + \mathbf{l} - \mathbf{g} + \gamma^{\lambda\mu\nu} \hat{\mathbf{z}})] \\ & \times [\sum_{ghl}^{\lambda'\mu'\nu'} X^{\lambda'\mu'\nu'} Z^{\lambda'\mu'\nu'} \phi(\mathbf{k} + \mathbf{h}' + \mathbf{l}' - \mathbf{g}' + \gamma^{\lambda'\mu'\nu'} \hat{\mathbf{z}})]^* \\ & \times \left(\frac{1}{|\mathbf{k}_0^\lambda + \mathbf{g} - \mathbf{k}_A^\mu - \mathbf{h}|^2 |\mathbf{k}_0^{\lambda'} + \mathbf{g}' - \mathbf{k}_A^{\mu'} - \mathbf{h}'|^2} - \frac{1}{|\mathbf{k}_0^\lambda + \mathbf{g} - \mathbf{k}_A^\mu - \mathbf{h}|^2 |\mathbf{k}_0^{\lambda'} + \mathbf{g}' - \mathbf{k}_B^{\mu'} - \mathbf{l}'|^2} \right. \\ & \left. - \frac{1}{|\mathbf{k}_0^\lambda + \mathbf{g} - \mathbf{k}_B^\nu - \mathbf{l}|^2 |\mathbf{k}_0^{\lambda'} + \mathbf{g}' - \mathbf{k}_A^{\mu'} - \mathbf{h}'|^2} + \frac{1}{|\mathbf{k}_0^\lambda + \mathbf{g} - \mathbf{k}_B^\nu - \mathbf{l}|^2 |\mathbf{k}_0^{\lambda'} + \mathbf{g}' - \mathbf{k}_B^{\nu'} - \mathbf{l}'|^2} \right) \\ & \times \frac{\exp\{i(\gamma^\lambda - \gamma^{\lambda'})d\} - \exp\{i(\gamma^\mu + \gamma^\nu - \gamma^{\mu'} - \gamma^{\nu'})d\}}{i d\{(\gamma^\lambda - \gamma^{\lambda'}) - (\gamma^\mu + \gamma^\nu - \gamma^{\mu'} - \gamma^{\nu'})\}}, \tag{37} \end{aligned}$$

where

$$a = \frac{1}{k_B^2} \left(k_{Bx} \frac{\partial \epsilon}{\partial k_x} + k_{By} \frac{\partial \epsilon}{\partial k_y} \right)_{\mathbf{k}=\mathbf{\kappa}_R}, \tag{38}$$

$$b = \frac{1}{k_{Bz}} \left(\frac{\partial \epsilon}{\partial k_z} \right)_{\mathbf{k}=\mathbf{\kappa}_R}. \tag{39}$$

5. Implications of Diffraction for (e, 2e) Experiments

Our expression (37) for the differential scattering cross section for an (e, 2e) reaction, which takes into account diffraction of the incident and outgoing electrons, is much more complicated than the corresponding expression

ignoring diffraction, equation (9), which is itself closely related to equation (2), the expression for an atom. Equation (37) does not provide for a 'clean' measurement of the wave function of a valence band state of the crystal.

If diffraction could be ignored, equation (37) would reduce to (9) except for a small difference in the energy dispersion factor resulting from the inclusion of crystal surfaces in the present model. One might therefore seek experimental conditions that avoid diffraction, and this seems quite feasible. Equation (37) can be considerably simplified without gross approximation even when diffraction cannot be ignored. Firstly, d is usually large enough and the final interference factor so oscillatory that only the diagonal elements of the sums over branch indices need be retained. Secondly, a , b and the γ are usually small. Thus, to a reasonable approximation, we have

$$\frac{d^5\sigma}{d\Omega_A d\Omega_B dE_A} \approx 4N \frac{k_A k_B}{k_0} \sum_{\mathbf{ghl}} \sum_{\mathbf{g'h'l'}} \phi(\boldsymbol{\kappa} + \mathbf{h} + \mathbf{l} - \mathbf{g}) \phi^*(\boldsymbol{\kappa} + \mathbf{h}' + \mathbf{l}' - \mathbf{g}') \times \left(\frac{1}{|\mathbf{k}_0 + \mathbf{g} - \mathbf{k}_A - \mathbf{h}|^2 |\mathbf{k}_0 + \mathbf{g}' - \mathbf{k}_A - \mathbf{h}'|^2} - \frac{1}{2} \frac{1}{|\mathbf{k}_0 + \mathbf{g} - \mathbf{k}_A - \mathbf{h}|^2 |\mathbf{k}_0 + \mathbf{g}' - \mathbf{k}_B - \mathbf{l}'|^2} - \frac{1}{2} \frac{1}{|\mathbf{k}_0 + \mathbf{g} - \mathbf{k}_B - \mathbf{l}|^2 |\mathbf{k}_0 + \mathbf{g}' - \mathbf{k}_A - \mathbf{h}'|^2} + \frac{1}{|\mathbf{k}_0 + \mathbf{g} - \mathbf{k}_B - \mathbf{l}|^2 |\mathbf{k}_0 + \mathbf{g}' - \mathbf{k}_B - \mathbf{l}'|^2} \right) \times \sum^{\lambda\mu\nu} |X^{\lambda\mu\nu}|^2 Z_{\mathbf{ghl}}^{\lambda\mu\nu} [Z_{\mathbf{g'h'l'}}^{\lambda\mu\nu}]^* \tag{40}$$

To appreciate the physical significance of equation (40) we recall that, in the absence of diffraction, a variation of scattering angles, with energies held fixed, yielded separate measurements of $|\phi(\boldsymbol{\kappa})|^2$, $|\phi(\boldsymbol{\kappa} + \mathbf{g})|^2$, ... Using many beam theory to describe the electron diffraction, these quantities are no longer obtained separately, but are coupled together in the form

$$\sum_{\mathbf{g}} \sum_{\mathbf{h}} A_{\mathbf{gh}} \phi(\boldsymbol{\kappa} + \mathbf{g}) \phi^*(\boldsymbol{\kappa} + \mathbf{h}) \tag{41}$$

Each measurement, with energies held fixed but with different scattering angles, now yields an expression of the same form as equation (41) but with different coefficients. These are available from the solution of the dynamical diffraction eigenvalue problem.

Can diffraction be used to advantage in (e, 2e) experiments? Apart from the complications of multiple inelastic scattering, low count rates are a major problem in (e, 2e) experiments on crystals. If the (e, 2e) reaction probability is sensitive to electron channelling then one might expect a substantial increase in count rate for an experimental arrangement such that the incident and outgoing electrons are all channelled. Williams and Bourdillon (1982) have provided theoretical arguments and experimental evidence from electron Compton scattering in favour of such an enhancement.

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