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On the impulse approximation in electron Compton scattering

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ABSTRACT

Electronic structure measurement via Compton scattering requires the impulse approximation to be satisfied. This states that the inelastic collision time is short, so that the 'secondary' electron ejected out of the atom is effectively free of the crystal potential. The robustness of the impulse approximation is tested for boron nitride and aluminium using momentum-resolved electron energy loss spectroscopy. Reliable (with respect to impulse approximation) electronic structure information is obtained for Compton peak energies at ~ 250 eV energy loss or higher. These experimental results are validated using a simple Kronig-Penney model of the secondary electron travelling through the crystal. For loosely bound valence electrons the impulse approximation is satisfied when the Compton peak energy is significantly larger than the mean inner potential of the crystal. This criterion provides a straightforward estimate of the experimental conditions required for extracting reliable Compton data from any given material.

1. Introduction

Electron Compton scattering is a technique for probing the ground state electronic structure of a solid using electron energy loss spectroscopy (EELS). A key advantage is that even a spectrometer with moderate energy resolution (e.g. ~1 eV) is suited for this purpose. Previous Compton EELS studies on 2D materials [1-2] have reported changes in electron density as small as 0.1% [1]. Compton spectroscopy measures the electron momentum density of states $J(p_z)$ for the solid projected along the scattering vector direction [3–4]. To extract reliable $J(p_z)$ data however the experimental conditions must satisfy the impulse approximation [5–6], which assumes the scattering time is sufficiently small to neglect any changes to the potential, such as hole screening [7-8]. Under these conditions the ejected solid-state electron, here referred to as the 'secondary' electron, is effectively 'free', i.e. the Bloch wavefunction collapses to the appropriate plane wave component in the Fourier series expansion (see Appendix). According to Eisenberger and Platzman [5], the impulse approximation has no effect on the first (mean) and second (variance) moments of the Compton signal, which are independent of the potential. However, the third moment (skewness) does depend on potential, meaning that the Compton signal becomes asymmetrical if the impulse approximation is not satisfied. It is then not possible to extract reliable information on $J(p_z)$.

From the energy-time version of the uncertainty principle, the collision time is small for high energy loss inelastic scattering events. For

Compton scattering, this means collecting an EELS spectrum at large momentum transfer, since the Compton peak energy increases monotonically with scattering angle [9]. However, the Compton signal intensity also decreases as q^{-4} , where q is the scattering vector magnitude [10–11]. Hence there is a trade-off between satisfying the impulse approximation (large *q*) and having good signal-to-noise ratio (small *q*). Talmantaite et al. [9]. compared experimental EELS Compton peak energies for amorphous carbon in the 100-600 eV energy loss range and found reasonable agreement with impulse approximation calculations. Feng et al. [12]. compared $J(p_z)$ profiles for graphite extracted from Compton signals with peak energies in the 500-1100 eV energy loss range. With increasing energy loss $J(p_z)$ became more symmetrical, such that full convergence was achieved for a Compton peak energy above \sim 1000 eV. For a single hydrogen atom, the fractional error in the third moment of the Compton signal is proportional to $(E_B/\Delta E)^2$, where E_B is the electron binding energy and ΔE is the energy transfer [5]. Equivalent analytical expressions are however not available for solids, and there is no general method for predicting the experimental conditions required for extracting reliable $J(p_z)$ data for a given material.

In this study the robustness of the impulse approximation in EELS Compton scattering is investigated for boron nitride and aluminium. The former is a wide band gap semiconductor, while the latter is metallic. This choice of materials therefore covers a broad range of (conduction band) electron density, and therefore hole screening times. For these low atomic number materials, a Compton peak energy of only $\sim 250 \text{ eV}$

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yields accurate $J(p_z)$ profiles, provided the high energy loss side of the signal is used for analysis. At energy losses below 100 eV however the Compton signal becomes highly asymmetric. These experimental trends are consistent with a simple Kronig-Penney model [13] of the secondary electron travelling through the crystal potential. The secondary electron is shown to be free if its kinetic energy is much larger than the mean inner potential of the solid. This is a far simpler criterion for the impulse approximation, compared to the scattering time previously described in the literature [5–6]. Furthermore, it can readily be applied to any solid under investigation. Together with previous work on minimising dynamical diffraction artefacts [14] and background subtraction [15] the results from this study help establish a robust methodology for accurate Compton EELS measurements.

2. Experimental methods

The boron nitride specimen consisted of thin flakes dispersed on a holey carbon grid. Only flakes suspended over vacuum were used for analysis. Electron transparent specimens of aluminium were extracted from the bulk material using a Helios 600 focussed ion-beam (FIB) microscope. The ion-beam voltage was reduced to 2 kV for the final stages of specimen thinning. Specimens were examined in a JEOL 2100F field emission gun transmission electron microscope (TEM) operating at 200 kV and equipped with a Gatan Tridiem EELS spectrometer. For Compton measurements the parallel incident beam was tilted using the microscope dark tilt coils and the dark-field EELS spectrum acquired in image mode using a 5.3 mrad radius objective aperture (Fig. 1). The EELS dispersion was 0.5 eV/channel. It is important to minimise artefacts due to Bragg diffraction [10,14]. BN flakes were therefore tilted away from any zone-axes and the Compton scattering vector chosen to avoid low index crystallographic directions. For Al however the Compton scattering vector was along 110. To minimise Bragg diffraction the specimen was tilted 19° away from the $[1\overline{1}0]$ zone-axis along the 220 Kikuchi band, so that the diffraction conditions were nominally two-beam. Furthermore, a positive deviation parameter was used to minimise the intensity of the 220 Bragg beam. The EELS measured specimen thickness for BN flakes was in the range $(0.4-0.7)\lambda$, i.e. \sim 45–79 nm, where λ is the inelastic mean free path. The Al specimen thickness was 0.9λ or ~ 85 nm.

Due to the broad width of the Compton signal the conventional EELS power law background subtraction routine [16] is not very accurate. The alternative procedure [15] used here relies on the fact that a conventional bright-field EELS spectrum does not contain a Compton signal. Fourier-log deconvolving the bright-field EELS spectrum gives the single scatter distribution, while further self-convolution generates higher



Fig. 1. Schematic of the Compton EELS scattering geometry. The collimated primary electron beam is tilted by an angle φ to the specimen. The spectrometer collects only those electrons scattered along the electron-optic axis. Reproduced with permission from Talmantaite et al. *Phys Rev B* **107** (2023) 235424 (DOI: 10.1103/PhysRevB.107.235424).

order scattering distributions as well. The single and multiple scattering distributions are least-squares fitted over a 10–100 eV pre-Compton energy window to simulate the background under the Compton signal. Further details of the least squares fitting can be found in [15]. The intensity of the background subtracted Compton profile is proportional to $J(p_z)$. The EELS energy loss axis is converted to momentum p_z using the formula [9]:

$$p_z = \delta E \sqrt{\frac{m}{2E_p}} \tag{1}$$

where *m* is the electron mass, E_p is the Compton peak energy and δE the Doppler broadened energy loss. p_z represents the momentum component of the solid-state electrons along the scattering vector direction. In this work p_z is expressed in atomic units and all $J(p_z)$ profiles are normalised to unity at $p_z = 0$. Note that a negative sign has been omitted from the right-hand side of Eq. (1) without any loss of generality.

3. Results and discussion

3.1. Experimental Compton profiles

Two Compton EELS data sets were acquired from two separate BN flakes, one at high (34.8-52.5 mrad) scattering angles and the other at low (6.2-23.5 mrad) scattering angles. Fig. 2a shows Compton spectra from the latter. The real (ϵ_1) and imaginary (ϵ_2) parts of the dielectric function (Figs. 2b and 2c, respectively), extracted via a Kramers-Kronig analysis of the bright-field EELS spectrum [16], are useful for identifying many of the peaks. For example, the π and $\pi{+}\sigma$ plasmons can be identified by ϵ_1 zero crossings with positive gradient [16]. The energy loss peak at 38 eV (labelled I in Fig. 2a) is due to an inter-band transition, as evidenced by the small peak in ϵ_2 . A similar feature is also observed in density functional theory calculations of the dielectric function parallel to the BN basal plane [17]. The oscillator strength for this inter-band transition is maximum at ~ 10 mrad scattering angle. The broad peak at energy losses above the inter-band transition *I* is the Compton profile, indicated by an asterisk sign in Fig. 2a. As the scattering angle is decreased the energy transfer and Compton peak energy become similar to the binding energy of the solid-state electrons, causing a breakdown in the impulse approximation. Consequently the Compton profiles become more skewed, with long tails on the high energy loss side, consistent with theory [5].

In Fig. 2d representative Compton spectra from the high scattering angle data set are shown. The Compton profiles appear more symmetric, due to the higher Compton peak energies. Some Compton peak energies, such as at 34.8 and 38.0 mrad scattering angle, lie between B and N K-core loss edges. For a solid-state electron to undergo Compton scattering the energy transfer must be greater than its binding energy. The shape of the Compton profile will therefore be altered either side of a core loss edge. For example, B 1s and N 1s core electrons are absent from the Compton signal at energy losses below 188 eV and 410 eV, respectively. The Compton peak energy at 52.5 mrad scattering angle is however greater than both B and N K-edges, so that all electrons in BN contribute to the high energy loss side of the Compton profile.

The $J(p_z)$ profiles for 34.8, 38.0 and 52.5 mrad scattering angles are shown in Figs. 3a, 3b and 3c, respectively. The p_z range is limited on the negative side by the energy window used for background fitting (see Experimental Methods) and on the positive side by the finite size of the EELS detector. The background subtraction routine [15] did not completely remove the B and N K-edges, and hence their residuals are also present as artefacts in the $J(p_z)$ profiles. To determine the symmetry of the profiles, the curve for negative p_z was mirror reflected to the positive p_z side (red dashed line). The two segments overlap more closely with increasing scattering angle, indicating more symmetric profiles, and therefore better agreement with the impulse approximation. However, in all cases the positive p_z portion shows a more gradual



Fig. 2. (a) BN EELS spectra at small scattering angles. The total intensity has been normalised for a direct visual comparison. The dashed vertical lines represent π and π + σ plasmons, as well an inter-band transition *I*. Compton peaks are indicated by an asterisk symbol. The real (ϵ_1) and imaginary (ϵ_2) part of the dielectric function for BN, extracted from a bright-field EELS spectrum, are shown in (b) and (c), respectively. The arrows in (b) are ϵ_1 zero crossings due to plasmons, while the inset in (c) shows an inter-band peak at 38 eV. (d) BN EELS spectra at high scattering angles. The total intensity has been normalised and the plots vertically shifted for visual clarity. The dashed vertical lines are B and N K-edges, while Compton peaks are indicated by an asterisk.

decrease of $J(p_z)$ at higher momenta. This is because the $J(p_z)$ contribution from B 1s and N 1s electrons are absent for large momenta on the negative p_z side. In particular, $J(p_z)$ due to localised core electrons is significantly broader than delocalised valence electrons [18], so that the former has a larger contribution to the overall $J(p_z)$ profile at large momenta.

In Fig. 3d $J(p_z)$ for all EELS spectra in the high scattering angle data set are superimposed. Only the positive p_z portion of the curve is displayed, since it includes contributions from core electrons as well. All $J(p_z)$ profiles have similar shape, especially the two largest scattering angles, i.e. 46.5 and 52.5 mrad, which have converged to within the measurement noise level. Taking the latter as the true $J(p_z)$ profile, it is possible to calculate the fractional error for any intermediate scattering angle θ . The fractional error is defined as $|J(p_z)_{\theta} - J(p_z)_{ref}|/J(p_z)_{ref}$, where subscript 'ref' denotes the reference $J(p_z)$ value at 52.5 mrad scattering angle and similarly for the subscript ' θ '. The | | symbol represents the absolute value. Fractional errors for 34.8 and 46.5 mrad scattering angles are plotted in Fig. 3e. For the former there is a step increase in the fractional error at $p_z \sim 1.3$ a.u. Examination of Fig. 3a

shows that this is due to the N K-edge artefact from incomplete background subtraction. The fractional error is otherwise largely within the noise level for both scattering angles.

EELS Compton spectra for Al at 33.0 and 53.8 mrad scattering angles are shown in Fig. 4a. The Compton peak energy is greater than the Al Ledge, but below the K-edge, so that only 1s core electrons are completely suppressed. $J(p_z)$ profiles are shown in Figs. 4b and 4c, respectively. For the latter the bright-field EELS background subtraction method ([15]; see Experimental Methods) did not produce good results, and therefore a power law was used to subtract the background instead. The negative p_z portion of the $J(p_z)$ profile decreased more rapidly compared to the positive p_z side, due to the absence of Al 2s and 2p semi-core contributions. A superposition of $J(p_z)$ profiles for positive p_z is shown in Fig. 4d, indicating a similar shape for the two scattering angles. The fractional error between the two curves is defined as $|J(p_z)_{33,0}$ - $J\big(p_z\big)_{53.8}|/J\big(p_z\big)_{53.8},$ the subscript identifying the scattering angle for a given $J(p_z)$. The fractional error (Fig. 4d) shows a small but systematic increase above $p_z \sim 1.5$ a.u, possibly due to errors associated with power law background subtraction.



Fig. 3. BN $J(p_z)$ profiles for (a) 34.8 mrad, (b) 38.0 mrad and (c) 52.5 mrad scattering angle. J(0) has been normalised to unity. The red dashed line is the mirror reflection of the negative p_z portion of the curve. The arrows are artefacts from residual B and N K-edge intensities. In (d) the positive p_z portion of the $J(p_z)$ profile is superimposed for different scattering angles. The fractional $J(p_z)$ error for 34.8 mrad and 46.5 mrad scattering angles are plotted in (e). See text for further details.

3.2. Kronig-Penney model for the secondary electron

Consider a solid-state electron undergoing Compton scattering. The secondary electron travels through the crystal along $-\mathbf{q}$, where \mathbf{q} is the

Compton scattering vector. It is therefore subject to the periodic potential $V_{-\mathbf{q}} = V_{\mathbf{q}}^*$, where $V_{\mathbf{q}}$ is the Fourier component of the crystal potential along \mathbf{q} and the asterisk denotes the complex conjugate. It will be assumed that the crystal is centro-symmetric, so that $V_{\mathbf{q}}^*$ is a real number



Fig. 4. (a) Al EELS spectra at different scattering angles. The total intensity has been normalised and the plots vertically shifted for visual clarity. The dashed vertical line is the Al L-edge, while Compton peaks are indicated by an asterisk symbol. (b) and (c) are Al $J(p_z)$ profiles for 33.0 mrad and 53.8 mrad scattering angles, respectively. J(0) has been normalised to unity. The red dashed line is the mirror reflection of the negative p_z portion of the curve. In (d) the positive p_z portion of the $J(p_z)$ profile is superimposed for different scattering angles. (e) shows the fractional error for 33.0 mrad scattering angle. See text for further details.

and is equal to V_q . The secondary electron kinetic energy *E* is equal to the difference between the Compton energy transfer and electron binding energy. For the secondary electron to be 'free' and satisfy the impulse approximation its propagation must not be affected by the potential wells due to the periodic potential V_q . This is schematically illustrated in Fig. 5, where the potential wells are assumed to be rectangular shaped, with width *b* and periodic spacing *a*. Note that V_q is measured with respect to the mean inner potential V_0 , which is arbitrarily assigned a value of zero. Due to Bloch's theorem [13], the secondary electron wavefunction must have the form $\psi(x) = u(x)e^{ikx}$, where *k* is the wavenumber and *u* is a periodic function of position *x*.

The Schrödinger equation for the 0 < x < a - b background region between the potential wells is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{\rm bg}}{dx^2} = E\psi_{\rm bg} \tag{2}$$

where \hbar is Planck's reduced constant, and e, m are the charge magnitude and mass of the electron, respectively. The wavefunction (ψ_{bg}) has the solution:

$$\psi_{\rm bg}(\mathbf{x}) = A e^{iax} + A' e^{-iax} = u_{\rm bg}(\mathbf{x}) e^{ikx}$$
(3a)

$$u_{\rm bg}(x) = A e^{i(\alpha - k)x} + A' e^{-i(\alpha + k)x}$$
(3b)

$$a^2 = \frac{2m}{\hbar^2}E\tag{3c}$$

A and *A*' are constants to be determined. Similarly, the Schrödinger equation for the -b < x < 0 potential well region is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{\rm pw}}{dx^2} = \left(E + eV_{\rm q}\right)\psi_{\rm pw} \tag{4}$$

which gives the following wavefunction solution:

$$\psi_{\rm pw}(\mathbf{x}) = Be^{i\beta x} + B'e^{-i\beta x} = u_{\rm pw}(\mathbf{x})e^{ikx}$$
(5a)

 $u_{pw}(x) = Be^{i(\beta-k)x} + B'e^{-i(\beta+k)x}$ (5b)

$$\beta^2 = \frac{2m}{\hbar^2} \left(E + eV_{\mathbf{q}} \right) \tag{5c}$$

with *B* and *B*' being constants. The two wavefunctions and their derivatives must be equal at x = 0, i.e. $\psi_{\rm bg}(0) = \psi_{\rm pw}(0)$ and $\psi_{\rm bg}'(0) = \psi_{\rm pw}'(0)$. From the periodicity and smoothness of the Bloch *u* functions, it is also required that $u_{\rm bg}(a-b) = u_{\rm pw}(-b)$ and $u_{\rm bg}'(a-b) = u_{\rm pw}'(-b)$. These boundary conditions lead to the following result:



Fig. 5. Schematic of the Kronig-Penney model. The secondary electron kinetic energy is *E*. The potential energy wells are modelled as rectangular slabs with width *b* and depth $-eV_q$. The potential wells have periodic spacing *a*.

$$\cos(ka) = \cos(\beta b)\cos[\alpha(a-b)] - \frac{\alpha^2 + \beta^2}{2\alpha\beta}\sin(\beta b)\sin[\alpha(a-b)]$$
(8)

If $\alpha = \beta$, Eq. (8) reduces to $k = \alpha$ or equivalently from Eq. (3c):

$$E = \frac{\left(\hbar k\right)^2}{2m} \tag{9}$$

Furthermore, from Eq. (6), A = B and A' = B' = 0, so that u_{bg} and u_{pw} are independent of position. These results are consistent with a plane wave of kinetic energy *E* propagating in a uniform potential, i.e. the secondary electron is free and satisfies the impulse approximation. In practice, for non-zero V_q the condition $\alpha = \beta$ can only be approximately satisfied provided $E \gg eV_q$.

The potential V_q in a crystal can be calculated using the formula [19]:

$$V_{\mathbf{q}} = \frac{h^2}{2\pi m e \Omega} \sum_{i} f_i(\mathbf{q}) \exp(-2\pi i \mathbf{q} \cdot \mathbf{r}_i)$$
(10)

where *h* is Planck's constant, Ω is the unit cell volume, and f_i is the atom scattering factor for the atom *i* in the unit cell with fractional coordinates \mathbf{r}_i . Scattering factors for individual neutral atoms and ions are widely available, although they do not include solid-state bonding effects. Nevertheless, subtle changes due to bonding can be ignored, since we are only interested in the condition $E \gg eV_q$. From Eq. (10) it is easy to see that V_q cannot be larger than the mean inner potential V_0 , since as $\mathbf{q} \rightarrow \mathbf{0}$, f_i approaches its maximum value and all atoms are in phase (recall that f_i is real for an individual atom or ion). Using Kirkland's atom scattering factors [20] V_0 is calculated to be 13 eV for BN and 17 eV for Al. For $(E/eV_0) > 10$ the secondary electron kinetic energy must therefore be larger than 130 eV for BN and 170 eV for Al. The Compton energy loss



For non-trivial solutions of the constants A, A', B and B' the determinant of the 4 \times 4 matrix on the left-hand side must be equal to zero. This is satisfied for the condition:

$$(\alpha + \beta)(D_{23} - D_{14}) + (\alpha - \beta)(D_{13} - D_{24}) = 2\alpha D_{34} + 2\beta D_{12}$$
(7)

where D_{ij} is a 2 \times 2 determinant containing elements from the last two rows of columns *i* and *j*. Simplifying further we obtain:

however includes both the secondary electron kinetic energy as well as its binding energy. For outermost valence electrons, which are largely shielded from the positively charged nuclei, it is reasonable to assume the binding energy is of a similar magnitude to eV_0 . Therefore, a large value of (E_p/eV_0) , where E_p is the Compton peak energy, would guarantee free space propagation for a loosely bound secondary electron. These predictions are consistent with experimental observations, where a Compton peak energy in the <100 eV low energy loss region (Fig. 2a) yielded highly asymmetric profiles. Compton peak energies at ~250 eV and above however produced converged $J(p_z)$ values for positive p_z (Figs. 3d and 4d).

The discussion thus far has focussed on only the secondary electron kinetic energy. For the secondary electron to be considered completely 'free' however several other criteria need to be satisfied. First there is electron screening of the hole left behind by the secondary electron. Several studies [7–8,21] have shown that plasmons play a dominant role in hole screening. For a metal the sudden appearance of a positively charged hole creates a 'shock wave' in the surrounding electron gas, which propagates outwards at the Fermi velocity [21]. Secondary electron kinetic energies of 100 eV or more are however much larger than the Fermi energy, and can therefore easily escape the screening region. Second there can also be relaxations at the atomic level, such as atomic recoil, perturbation of core electronic states, shake up and shake off processes [7]. For a hydrogen atom these effects lead to a $(E_B/\Delta E)^2$ error term in Compton measurements [5]. For a loosely bound electron in a solid the equivalent error is $(eV_0/E_p)^2$, although it is not clear if this expression, which is based on the hydrogen atom, holds true for a multi-electron solid. If it is valid, then satisfying the kinetic energy criterion (i.e. $E_p \gg eV_0$) would also simultaneously minimise errors due to atomic relaxation. The experimental $J(p_z)$ results for BN and Al suggest that this is indeed the case, at least for light element solids.

4. Summary

Accuracy of $J(p_z)$ profiles have been experimentally investigated for momentum resolved EELS spectra in BN and Al. At small scattering angles, where the Compton peak energy E_p is below 100 eV, the Compton EELS signal becomes highly skewed, indicating breakdown of

the impulse approximation. The Compton profile becomes more symmetrical with increasing scattering angle, especially for Compton peak energies at ~250 eV or higher. $J(p_z)$ profiles for these spectra are converged for positive p_z values, i.e. the high energy loss side of the Compton signal. However, $J(p_z)$ values for the negative p_z side can be underestimated at large momenta. This is because Compton scattering of core or semi-core electronic states are suppressed by the low energy loss. The experimental results are rationalised using a simple Kronig-Penney model of the secondary electron travelling through the crystal. For the secondary electron to be effectively 'free' its kinetic energy must be much larger than the periodic potential well energy eV_q along the scattering vector direction. For loosely bound valence electrons this implies that $E_p \gg eV_0$, where V_0 is the mean inner potential of the crystal. For such a scenario the secondary electron is also likely unaffected by atomic relaxation and hole screening. The mean inner potential can be easily estimated from atom scattering factors [22], while the Compton peak energy is an analytic function of the scattering angle. $E_p \gg eV_0$ is therefore a straightforward criterion for extracting reliable $J(p_z)$ data from valence electrons in any given solid.

CRediT authorship contribution statement

BG Mendis: Writing – review & editing, Writing – original draft, Formal analysis, Conceptualization.

Declaration of competing interest

I have nothing to declare.

Appendix

Here we apply sudden perturbation theory [23] to prove that in the limit of zero collision time Compton scattering measures the electron momentum density of states in a solid. The Bloch wavefunction (ψ_{kn}) for a solid-state electron in the initial state is given by:

$$\psi_{\mathbf{k}n}(\mathbf{r}) = \sum_{\mathbf{g}} C_{\mathbf{g}n}(\mathbf{k}) \exp[i(\mathbf{k} + \mathbf{g}) \cdot \mathbf{r}]$$
(11)

where $C_{gn}(\mathbf{k})$ is the Fourier coefficient for reciprocal vector **g**, Bloch band index *n* and wavevector **k**. The position vector of the electron is **r**. Assume now that the solid-state electron instantaneously becomes 'free', for example through Compton scattering. The new Hamiltonian consists of the kinetic energy operator and a constant potential energy (say V_0). The wavefunction (ψ_{α}) for this new Hamiltonian is a plane wave:

$$\psi_{\mathbf{q}}(\mathbf{r}) = \frac{a_{\mathbf{q}}}{\sqrt{N}} \exp(i\mathbf{q}\cdot\mathbf{r}) \tag{12}$$

where N is a normalisation constant. Since the wavefunction must be continuous in time:

$$\sum_{\mathbf{g}} C_{\mathbf{g}n}(\mathbf{k}) \exp[i(\mathbf{k} + \mathbf{g}) \cdot \mathbf{r}] = \frac{a_{\mathbf{q}}}{\sqrt{N}} \exp(i\mathbf{q} \cdot \mathbf{r})$$
(13)

Multiplying both sides by $\frac{1}{\sqrt{N}} \exp(-i\mathbf{q}\cdot\mathbf{r})$ and integrating over all \mathbf{r} values gives:

$$a_{\mathbf{q}} = \frac{2\pi}{\sqrt{N}} C_{\mathbf{g}n}(\mathbf{k}) \delta(\mathbf{k} + \mathbf{g} - \mathbf{q})$$
(14)

where δ is the Dirac delta function. The measurement amplitude for a final state plane wave with wavevector **q** is given by $|a_{\mathbf{q}}|^2$, i.e. $\frac{4\pi^2}{N}|C_{gn}(\mathbf{k})|^2\delta(\mathbf{k} + \mathbf{g} - \mathbf{q})$. Summing over all occupied electron states we therefore obtain the momentum density of states along the measurement direction.

Data availability

Data will be made available on request.

References

A. Talmantaite, Y. Xie, A. Cohen, P.K. Mohapatra, A. Ismach, T. Mizoguchi, S. J. Clark, B.G. Mendis, Twist-induced interlayer charge buildup in a WS₂ bilayer revealed by electron Compton scattering and density functional theory, Phys. Rev. B 107 (2023) 235424.

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- [2] Z. Feng, X. Zhang, Y. Sakurai, Z. Wang, H. Li, H. Hu, Compton profile of few-layer graphene investigated by electron energy-loss spectroscopy, Sci. Rep. 9 (2019) 17313.
- [3] B.G. Williams, T.G. Sparrow, R.F. Egerton, Electron Compton scattering of solids, Proc. R. Soc. Lond. A 393 (1984) 409–422.
- [4] P. Schattschneider, A. Exner, Progress in electron Compton scattering, Ultramicroscopy 59 (1995) 241.
- [5] P. Eisenberger, P.M. Platzman, Compton scattering of X rays from bound electrons, Phys. Rev. A 2 (1970) 415.
- [6] P. Schattschneider, P. Pongratz, H. Hohenegger, Compton scattering in electron energy loss spectroscopy, Scanning Microsc. 4 (1990) 35.
- [7] C. Noguera, D. Spanjaard, J. Friedel, Dynamic screeening of a core hole: i semiclassical model, J. Phys. F: Metal Phys. 9 (1979) 1189.
- [8] B.G. Mendis, Q.M. Ramasse, Removal of core hole distortion from ionization edges in electron energy loss spectroscopy, Phys. Rev. B 103 (2021) 205102.
- [9] A. Talmantaite, M.R.C. Hunt, B.G. Mendis, Electron compton scattering and the measurement of electron momentum distribution in solids, J. Microsc. 279 (2020) 185.
- [10] B.G. Williams, M.K. Uppal, R.D. Brydson, Dynamicalal scattering effects in electron scattering measurements of the Compton profiles of solids, Proc. R Soc. Lond. A 409 (1987) 161.
- [11] B.G. Mendis, Coherent electron compton scattering and the non-diagonal electron momentum density of solids, Ultramicroscopy 245 (2023) 113664.

- [12] Z. Feng, S. Löffler, F. Eder, D. Su, J.C. Meyer, P. Schattschneider, Combined study of the ground and unoccupied electronic states of graphite by electron energy-loss spectroscopy, J. Appl. Phys. 114 (2013) 183716.
- [13] C. Kittel, Introduction to Solid State Physics, 8th Edition, John Wiley and Sons, USA, 2005.
- [14] B.G. Mendis, A. Talmantaite, Towards electron energy loss Compton spectra free from dynamical diffraction artefacts, Microsc. Microanal. 28 (2022) 1971.
- [15] B.G. Mendis, Background subtraction in electron Compton spectroscopy, Micron 163 (2022) 103363.
- [16] R.F. Egerton, Electron Energy-Loss Spectroscopy in the Electron Microscope, Plenum Press, New York, 1996.
- [17] P. Moreau, M.C. Cheyner, Improved comparison of low energy loss spectra with band structure calculations: the example of BN filaments, Ultramicroscopy 94 (2003) 293.
- [18] M.J. Cooper, P.E. Mijnarends, N. Shiotani, N. Sakai, A. Bansil, X-Ray Compton Scattering, Oxford University Press, Oxford, 2004.
- [19] J.C.H. Spence, J.M. Zuo, Electron Microdiffraction, Plenum Press, New York, 1992.
 [20] E.J. Kirkland, Advanced Computing in Electron Microscopy, 2nd ed, Springer, New
- York, 2010. [21] G.S. Canright, Time-dependent screening in the electron gas, Phys. Rev. B 38 (1988) 1647.
- [22] P. Kruse, M. Schowalter, D. Lamoen, A. Rosenauer, D. Gerthsen, Determination of the mean inner potential in III-V semiconductors, Si and Ge by density functional theory and electron holography, Ultramicroscopy 106 (2006) 105.
- [23] A.I.M. Rae, Quantum Mechanics, 5thEdition, Taylor and Francis, USA, 2008.