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Coherent electron Compton scattering in crystals

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Abstract. An expression for the double differential cross section for electron Compton scattering with emphasis on coherent scattering in a crystal is derived. The resulting expression is evaluated for two beam conditions neglecting absorption. It is shown for this special case that the influence of coherent effects for s states is too small to be detected in the resulting Compton profiles.

1. Introduction

The momentum density distribution of electrons in solids can be probed by a Compton scattering experiment, in which the energy shift of an inelastically scattered x-ray is measured. More recently it has been demonstrated that equivalent results can be obtained in a transmission electron microscope by determining the energy loss of fast incident electrons, which have been scattered into large angles (Jonas and Schattschneider 1993a, b). Focusing the electron beam it is even possible to obtain the anisotropical shape of the Compton profile for small crystallites, which are only about $1\ \mu\text{m}$ in extension.

For the case of scattering in a crystal, however, we have to account for the fact that an incident electron passing through the specimen can no longer be described by a plane wave, but is represented by a sum of Bloch waves, leading to coherent scattering effects. In section 2 we derive an expression for the Compton scattering cross section treating the initial electron wavefunction as a sum of Bloch waves. For the sake of simplicity, absorption will be neglected. Section 4 presents the analytical evaluation of this expression in a one-electron approximation using silicon 3s wavefunctions. The impact of coherence upon electron Compton scattering experiments will be discussed in section 5 for a two-beam case.

2. The mixed dynamic form factor

According to Bloch's theorem the steady state solution of the Schrödinger equation for an electron propagating in a periodic medium is a superposition of Bloch waves (Metherell 1973)

$$\Psi_a(\mathbf{r}) = \sum_{j,g} u_g^{(j)} \exp[i(\mathbf{k}^{(j)} + \mathbf{g})\mathbf{r}] \quad \mathbf{k}^{(j)} = \mathbf{k}_a + \boldsymbol{\gamma}^{(j)}$$

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where the sum is taken over all possible reciprocal lattice vectors g and all degenerate Bloch waves $k^{(j)}$. We intend to investigate the scattering of an incident electron represented by Bloch waves into a free plane-wave state

$$\Psi_b(\mathbf{r}) = e^{i\mathbf{k}_b \mathbf{r}}.$$

The transition matrix element is then given by

$$\begin{aligned} \langle b|V|a\rangle &= \sum_{j,g} u_g^{(j)} \frac{1}{Q_{jg}^2} \langle f| \sum_n e^{iQ_{jg} r_n} |i\rangle \\ Q_{jg} &= k^{(j)} + g - k_b. \end{aligned} \quad (1)$$

This expression is valid for weak interactions so that the state vectors can be factorized since exchange effects are negligible; $|a\rangle = |\Psi_a\rangle \otimes |i\rangle$, $|b\rangle = |\Psi_b\rangle \otimes |f\rangle$ are the initial, resp. the final states of the combined crystal-probe electron system, and $|i\rangle$, $|f\rangle$ the initial, resp. final state of the crystal. The double differential cross section is proportional to

$$\frac{\partial^2 \sigma}{\partial E \partial \Omega} \propto \sum_b |\langle b|V|a\rangle|^2 \delta(E_i - E_f + E). \quad (2)$$

We obtain

$$\begin{aligned} \sum_b |\langle b|V|a\rangle|^2 \delta(E_i - E_f + E) &= \sum_f \sum_{\substack{j,g \\ j',g'}} u_g^{(j)*} u_{g'}^{(j')} \frac{1}{Q_{jg}^2 Q_{j'g'}^2} \left\langle i \left| \sum_n e^{-iQ_{jg} r_n} \right| f \right\rangle \\ &\quad \times \left\langle f \left| \sum_n e^{iQ_{j'g'} r_n} \right| i \right\rangle \delta(E_i - E_f + E) \\ &= \sum_{\substack{j,g \\ j',g'}} u_g^{(j)*} u_{g'}^{(j')} \frac{1}{Q_{jg}^2 Q_{j'g'}^2} S(Q_{jg}, Q_{j'g'}, E). \end{aligned} \quad (3)$$

Here we have introduced the mixed dynamic form factor $S(K := Q_{jg}, K' := Q_{j'g'}, E)$ which is formally defined as (Kohl and Rose 1985)

$$S(K, K', E) := \frac{1}{2\pi} \int_{-\infty}^{\infty} \langle i | \rho_K(t) \rho_{-K'} | i \rangle e^{iEt} dt.$$

Note that $\hbar = 1$ since we have used atomic units. We have used the integral representation of the δ function

$$\delta(E) = \frac{1}{2\pi} \int e^{iEt} dt$$

and the fact that

$$\rho_K = \sum_n e^{-iK r_n}$$

is the Fourier transform of the electron density operator $\rho(\mathbf{r})$; additionally the completeness relation $\sum_f |f\rangle \langle f| = 1$ was applied. The exact form factor obeys the symmetry relation

$S^*(K, K', E) = S(K', K, E)$, which is due to the invariance with respect to time reversal. In order to preserve this symmetry under the conditions of the impulse approximation (Eisenberger and Platzman 1970, Platzman and Tzoar 1965, Schattschneider *et al* 1990)

$$e^{iHt} = e^{iH_0t} e^{iVt} \underbrace{e^{-\frac{1}{2}(H_0, V)t^2} e^{\dots}}_{\simeq 1}$$

we use the fact that $S(K, K', E)$ is invariant with respect to time translations, thus we rewrite $S(K, K', E)$

$$\begin{aligned} S(K, K', E) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \langle i | \rho_K(t/2) \rho_{-K'}(-t/2) | i \rangle e^{iEt} dt \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \langle i | e^{iHt/2} \rho_K e^{-iHt/2} e^{-iHt/2} \rho_{-K} e^{iHt/2} e^{i\omega t} | i \rangle dt. \end{aligned} \tag{4}$$

The Hamiltonian of the scattering system is written as $H = H_0 + V$, together with the impulse approximation and $[\rho_K, V] = 0$ we obtain for the matrix element

$$\langle i | e^{iH_0t/2} \rho_K e^{-iH_0t/2} e^{-iH_0t/2} \rho_{-K} e^{iH_0t/2} | i \rangle.$$

Finally, the insertion of a complete system of momentum eigenfunctions $|p\rangle$ of H_0 , together with

$$e^{iH_0t} |p\rangle = e^{i\epsilon_p t} |p\rangle \quad \epsilon_p \equiv \frac{p^2}{2}$$

transforms (4) into

$$S(K, K', E) = \int \langle i | p - K \rangle \langle p - K' | i \rangle \delta \left\{ E - \frac{1}{2} [p(K + K')] - \frac{1}{2} (K^2 + K'^2) \right\} d^3p. \tag{5}$$

In a Wannier representation (Madelung 1972) the function $a_n(r - R_a)$ is a wave packet localized at the lattice sites R_a ; the functions are orthogonal with respect to different energy bands (n, n') and also to different lattice sites ($R_a, R_{a'}$). For the matrix elements we then have

$$\begin{aligned} \langle i | p - K \rangle \langle p - K' | i \rangle &= \sum_n \sum_{R_a} \int a_n^*(r - R_a) e^{i(p-K)r} d^3r \int a_n(r - R_a) e^{-i(p-K')r} d^3r \\ &= \sum_n a_n^*(p - K) a_n(p - K') \sum_{R_a} e^{i(\gamma^{(j')} - \gamma^{(j)} + g' - g)R_a}. \end{aligned} \tag{6}$$

The sum over atomic sites R_a may be split into a sum within the unit cell and a sum over all unit cells in the volume. The lattice vector in the z direction, chosen to be perpendicular to the surface, is a_z

$$\begin{aligned} \sum_{R_a} e^{i(\gamma^{(j')} - \gamma^{(j)} + g' - g)R_a} &= N_{xy} \underbrace{\sum_{\tau} e^{i(g' - g)\tau}}_{:=K_{g' - g}} \underbrace{e^{i(\gamma^{(j')} - \gamma^{(j)})\tau}}_{\simeq 1} \sum_{n=-d/2a_z}^{d/2a_z} e^{i(\gamma^{(j')} - \gamma^{(j)})a_z n} \\ &= N_{xy} K_{g' - g} \frac{\sin[(\gamma^{(j')} - \gamma^{(j)})d]}{\sin[(\gamma^{(j')} - \gamma^{(j)})a_z]} \simeq N K_{g' - g} \frac{\sin[(\gamma^{(j')} - \gamma^{(j)})d]}{(\gamma^{(j')} - \gamma^{(j)})d} \end{aligned}$$

where N_{xy} , N is the number of unit cells in the plane, resp. the volume. Finally, we end up for the double differential cross section for inelastic scattering from a crystal within the impulse approximation with

$$\begin{aligned} \frac{\partial^2 \sigma}{\partial E \partial \Omega} \propto & \sum_{j', g'} u_g^{(j)*} u_{g'}^{(j)} \frac{N K_{g'-g} \sin[(\gamma^{(j')} - \gamma^{(j)})d]}{Q_{jg}^2 Q_{j'g'}^2 (\gamma^{(j')} - \gamma^{(j)})d} \\ & \times \sum_n \int a_n^*(\mathbf{p} - \mathbf{Q}_{jg}) a_n(\mathbf{p} - \mathbf{Q}_{j'g'}) \delta\{E - \frac{1}{2}[\mathbf{p}(\mathbf{Q}_{jg} + \mathbf{Q}_{j'g'}) \\ & - \frac{1}{2}(\mathbf{Q}_{jg}^2 + \mathbf{Q}_{j'g'}^2)]\} d^3 \mathbf{p}. \end{aligned} \quad (7)$$

Table 1. Extinction distance ξ_g for silicon at a primary beam energy of $E_a = 200$ keV.

hkl	111	220	400	422
ξ_g [nm]	78.1	95.9	160.7	211.1

3. Coherent Compton scattering for a two-beam case

Expression (7) will now be evaluated for a two-beam case and atomic single-particle 3s wavefunctions for silicon. The $\gamma^{(j)}$ for the two-beam case are given by

$$\gamma^{(j)} = \pi [s - (-1)^j \sqrt{1/\xi_g^2 + s^2}]$$

with the excitation error s and the excitation distance ξ_g . For $u_0^{(j)}$ and $u_g^{(j)}$ we have

$$u_0^{(j)} = \frac{1}{2} \left(1 + (-1)^j \frac{w}{\sqrt{1+w^2}} \right) \quad u_g^{(j)} = -\frac{1}{2} \frac{(-1)^j}{\sqrt{1+w^2}}$$

with the dimensionless parameter $w = s\xi_g$ characterizing the tilt out of the Bragg condition (Reimer 1984). Since under practical conditions the extinction distance ξ_g in silicon (see table 1) far exceeds the lattice constant a_0 ($a_0 = 0.357$ nm) it follows that

$$|\gamma^{(1)} - \gamma^{(2)}| \ll |g| \neq 0$$

and finally

$$\mathbf{Q}_{jg} - \mathbf{Q}_{j'g'} \simeq \mathbf{g} - \mathbf{g}' \quad \rightarrow \quad \mathbf{Q}_g := \mathbf{k} + \mathbf{g} - \mathbf{k}_f.$$

With this approximation and the relations for $\gamma^{(j)}$ and $u_g^{(j)}$ we obtain an expression for the double differential scattering cross section including coherent scattering:

$$\begin{aligned} \frac{\partial^2 \sigma}{\partial E \partial \Omega} \propto & \frac{K_0}{2Q_0^4} \left(\frac{1+2w^2}{1+w^2} + \frac{1}{1+w^2} \frac{\sin \delta}{\delta} \right) S(\mathbf{Q}_0, \mathbf{Q}_0, E) \\ & + \frac{K_0}{2Q_g^4} \left[\frac{1}{1+w^2} \left(1 - \frac{\sin \delta}{\delta} \right) \right] S(\mathbf{Q}_g, \mathbf{Q}_g, E) \\ & - \frac{K_g}{2Q_0^2 Q_g^2} \left[\frac{2w}{1+w^2} \left(1 - \frac{\sin \delta}{\delta} \right) \right] S(\mathbf{Q}_0, \mathbf{Q}_g, E) \end{aligned} \quad (8)$$

where we have introduced the definition $\delta = (\gamma^{(1)} - \gamma^{(2)})d$; K_0 is simply the number of atoms in the unit cell and for K_g we get for the case of silicon

$$K_g = K_0 \cos \left[\frac{\pi}{4} (h + k + l) \right].$$

The first and the second part of (8) represent the incoherent scattering from the transmitted (0), resp. the Bragg-reflected beam (g), and is termed the 'direct term' in what follows; the third part arises from the coherent superposition of amplitudes from (0) and (g), and is referred to as the 'indirect term'.

4. Analytical evaluation of the mixed dynamic form factor

Within the limits of a one-electron approximation, the one-particle density matrix in momentum space will be discussed for a crystal composed of free atoms at the positions R_a . For this purpose we take atomic silicon single-particle wavefunctions given in position space (Duncanson 1947)

$$\Psi_{nlm}(\mathbf{r}) = N_r N_\theta N_\phi r^{n'-1} e^{-cr} P_l^m(\cos \theta) e^{im\phi}.$$

Of the occupied p and s states the latter lead to an expression for $S(K, K', E)$ that can be evaluated analytically. It was not possible to find a similar treatment for the p states, so calculation of the 3p contribution would necessitate lengthy numerical integration. We plan to perform these calculations in a forthcoming paper. Here we derive an analytical expression for the contribution of the 3s states to the indirect term.

Fourier transformation yields the normalized single-particle wavefunction in the momentum representation:

$$\begin{aligned} \Phi_{nlm}(\mathbf{p}) &= (-i)^l \left(\frac{2l+1}{\pi} \frac{(2c)^{n'+1}}{(2n)!} \right)^{1/2} P_l^m(\cos \theta) e^{im\phi} R_l(p) \\ R_l(p) &= \int_0^\infty r^{n'-1} \exp(-cr) j_l(pr) r^2 dr \end{aligned} \quad (9)$$

where n' is the effective principal quantum number whose value is equal to the true quantum number for levels up to $n = 3$ (Duncanson 1947); c is a quantity related to the nuclear charge Z and the screening constant σ by $c = (Z - \sigma)/n'$. The constant s determines the extent of the wavefunction in momentum space and hence the width of the Compton profile; for the calculations we chose $\sigma = 9.25$ so that the resulting direct Compton profile fitted the Hartree-Fock profiles given by Biggs (Biggs *et al* 1975). For 3s electrons ($n = 3$, $l = m_l = 0$) we obtain

$$R_0(p) = 24c \frac{c^2 - p^2}{(c^2 + p^2)^4} \quad \rightarrow \quad \Phi_{300}(\mathbf{p}) = \frac{c^2}{3\sqrt{5}\pi} R_0(p).$$

We will now briefly discuss the analytical evaluation of the integral

$$S_{\text{AI}}(K, K', E) = \int \Phi_{300}(\mathbf{p} - K) \Phi_{300}(\mathbf{p} - K') \delta \left\{ E - \frac{1}{2} [\mathbf{p} \cdot (K + K') - \frac{1}{2} (K^2 + K'^2)] \right\} d^3 p \quad (10)$$

of the atomic scattering factor $S_{\text{At}}(K, K', E)$, for which we will use the abbreviation \mathfrak{S} . We assume a symmetric two-beam scattering geometry, i.e. $g \cdot (K + K') = 0$ and therefore $|K| = |K'|$. The results presented below all refer to this kind of scattering geometry (Jonas and Schattschneider 1993a, b).

For the case $g = 0$, which is equivalent to $K = K'$, equation (10) leads to the result for the direct term:

$$S_{\text{At}}(K, K, E) = \frac{64c^6}{5K} \frac{(12\xi_{z0}^4 - 28c^2\xi_{z0}^2 + 11c^2)}{105(\xi_{z0}^2 + c^2)^7} \quad (11)$$

with

$$\xi_{z0} = \frac{2E - K^2}{2K}.$$

The integration of the indirect term ($g \neq 0$) requires a more detailed discussion. Using cylindrical coordinates, choosing the z axis parallel to $(K + K')$, the δ function transforms into

$$\delta[E - \frac{1}{2}(\xi_z |K + K'| + K \cdot K')] = \frac{2}{|K + K'|} \delta(\xi_z - \xi_{z0})$$

where we have introduced $\xi = p - K$ and defined $\xi_{z0} := (2E - K \cdot K') / (|K + K'|)$. Inserting the expression for $\Phi_{300}(p)$ into (10) and performing the ξ_z integration, \mathfrak{S} takes the form

$$\mathfrak{S} = \frac{2A}{\pi} \int_0^\infty \xi_r d\xi_r \int_0^{2\pi} d\phi \frac{(c^2 - \xi_{z0}^2 - \xi_r^2)(c^2 - g^2 - \xi_{z0}^2 - \xi_r^2 - 2g\xi_r \cos \phi)}{(c^2 + \xi_{z0}^2 + \xi_r^2)^4 (c^2 + g^2 + \xi_{z0}^2 + \xi_r^2 + 2g\xi_r \cos \phi)^4}$$

with

$$A = \frac{64c^6}{5 |K + K'|}.$$

The second factor of the integrand can be split into two parts:

$$\frac{2c^2}{(c^2 + g^2 + \xi_{z0}^2 + \xi_r^2 + 2g\xi_r \cos \phi)^4} - \frac{1}{(c^2 + g^2 + \xi_{z0}^2 + \xi_r^2 + 2g\xi_r \cos \phi)^3}.$$

Using the formulae

$$\int_0^{2\pi} \frac{d\phi}{(a + b \cos \phi)^3} = \pi \frac{2a^2 + b^2}{(a^2 - b^2)^{5/2}}$$

and

$$\int_0^{2\pi} \frac{d\phi}{(a + b \cos \phi)^4} = \pi a \frac{2a^2 + 3b^2}{(a^2 - b^2)^{7/2}}$$

derived† (Gradstein and Ryzhik 1981) from

$$\int_0^\pi \frac{d\phi}{(a + b \cos \phi)} = \frac{\pi}{\sqrt{a^2 - b^2}}$$

† The given formulae are only valid for $a > |b|$, a condition which for our case, as can be easily shown, will always be satisfied.

we perform the ϕ integration, obtaining

$$S = 2c^2 A \int_{c^2 + \xi_{20}^2}^{\infty} dy \frac{(2c^2 - y)(y + g^2) \{2y^2 + 16g^2y + 2g^2[g^2 - 6(c^2 + \xi_{20}^2)]\}}{y^4 (y^2 + py + q)^{7/2}}$$

$$- A \int_{c^2 + \xi_{20}^2}^{\infty} dy \frac{(2c^2 - y) \{2y^2 + 8g^2y + 2g^2[g^2 - 2(c^2 + \xi_{20}^2)]\}}{y^4 (y^2 + py + q)^{5/2}}$$

where we have made the substitution $y := \xi_r^2 + \xi_{20}^2 + c^2$ and used the abbreviations $p := -2g^2$ and $q := g^4 + 4g^2(c^2 + \xi_{20}^2)$. To solve the integrals we use the following formulae from Gradstein and Ryshik (1981):

$$I_m^n := \int \frac{dy}{y^m \sqrt{R^{2n+1}}} = -\frac{1}{(m-1)q y^{m-1} \sqrt{R^{2n-1}}} - \frac{(2n+2m-3)p}{2(m-1)q} I_{m-1}^n$$

$$- \frac{(2n+m-2)}{(m-1)q} I_{m-2}^n \quad m > 1$$

$$I_1^n := \int \frac{dy}{y \sqrt{R^{2n+1}}} = \frac{1}{(2n-1)q \sqrt{R^{2n-1}}} - \frac{p}{2q} I_0^n + \frac{1}{q} I_1^{n-1}$$

$$I_0^n := \int \frac{dy}{\sqrt{R^{2n+1}}} = \frac{2(2y+p)}{(2n-1)(4q-p^2)\sqrt{R^{2n-1}}}$$

$$\times \left(1 + \sum_{k=1}^{n-1} \frac{8^k (n-1)(n-2) \dots (n-k) R^k}{(2n-3)(2n-5) \dots (2n-2k-1)(4q-p^2)^k} \right) \quad n \geq 1$$

$$R := y^2 + py + q.$$

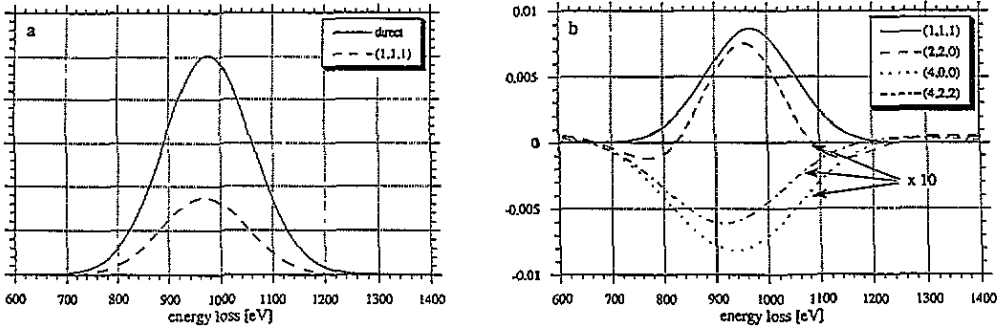


Figure 1. Dynamical form factor $S(K, K', E)$. (a) Direct term $S(K, K, E)$ compared to the indirect term $S(K, K + g, E)$ for $g_{1,1,1}$, momentum transfer $q = 16 \text{ \AA}^{-1}$. (b) Indirect term for reflections (1) $g_{1,1,1}$, (2) $g_{2,2,0}$, (3) $g_{4,0,0}$ and (4) $g_{4,2,2}$. Note the scale change from (1) to (2).

A decomposition into partial fractions allows us to apply the formulae to the integral immediately, leading finally to the result

$$S_{At}(K, K', E) = A \left(\delta_1 I_4^3 + \delta_2 I_3^3 + \delta_3 I_2^3 + \delta_4 I_1^3 + \delta_5 I_0^3 - \frac{2}{5(y^2 + py + q)^{5/2}} \right) \quad (12)$$

with

$$\delta_1 = 4c^2g^6(2c^2 - g^2) - 8c^2g^4(c^2 + \xi_{z0}^2)(6c^2 + g^2) + 32c^2g^4(c^2 + \xi_{z0}^2)^2$$

$$\delta_2 = 2g^4(g^4 - 6c^2g^2 + 36c^4) + 4g^2(g^4 - 14c^2g^2 - 12c^4)(c^2 + \xi_{z0}^2) - 16g^4(c^2 + \xi_{z0}^2)^2$$

$$\delta_3 = 12g^2c^2(6c^2 - g^2) + 4g^6 + 8g^2(c^2 + \xi_{z0}^2)(2c^2 + 5g^2)$$

$$\delta_4 = 4[2c^4 - 11g^2c^2 - 3g^4 + g^2(c^2 + \xi_{z0}^2)]$$

$$\delta_5 = 6g^2 - 8c^2.$$

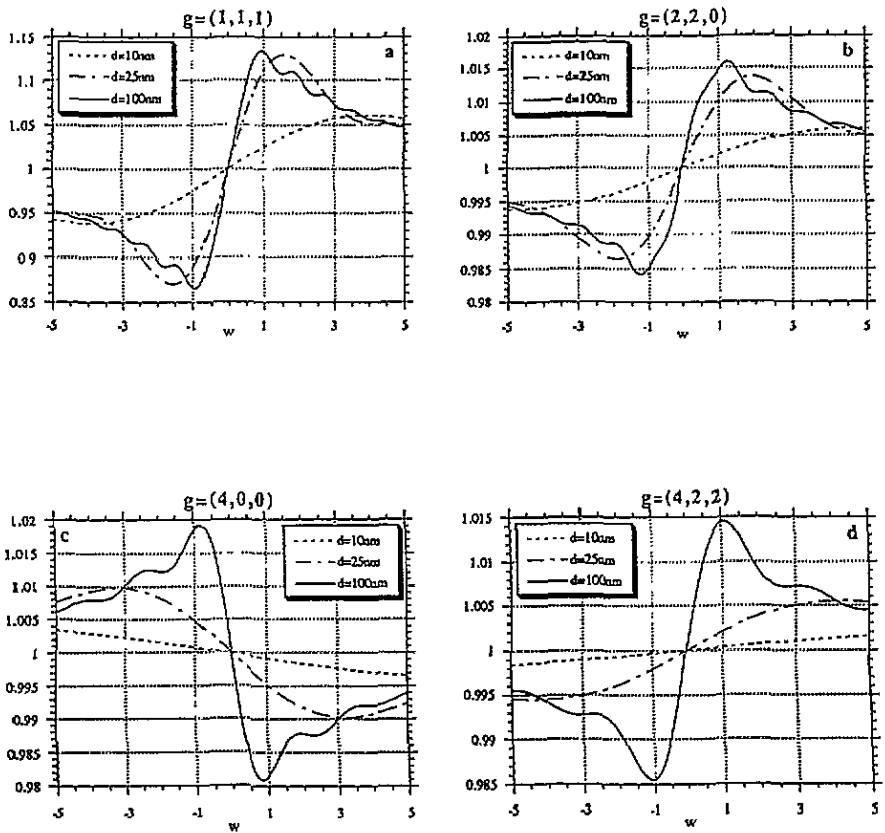


Figure 2. Expression (13) plotted against the deviation parameter w for various specimen thicknesses d . (a) $g_{1,1,1}$; (b) $g_{2,2,0}$; (c) $g_{4,0,0}$; (d) $g_{4,2,2}$.

5. Results

Figure 1(a) shows the direct form factor $S(K, K, E)$ compared to the strongest possible coherent contribution $S(K, K + g, E)$, caused by the Bragg reflection $g_{1,1,1}$. The mixed form factors $S(K, K + g, E)$ for Bragg reflections up to $g_{4,2,2}$ are shown in figure 1(b); we

obtain a rapid decrease in the intensity of the coherent contribution as we change g from $g_{1,1,1}$ to $g_{2,2,0}$. This is obvious from the structure of the integral (10) and the respective integrand $\Phi_{300}(p)$, as well as the fact that, for large g , the shape of the indirect term shows only a slow variation as a function of g . The symmetry axis of the indirect term shifts to lower energy loss when g is increased; this is caused by the argument of the δ function in (10) causing the integral to be symmetric with respect to an energy-loss value given by $E = \hbar^2 K \cdot K' / 2m_e$.

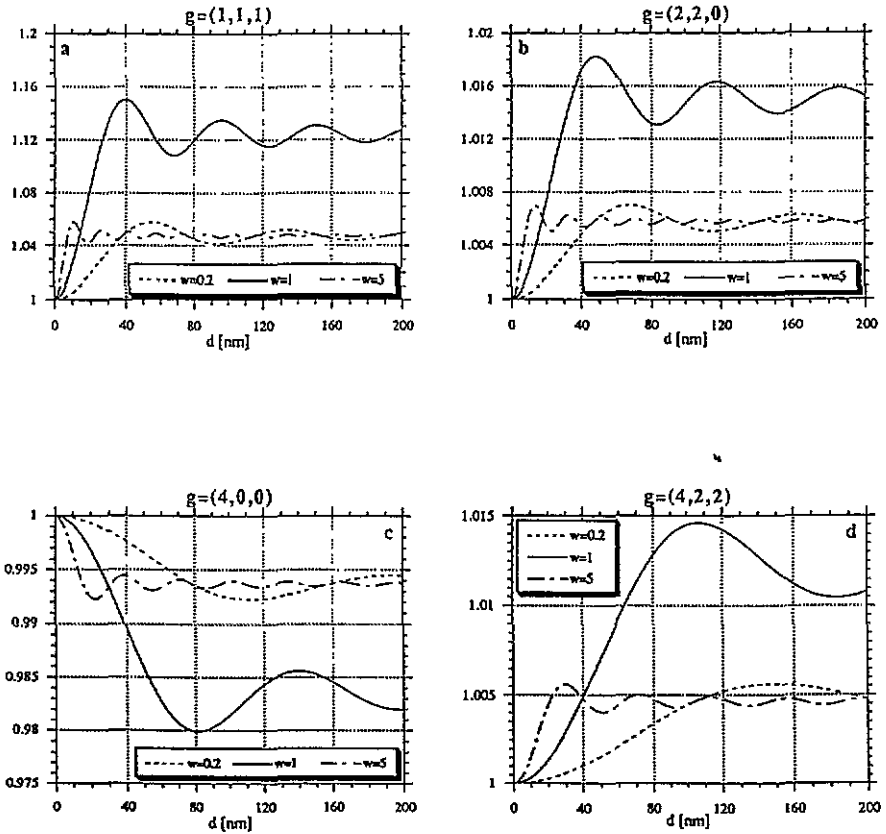


Figure 3. Expression (13) plotted against the specimen thickness d for various deviation parameters w . (a) $g_{1,1,1}$; (b) $g_{2,2,0}$; (c) $g_{4,0,0}$; (d) $g_{4,2,2}$.

In order to estimate the contribution of the indirect term to the total profile we rewrite (8) as

$$\frac{\partial^2 \sigma}{\partial E \partial \Omega} \propto \left[a_0 - a_1 \cos \left(\frac{\pi}{4} (h + k + l) \right) \frac{w}{1 + w^2} \left(1 - \frac{\sin \delta}{\delta} \right) \right] \quad (13)$$

where a_0 and a_1 stand for the contribution of the direct and the indirect term, respectively[†]. Expression (13) as a function of the deviation parameter w for Bragg reflections up to

[†] For the following estimation it is sufficient to take for a_0 and a_1 the values at the maximum of the respective $S(K, K', E)$, and define $a_0 := 1$.

$g_{4,2,2}$, is displayed in figure 2. The fact that catches the eye is that the indirect term contributes zero for $w = 0$, a rather simple consequence of (13). Tilting the crystal out of the Bragg condition enhances the weight of the coherent part until a maximum is reached; this maximum with respect to the modulus of its contribution lies for each g in the vicinity of $w = \pm 1$, dependent on d such that w_{\max} approaches $w = 1$ for a thickness $d > \xi_g/2$. The amount of the coherent part as a function of specimen thickness oscillates with a period proportional to ξ_g/w , see figure 3.

6. Conclusion

From our explicit calculations we find that for sufficiently large reciprocal lattice vectors the contribution of the indirect terms for s states is negligibly small. In that case the resulting Compton spectrum can be obtained by adding the relevant direct terms. For small reciprocal lattice vectors (e.g. Si-111) however, the indirect term contributes noticeably to the measured signal. As the energy loss spectrum of the indirect term is very similar to that of the direct term, the normalized spectra remain practically unchanged. In particular, it can be said that when working in a symmetric two-beam scattering geometry, the contributions of coherent scattering from 3s electrons—even when the incident electron beam is not exactly parallel—are negligible in electron Compton scattering experiments. It remains to be seen whether the same is true for the 3p states.

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