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Cross sections for X-ray plasmon and Compton scatterings

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An attempt has been made to bring together for the first time the different formulae for X-ray plasmon and Compton scatterings in a unified formalism. Numerical calculations are presented for beryllium and lithium in order to arrive at the optimum condition for observing the pure plasmon scattered spectrum. It has been shown that for beryllium it should correspond to $k/k_F \sim 0.5$ and for lithium $k/k_F \sim 0.8$. A new and simple method to obtain the plasmon scattering cross section is also described.

1. Introduction

Several workers (Priftis *et al* 1968, 1970, Tanokura *et al* 1970, Suzuki *et al* 1970, Alexandropoulos 1971, Miliotis 1971) have recently observed plasmon excitation in X-ray scattering experiments from solids of low atomic number, such as, beryllium, lithium and graphite. Very often the plasmon, Compton and the elastic (Rayleigh-Thomson) components of the scattered radiation overlap on one another making it very difficul to separate the plasmon spectrum. There exists considerable theoretical work (Pines 1963, Pimpale & Mande 1971, Kliewer & Raether 1973) on the cross section for the X-ray plasmon scattering and the shape of the plasmon scattered spectrum for different scattering angles. Most of this work is either within the random phase approximation (RPA) or seeks simple modifications of the RPA. It is generally recognised that the plasmon excitation predominates the scattered spectrum for small scattering angles and the Compton process dominates for large scattering angles. However, there do not exist any specific calculations of the relative amplitudes of the different components of the scattered radiation which may be present in the experimental curves. The purpose of this note is to bring the different formulae for the cross sections in a unified formalism and to present specific calculations of these for the most often studied experimental materials beryllium and lithium. An attempt is made from this study to see whether it is necessary to unfold the experimental spectrum in its different components for a particular scattering angle and whether it is possible to obtain the experimental condition in which only plasmon excitation predominates. A new and simple method to obtain the pure plasmon scattering cross section within RPA is discussed in appendix 1.

2. Cross Sections for the Different Scattering Processes

The most general expression for the scattering cross section from an interacting many electron system, such as a solid is given by Pines (1963) as,

$$d^2\sigma/d\Omega d\omega = (e^2/mc^2)^2(e_i \, . \, e_s)^2 S(\boldsymbol{k}, \omega), \qquad \ldots \quad (1)$$

where

$$S(\boldsymbol{k}, \omega) = \sum_n |(\rho_{\boldsymbol{k}}{}^\dagger)_{n0}|^2 \, \delta(\omega - \omega_{n0}) \qquad \ldots \quad (2)$$

is the scattering form factor. In the above equations e_i and e_s are polarization vectors for the incident and the scattered photons, $\hbar\omega$ and $\hbar\boldsymbol{k}$ are respectively the energy and momentum transferred by the photon to the system in the act of scattering, $\rho_{\boldsymbol{k}}{}^\dagger$ is the electronic density fluctuation operator, $\hbar\omega_{n0}$ is the system excitation energy for the n-th state and the other symbols have their usual significance. The cross sections for the plasmon, Compton and elastic scattering processes can be obtained as special cases from eq. (1) by considering appropriate physical situations.

Although the plasmon cross section within RPA can be derived in many ways, we find it convenient to obtain it by a new and simple method (which is described in the appendix) by employing the Bohm-Pines collective formalism and utilizing their subsidiary conditions to obtain the plasmon wave function in terms of the electronic density fluctuations. The value of $S(\boldsymbol{k}, \omega)$ for plasmon scattering is obtained as,

$$S_{pl}(\boldsymbol{k}, \omega) = (N\hbar \boldsymbol{k}^2/2m\omega_p)\delta(\omega - \omega_p), \qquad \ldots \quad (3)$$

where N is the number of electrons per unit volume in the system and ω_p is the plasma frequency. From eq. (3) it is seen that the shape of the plasmon scattered spectrum is given by a delta function. This has to be modified as shown by Kliewer & Raether (1973) to obtain a more realistic shape of the plasmon scattered line. However, we are not interested in this line shape but in the total intensity under for a particular scattering angle ϕ. This can be obtained from eq. (3) by integrating it over all frequencies, as accurately as from the more elaborate formulae. Since in the usual experiments no attention is generally paid to the polarization of X-rays we average over the incident photon polarizations and sum over the final photon polarizations. We thus obtain the angular dependence of the plasmon scattering cross section as,

$$d\sigma/d\Omega \text{ (plasmon)} = (e^2/mc^2)^2(1 - \tfrac{1}{2}\sin^2\phi)S_{pl}(k), \qquad \ldots \quad (4)$$

with

$$S_{pl}(k) = (\hbar k^2/2m\omega_p) = (E_F/\hbar\omega_p)(k/k_F)^2. \qquad \ldots \quad (5)$$

In the above equation $E_F = \hbar^2 k_F/2m$ and k_F is the value of the wave vector at the Fermi surface.

The Klein-Nishina cross section for the usual Compton scattering by an ideally free electron (after averaging over the incident photon polarizations and summing over the final photon polarizations) is given by Feynman (1962) as

$$d\sigma/d\Omega(KN) = (e^2/mc^2)^2\tfrac{1}{2}(\omega_s/\omega_i)(\omega_s\omega_i+\omega_i/\omega_s-\sin^2\phi), \tag{6}$$

where ω_i and ω_s are the frequencies of the incident and scattered photons and ϕ is the scattering angle. When $\omega_i \simeq \omega_s$, eq. (4) reduces to the Rayleigh -Thomsón scattring cross section,.

$$d\sigma/d\Omega(KN) \approx d\sigma/d\Omega(RT) = (e^2/mc^2)^2(1-\tfrac{1}{2}\sin^2\phi)S_{el}(k). \tag{7}$$

It is easily seen that

$$S_{el}(k) = 1. \tag{8}$$

For calculating the cross section for Compton scattering from electrons in solids eq. (7) is inadequate since it does not take account of the Pauli exclusion principle. We therefore make use of the Hartree-Fock approximation to calculate this cross section. In this approximation one obtains, as shown by Pines (1963),

$$S_{CHF}(\boldsymbol{k}, \omega) = \sum_q \delta(\omega-\omega_{qk}), \tag{9}$$

where

$$\omega_{qk} = \hbar \boldsymbol{q}^2/2m+\hbar\boldsymbol{k}\cdot\boldsymbol{q}/m. \tag{10}$$

In the above equation the summation over $\boldsymbol{q}$ runs over the electronic states satisfying $|\boldsymbol{q}| \leqslant k_F$, $|\boldsymbol{q}+\boldsymbol{k}| > k_F$, where k_F is the value of the wave vector at the Fermi surface. Integrating eq (9) over all frequencies we obtain the cross section for Compton scattering in HFA as,

$$d\sigma/d\Omega(\mathrm{CHF}) = (e^2/mc^2)^2\,(1-\tfrac{1}{2}\sin^2\phi)\; S_{CHF}(k) \tag{11}$$

with

$$S_{CHF}(k) = \frac{3}{4}\,\frac{k}{k_F} - k^3/16\,k^3{}_F. \tag{12}$$

If we take into account the electronic correlations, then, within the RPA, the scattering form factor for Compton scattering becomes

$$S_{CRP}(\boldsymbol{k}, \omega) = S_{CHF}(\boldsymbol{k}, \omega)/|\epsilon|^2, \tag{13}$$

where ϵ is the RPA dielectric function. Noting that the ω's involved in eqs. (6) and (10) are small as compared to ω_p, we may use the following approximate value of ϵ as

$$\epsilon = 1+k^2{}_{FT}/k^2, \tag{14}$$

where k_{FT} is the Fermi-Thomas screening wave vector given by

$$k_{FT} = \sqrt{3}m\omega_p/\hbar k_F. \tag{15}$$

Using eqs. (13) and (14) we easily obtain

$$d\sigma/d\Omega(\text{CRP}) = (e^2/mc^2)^2(1-\tfrac{1}{2}\sin^2\phi)S_{CRP}(k), \quad \cdots \quad (16)$$

where

$$S_{CRP}(k) = \left\{\frac{3}{4}\frac{k}{k_F} - \frac{k^3}{16k^3_F}\right\} \Big/ (1+k^2_{FT}/k^2)^2. \quad \cdots \quad (17)$$

3. Calculations

Since considerable experimental work on X-ray plasmon scattering has been reported on beryllium and lithium, we have numerically calculated the values of $S_{pl}(k)$ and $S_{CRP}(k)$ for these solids for the values of k/k_F ranging from 0 to 1. For these calculations the values of the plasma energy $\hbar\omega_p$ and the Fermi energy E_F are necessary. We have employed in our calculations the recent experimental values of $\hbar\omega_p$(Pines 1963) and E_F (Wallace 1960, Crisp & Williams 1960). For beryllium $\hbar\omega_p = 19$ eV, $E_F = 13.8$ eV and for lithium $\hbar\omega_p = 8$ eV, $E_F = 3.0$eV The variation of $S_{pl}(k)$ and $S_{CRP}(k)$ thus calculated for beryllium and lithium is depicted graphically in figure 1. The points corresponding to k_c/k_F where k is the plasmon cut-off wave vector are also shown on the $S_{pl}(k)$ curves.

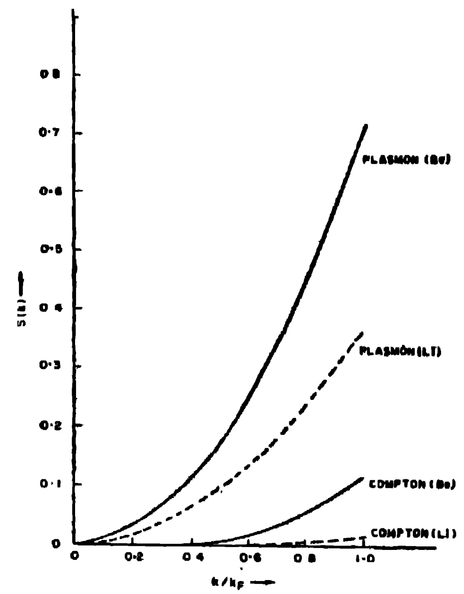

Fig.. 1. The variation of the scattering form factor $S(k)$with k/k_F for Compton and plasmon processes for beryllium and lithium.

4. Discussion

The optimum experimental conditions can be determined from figure 1 in association with the following points :

1. The plasmon width increases slowly with k for $k < k_c$ and it is not a well defined excitation for $k > k_c$ in that the plasmon width increases rapidly with k when it has crossed the cut-off value k_c.

2. The Compton line profile given approximately by $S_{CHF}(\boldsymbol{k}, \omega)/|\epsilon|^2$ [eqs. (6) and (8)] is highly asymmetric and its width on the high energy side is much lower than that on the low energy side. Further, for values of $k/k_F < 1$, the energy of the Compton profile peaks is, generally, considerably less than $\hbar\omega_p$.

From figure 1, with due cognizance to the above points, we note that in the case of beryllium the best plasmon spectrum with practically no other inelastic component would appear for $k/k_F \sim 0.5$ to 0.6. For $k/k_F > 0.6$ the plasmon width would be considerably large and so also would be the width and intensity of the Compton profile. In the range $1 \gtrsim k/k_F \gtrsim 0.5$ one would have a superposition of a wide plasmon spectrum and the Compton profile. In the case of lithium the best plasmon spectrum would appear at $k/k_F \sim 0.8$. From figure 1 it is also evident that one would obtain a better contrast for lithium than for beryllium since the probability of Compton scattering is very much lower in lithium.

For the $\mathrm{Cr}K_{\beta 1}$ radiation which is often used in experiments ($\lambda = 2.085$Å, $k_i = 3.0135$Å^{-1}) the above condition of k/k_F corresponds to the scattering angle $\phi \approx 20° \pm 2°$ for beryllium and for lithium it corresponds to the scattering angle $\phi \approx 14° \pm 2°$. At these angles one can expect to get the plasmon spectrum with practically no superposed Compton spectrum, *i.e.*, a *pure* plasmon spectrum and it would not be necessary to separate out different components of the inelastic spectrum. For increasing the scattering angles one may employ low energy radiation such as $T_i K_{\beta 1}$ (~ 4.9 KeV) for which the optimum scattering angle for beryllium is 27° and for lithium 20°.

Appendix I

A new method to obtain the RPA X-ray Plasmon scattering cross section

In the Bohm-Pines collective formalism the system wave function is given by

$$|\psi> = \psi \times \phi \text{ (plasmon)}, \tag{A.1}$$

where ψ is the determinant wave function of the electrons and ϕ is the plasmon wave function. In the ground state the plasmon execute only the zero point oscillations and their wave function (in momentum space) is given by

$$\phi \text{ (plasmon)} = \exp\left\{-\sum_{k<k_c} \frac{P_k^{\dagger} P_k}{2\hbar\omega_p}\right\}, \tag{A.2}$$

where P_k is the collective momentum variable. P_k is connected with the density fluctuation ρ_k through the subsidiary condition

$$\{P_k - M_k \rho_k\} | \psi > = 0, \qquad \text{... (A.3)}$$

where $M_k^2 = 4\pi e^2/k^2$. From eq. (A.3) we can write

$$\phi\,(\text{plasmon}) = \prod_{k<k_c} \exp\{-M_k^2 \rho_k^\dagger \rho_k / 2\hbar\omega_p\}. \qquad \text{... (A.4)}$$

Eq. (A.4) resembles the unnormalized wave function for an assembly of $k_c^3/6\pi^2$ independent harmonic oscillators in their ground state, each with frequency ω_p. M_k^2 and $\rho_k^\dagger \rho_k$ play the roles of the force constant and the square of the position coordinate for the k-th oscillator. The first excited state for the k-th oscillator is then given by

$$\phi^1(k\text{-th oscillator}) = N_k \rho_k \exp(-M_k^2 \rho_k^\dagger \rho_k / 2\hbar\omega_p), \qquad \text{... (A.5)}$$

where N_k is the normalization constant. From eqs (1), (A.1), (A.4) and (A.5), using proper normalization constants, and assuming that only a plasmon is excited in the act of scattering, we obtain the value of $S_{pl}(k)$ as given in eq. (3).

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