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X-ray polaroids based on the total external reflection in anomalous-dispersion regions

V Sh Machavariani

Raymond and Beverley Sackler School of Physics and Astronomy, Tel-Aviv University, 69978, Tel-Aviv, Israel

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Abstract. A new method of development of x-ray polaroids is suggested. The idea is based on the effect of total external reflection from an anisotropic crystal in the anomalous-dispersion region. The polarization coefficient for hexagonal BN crystal near the boron K absorption edge is calculated for different glancing angles and thicknesses of sample. It is shown that the method treated provides a simple way of constructing an effective x-ray polaroid.

1. Introduction

X-ray scattering in condensed matter in a normal-dispersion region of photon energies can be described satisfactorily within the framework of the free-atom approach to the calculation of a permittivity tensor (PT). In this frequency region the PT is an isotropic tensor [1], and the small anisotropic correction which is needed because of the anisotropy of the crystalline potential is negligible. This anisotropy is insufficient for creating x-ray polaroids.

Nevertheless, there have been several experiments performed such as the studies of the orientational dependence of the XANES [2] and the polarization dependence of x-ray reflectivity fine structure (XRFS) in hexagonal BN crystals [3, 4] which prove that there is an appreciable anisotropy of the PT in low-symmetry crystals if the photon energy is near the absorption edge of any atomic core level. In this case the PT depends appreciably on the chemical state and environment of the scattering atoms. Earlier we showed [5, 6] that this is caused by the scattering of the photoelectrons or virtual electrons from the neighbouring atoms (in the case of the x-ray elastic scattering process, photoelectrons do not appear in the final state, but in the intermediate state virtual electrons exist). Due to photoelectron and virtual-electron interactions with surrounding atoms the PT becomes an anisotropic tensor with a sharp photon energy dependence in the anomalous-dispersion region. Our calculations of the XRFS [6] appear to be in reasonable agreement with experimental spectra [3]. We have shown that the anisotropy of the PT leads to crystal optic effects both in reflectivity [6] and in absorption [7] x-ray spectra, such as polarization and orientation dependencies of the x-ray reflectivity fine structure, and differences in the fine structures of left- and right-hand circularly polarized radiation both in reflection and absorption spectra. In this paper we suggest using the effect of total external reflection of x-ray radiation for the development of efficient x-ray polaroids. The idea of the polaroid is based on the difference between the critical angles of total external reflection for two different polarizations of the incident radiation in low-symmetry crystals in the anomalous-dispersion region.

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2. The x-ray polaroid effect in uniaxial crystals in the anomalous-dispersion region

In the x-ray region the permittivity of the crystal has the form $\varepsilon = 1 - \alpha + \mathrm{i}\beta$. The minus sign before the second term indicates that a crystal is a material which is optically less dense than vacuum. This leads to the effect of total external reflection. Let us consider refraction within the sample when the glancing angle θ is close to the critical value $\theta^{crit} = \sqrt{\alpha}$ (if α^2 and $\beta^2 \ll \alpha$) of the total external reflection. In this case the depth of penetration of the radiation into the sample depends very strongly on the glancing angle. If the absorption is negligible, the intensity of the radiation does not depend on the distance from the surface for all angles $\theta > \theta^{crit}$ and decreases exponentially for $\theta < \theta^{crit}$. In real crystals the dependence of the penetration depth on the glancing angle is not so strong, but it is very strong when θ is close to θ^{crit}. For anisotropic crystals there are two different critical angles for two different polarizations of the incident radiation.

Let us consider for simplicity the case of a uniaxial crystal in an anomalous-dispersion region. The PT of the uniaxial crystal is a diagonal tensor in the rectangular coordinate system x, y, z if one of the axes of this system coincides with the optical axis of the crystal. This is correct even in the case of a complex PT with absorption taken into account. We shall call the plane parallel to the wave vectors of the incident and reflected radiation the scattering plane hereafter. Let us consider first the case where the crystal face is perpendicular to the optical axis. In such a case there are two different critical angles θ_s^{crit} and θ_p^{crit} for s- and p-polarized incident radiation. The critical angle θ_s^{crit} is determined by $\varepsilon_\perp$, and θ_p^{crit} is determined by $\varepsilon_\parallel$, where $\varepsilon_\parallel$ and $\varepsilon_\perp$ are the permittivities for the electric field parallel and perpendicular to the optical axis. Thus we can choose the glancing angle θ to be less than θ_s^{crit} and more than θ_p^{crit} if $\theta_s^{crit} > \theta_p^{crit}$ or to be more than θ_s^{crit} and less than θ_p^{crit} if $\theta_s^{crit} < \theta_p^{crit}$:

$$\min(\theta_s^{crit}, \theta_p^{crit}) < \theta < \max(\theta_s^{crit}, \theta_p^{crit}). \tag{1}$$

In this case the s- (or p-) polarized radiation will decrease in the sample more strongly than the p (or s) radiation. Because of the small difference between the critical values θ_s^{crit} and θ_p^{crit}, the incident x-ray radiation must be collimated.

To use this effect for the creation of x-ray polaroids we suggest the following scheme: x-ray radiation is passed through the plane-parallel sample provided that the angle between the incident wave and the crystal face is near to the critical value for total external reflection. For the case where the glancing angle θ is chosen according to (1), transmitted radiation will be strongly polarized.

In the case where the x- and y-axes belong to the crystal face and the y- and z-axes belong to the scattering plane it is easy to write boundary conditions for incident, reflected, refracted and transmitted waves and obtain explicit formulae for the transmission of s- and p-polarized incident radiation:

$$T_s = \left| \frac{4k_z^{(s)}(\omega/c)\sin\theta}{((\omega/c)\sin\theta + k_z^{(s)})^2 \exp(-\mathrm{i}k_z^{(s)}L) - ((\omega/c)\sin\theta - k_z^{(s)})^2 \exp(+\mathrm{i}k_z^{(s)}L)} \right|^2 \tag{2}$$

$$T_p = \left| \frac{4\varepsilon_{yy}k_z^{(p)}(\omega/c)\sin\theta}{(\varepsilon_{yy}(\omega/c)\sin\theta + k_z^{(p)})^2 \exp(-\mathrm{i}k_z^{(p)}L) - (\varepsilon_{yy}(\omega/c)\sin\theta - k_z^{(p)})^2 \exp(+\mathrm{i}k_z^{(p)}L)} \right|^2 \tag{3}$$

where T_s and T_p are transmission coefficients for s- and p-polarized radiation respectively, $T = I/I_0$, I_0 and I are the intensities of the incident and transmitted radiation, $\varepsilon_{\alpha\beta}$ is the

PT, L is the thickness of the sample, $k_z^{(s)}$ and $k_z^{(p)}$ are the z-components of the wave vector in the sample for s and p polarization, and

$$k_z^{(s)} = \frac{\omega}{c}\sqrt{\varepsilon_{xx} - \cos^2\theta} \tag{4}$$

$$k_z^{(p)} = \frac{\omega}{c}\sqrt{\varepsilon_{yy} - \frac{\varepsilon_{yy}\cos^2\theta}{\varepsilon_{zz}}}. \tag{5}$$

Also ω is the frequency of radiation, and c is the velocity of light.

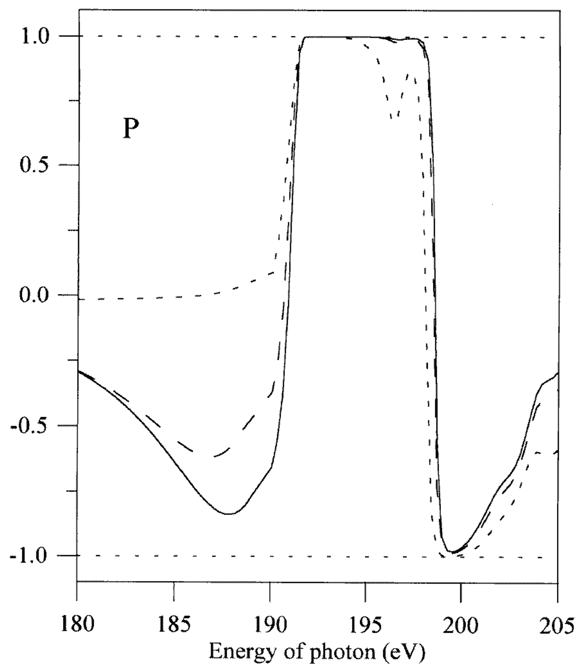

Figure 1. The polarization coefficient P for h-BN crystal for the glancing angles $\theta = 3^\circ$ (solid line), 5° (dashed line) and 10° (dotted line) versus the photon energy. The optical axis is perpendicular to the crystal face. The thickness of the sample is $L = 0.03\ \mu$m.

3. Calculation of the polarization coefficient in a hexagonal BN crystal

To demonstrate the method proposed we have applied it to hexagonal BN (h-BN) crystal near the boron K edge of photon energies. The crystal of h-BN has a graphite-like structure and therefore it is a uniaxial crystal. Earlier we calculated the PT of h-BN crystal [5, 6]. It was found that our calculation of the PT was in good agreement with experimental absorption spectra. Let us determine the polarization coefficient $P = (T_s - T_p)/(T_s + T_p)$. This coefficient shows the degree of polarization of transmitted radiation if the incident radiation is completely unpolarized. Thus, if $P = +1$, then the transmitted radiation has s polarization, if $P = -1$, then the transmitted radiation has p polarization, and if $P = 0$, then the transmitted radiation is completely unpolarized. We calculated the polarization coefficient P for h-BN crystal for the different glancing angles and thicknesses of the sample in the case when the optical axis of the crystal is perpendicular to the crystal face.

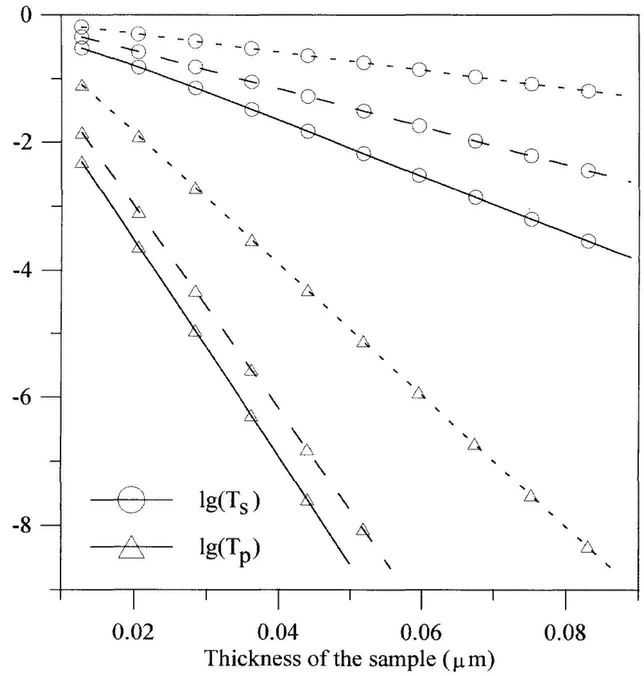

Figure 2. $\lg(T_s)$ and $\lg(T_p)$ for $\theta = 3^\circ$ (solid lines), 5° (dashed lines) and 10° (dotted lines) versus the thickness of the sample for a photon energy of 194 eV.

In figure 1 one can see P for $L = 0.03$ μm and $\theta = 3^\circ$ (the solid line), $\theta = 5^\circ$ (the dashed line) and $\theta = 10^\circ$ (the dotted line). One can see from figure 1 that for the energy region from 191 eV to 196 eV there is a strong polarization effect, and the transmitted radiation will have s polarization ($P = +1$). One can also see from figure 1 that in the case of small glancing angles the values of P are closer to $+1$ or to -1, and thereby small glancing angles are more convenient for the creation of x-ray polaroids. To understand the rate of decrease of the transmitted radiation we calculate T_s and T_p for the photon energy 194 eV versus the thickness of the sample for several glancing angles. In figure 2, $\lg(T_s)$ and $\lg(T_p)$ are shown for $\theta = 3^\circ$ (solid lines), $\theta = 5^\circ$ (dashed lines) and $\theta = 10^\circ$ (dotted lines) for a photon energy of 194 eV. One can see from figure 2 that even for a small thickness of sample there is a strong x-ray polaroid effect. Thus x-ray polaroids can be made even using thin films. Also figure 2 shows that the intensity of the transmitted radiation is quite sufficient for practical use.

4. Conclusions

In this paper a method of creation of x-ray polaroids in the soft-x-ray region is proposed. It is shown that in the case of h-BN crystal there is a strong polarization effect in the anomalous-dispersion region. It is found that in the h-BN crystal the most convenient conditions for building x-ray polaroids are found for a photon energy of 194 eV (s polarization) and a glancing angle of $\theta = 3^\circ$.

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