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The crystal optic effects in x-ray absorption spectroscopy in the anomalous dispersion region

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Abstract. Calculations of the permittivity tensor (PT) of a hexagonal BN (h-BN) crystal carried out near the B K edge by the Green function method show that the anisotropy of the PT can be considerable in the x-ray region of the spectra. Such anisotropy causes pronounced crystal optic effects in x-ray absorption spectroscopy such as the existence of x-ray polaroid and quarter-wave plate effects. It is shown that absorption spectra of the left and right circularly polarized radiation can differ from each other in biaxial crystals. Anisotropy of PT leads to violation of the exponential decrease of x-ray intensity.

The permittivity tensor (PT) in condensed matter in the normal dispersion region of photon energy can be calculated satisfactorily within the framework of the free-atom approach. The isotropy of the PT in this frequency region is usually assumed. Meanwhile experimental studies of the XAFS polarization and orientational dependences have shown that imaginary parts of the PT could be essentially anisotropic tensors in the vicinity of the K and L atomic edges in the case of low-symmetry crystals [1]. As was shown in [2] the PT tensor of low-symmetry crystals could be essentially anisotropic in the soft-x-ray region if the wavelength is close to some atomic core level absorption edge. In the present paper we show that anisotropy of the PT leads to such crystal optic phenomena in x-ray absorption spectroscopy as the existence of the x-ray polaroid and quarter-wave plate effects. It is shown also that x-ray absorption spectra of the left and right circularly polarized radiation can differ from each other in biaxial crystals. Anisotropy of the PT leads to violation of the exponential decrease of the x-ray intensity and this phenomenon can lead to dependence of the experimental XAFS on the sample width.

In the case of x-ray absorption by low-symmetry crystals in the vicinity of the K and L atomic edges we study the polarization dependence of the spectra. In this case the electric field components $E_x^{(1)}$ and $E_y^{(1)}$ of the transmitted radiation are connected with the components $E_x^{(0)}$ and $E_y^{(0)}$ of the incident wave as follows:

$$\begin{bmatrix} E_x^{(1)} \\ E_y^{(1)} \end{bmatrix} = \begin{bmatrix} A+B & C \\ C & A-B \end{bmatrix} \begin{bmatrix} E_x^{(0)} \\ E_y^{(0)} \end{bmatrix} \tag{1}$$

where

$$A = \tfrac{1}{2}[\exp(\mathrm{i}Lk_1) + \exp(\mathrm{i}Lk_2)] \tag{2}$$

$$B = \frac{a}{2(a^2+b^2)^{1/2}}[\exp(\mathrm{i}Lk_1) - \exp(\mathrm{i}Lk_2)] \tag{3}$$

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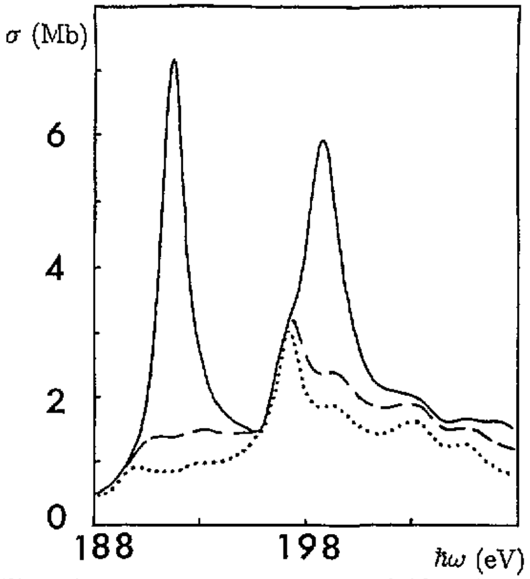

Figure 1. Absorption cross section of the primitive volume of a h-BN crystal near the boron K edge for sample widths 0.01 μm (——), 0.2 μm (- - - -) and 1.6 μm (· · · · · ·).

$$C = \frac{b}{2(a^2+b^2)^{1/2}}[\exp(\mathrm{i}Lk_1) - \exp(\mathrm{i}Lk_2)] \tag{4}$$

$$k_1 = \frac{\omega}{4c}\left(\varepsilon_{11} + \varepsilon_{22} - \frac{\varepsilon_{13}^2}{\varepsilon_{33}} - \frac{\varepsilon_{23}^2}{\varepsilon_{33}} + (a^2+b^2)^{1/2}\right) \tag{5}$$

$$k_2 = \frac{\omega}{4c}\left(\varepsilon_{11} + \varepsilon_{22} - \frac{\varepsilon_{13}^2}{\varepsilon_{33}} - \frac{\varepsilon_{23}^2}{\varepsilon_{33}} - (a^2+b^2)^{1/2}\right) \tag{6}$$

$$a = \varepsilon_{11} - \varepsilon_{22} - \frac{\varepsilon_{13}^2}{\varepsilon_{33}} + \frac{\varepsilon_{23}^2}{\varepsilon_{33}} \tag{7}$$

$$b = 2\left(\varepsilon_{12} - \frac{\varepsilon_{13}\varepsilon_{23}}{\varepsilon_{33}}\right). \tag{8}$$

ω is the radiation frequency, c is the light velocity, the O_z axis is perpendicular to the sample surface, L is the sample width and $\varepsilon_{\alpha\beta}$ is the PT. The total intensity I_1 of the transmitted radiation takes the form

$$I_1 = I_0[|A|^2 + |B|^2 + |C|^2 + 2\,\mathrm{Im}(B^*C)] \tag{9}$$

for the right circularly polarized incident radiation and

$$I_1 = I_0[|A|^2 + |B|^2 + |C|^2 - 2\,\mathrm{Im}(B^*C)] \tag{10}$$

for the left circularly polarized incident radiation, where I_0 is the incident radiation intensity. One can see from equations (9) and (10) that the transmitted radiation intensities for the left and right circularly polarized incident radiation can differ from each other. In the case of unpolarized incident radiation we have

$$I_1 = I_0(|A|^2 + |B|^2 + |C|^2). \tag{11}$$

If experimental absorption spectra of a low-symmetry crystal are analysed by means of the usual formula $\sigma = (1/nL)\ln(I_1/I_0)$, then the absorption cross section σ depends on the sample width. This is illustrated in figure 1 where the XANES of a h-BN crystal near the boron K edge for sample widths 0.01, 0.2 and 1.6 μm for unpolarized incident radiation are shown. The details of the PT calculations for a h-BN crystal have been presented in [3].

We draw attention to the fact that even in the x-ray region the crystal optic effects such as the x-ray polaroid and quarter-wave plate effects could exist. If we consider a photon energy which is several electronvolts less than the absorption threshold in a low-symmetry crystal, then the imaginary parts of the PT components are small and consequently the photon mean free path is large. Nevertheless the real parts of the PT components can differ from each other significantly. This leads to the quarter-wave plate effect. If we consider a photon energy which exceeds some absorption threshold in a low-symmetry crystal, then the imaginary parts of the PT components strongly depend on the photon energy and it is possible that for some energy the imaginary part of one component of the PT is significantly less than the imaginary part of the other PT component. In this case the absorption coefficients for the different polarization directions of incident radiation could differ significantly from each other. This leads to the x-ray polaroid effect.

Acknowledgments

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References

[1] Brouder C 1990 *J. Phys.: Condens. Matter* 2 701
[2] Vedrinskii R V, Kraizman V L, Novakovich A A and Machavariani V Sh 1992 *J. Phys.: Condens. Matter* 4 6155
[3] Vedrinskii R V, Kraizman V L, Novakovich A A and Machavariani V Sh 1993 *J. Phys.: Condens. Matter* 5 8643