X-RAY CRYSTAL OPTICS FOR ANALYSER BASED IMAGING

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1. Introduction

X-ray crystal optics providing asymmetric diffraction can be designed for a number of applications. For metrological applications [1]the most important is high intensity throughput, while the imaging applications [2, 3] moreover require the spatial homogeneity of the wave-field impinging on an X-ray detector. Analyser based imaging (ABI) technique [4] utilizes at least two single optical elements. The first optical element placed before the sample is used as a monochromator and collimator and the second optical element is used to analyze the wave-field after traversing the object (sample). The magnification of the sample requires placing additional magnification optical elements using the asymmetric diffraction behind the sample. High asymmetric diffraction for the X-ray beam expansion in grazing incidence (gi) mode provides a high magnification factor and in this case the spatial homogeneity of the X-ray wave-field is influenced mainly by the quality of the diffraction surface preparation [5].

2. Theoretical background

The first crystal in the ABI setup can act as monochromator and collimator simultaneously. Asymmetrically cut crystal allows the function of magnifier. Asymmetrically cut crystal provides the asymmetric diffraction which will in gi mode effectively increase the propagation distance and preserve sufficient magnification of the sample, which for one diffraction (1D) is given by

$$m = \frac{\sin(\theta_B + \delta_h + \alpha)}{\sin(\theta_B + \delta_i - \alpha)}, \tag{1}$$

where θ_B is the Bragg angle, α is the asymmetry angle(the inclination angle of the diffraction planes with respect to the surface), and $\delta_{i,h}$ are the refraction corrections for the input and output beam, respectively [6].The magnification factor affects the effective pixel size of the detector by this means *Effective pixel size = Real pixel size/m*. Small effective pixel size of the detector contributes to the improvement of the spatial resolution of the X-ray imaging system.

The second crystal in the ABI setup acts as the analyser of the wave-field after traversing the sample. The principle of operation of the analyser crystal is given by the shape of its diffraction (rocking) curve. A small angular change of the analyser crystal causes the significant change in the intensity profile due to large slope of the rocking curve. Setting of the analyser to 50% of the peak intensity of the rocking curve makes acceptance only for a very small angular range. Therefore, the divergence of the incident X-ray beam has to be very small and then the phase gradient in the sample as the intensity profile can be directly observable as depicted in Fig. 1(c).

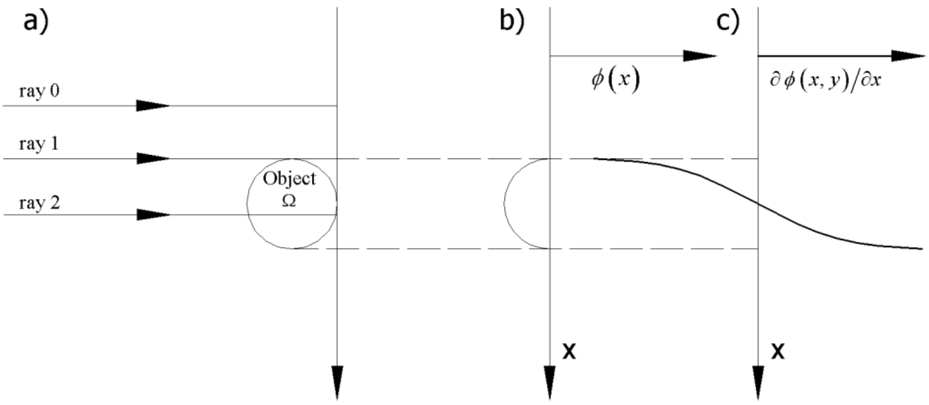

Fig.1:*a) Schematic illustration of the formation of phase contrast when a parallel X-ray beam is passing through the object Ω with the circular cross-section.. b) The phase difference, ø(x), after passing through the object. c) Intensity profile of the phase gradient in the x-direction ∂ø(x,y)/∂x (thick curve)[7].*

Phase gradient increases the contrast (phase contrast) of weakly absorbing samples. Using appropriate phase/amplitude retrieval method allows one to recover the phase information from the ABI image [8]. The retrieved phase is directly proportional to the projected electron density in the sample, and can be used for Computerized Tomography (CT)

3. Experimental setup

Schematic representation of the ABI X-ray system using Germanium Ge (111) crystal as one dimensional (1D) magnifier and Ge(400) crystal as the analyser is depicted in Fig. 2.

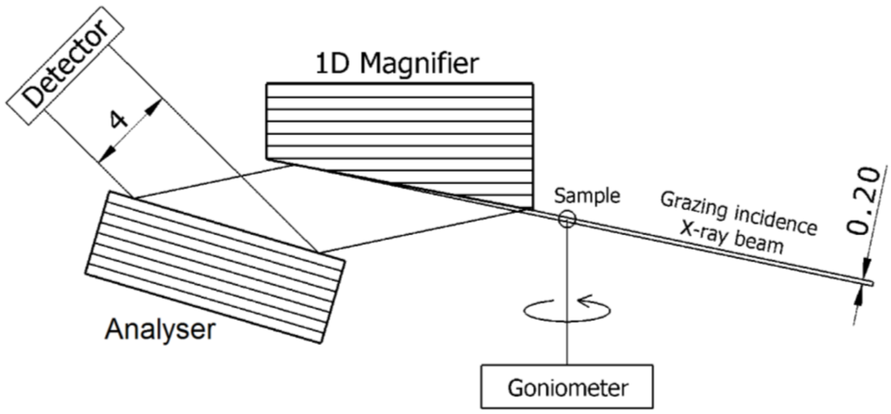

Fig.2:*1D ABI X-ray system.*

We suppose the gallium X-ray source with Kα emission of 9.2 keV which is close to the copper CuKα emission line at 8.048 keV. The X-ray beam of 200 µm wide is passing through the sample and impinges in grazing incidence mode on the surface of 1D magnifier crystal. The 1D (one dimensional) Magnifier Ge(111) is asymmetrically cut at the angle α=10.8 deg providing a 20-fold magnification. Magnified X-ray image of the sample impinges on symmetrically cut Ge(400) crystal which acts as the analyser crystal. Results of the simulations of the intrinsic rocking curves of single crystals and intensity throughput versus spatial resolution and angular sensitivity of the ABI setup using optionally Ge (111) and Ge (400) analysers are compared in the next section of this contribution.

4. Simulations and Calculations

Figure 3 shows calculated diffraction curves of crystal elements in the ABI setup described in the previous section. The GaKα1 radiation with s-polarization was used.

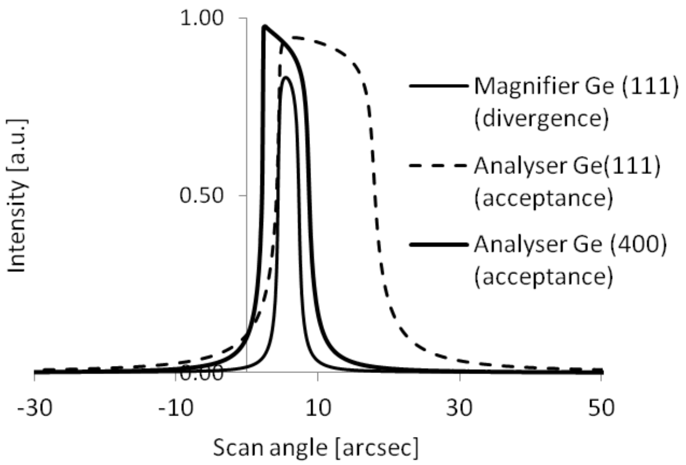

Fig.2:*Diffraction curves of single crystal elements in the proposed ABI X-ray system.*

Magnifying crystal Ge(111) provides the angular divergence of 3.09 arcsec (FWHM) what is acceptable using both analysers Ge(111) and Ge(400) with angular acceptance 13.42 [arcsec] and 6.71 [arcsec] respectively. The spatial resolution limit of the magnifier can be calculated according to Abbe's resolution criterion $d=\lambda/2NA$, where λ is the wavelength and NA is the numerical aperture. The numerical aperture of the crystal optics equal to half the width of the diffraction curve, thus $d=\lambda/\omega_i$, where ω_i is the angular acceptance (FWHM) of the magnifier [6]. For the Ge(111) magnifier (20-fold) using s-polarizedGaKα1 radiation is the angular acceptance of 1382.2 μrad and in case of neglecting of other parameters the spatial resolution limit equal to 0.1 μm. The spatial resolution limits of the symmetrically cut analyser crystals optionally Ge(111) or Ge(400) are 2.1 μm or 4.1μm, respectively. From this one can expected that using of the Ge(111) analyser will cause less deterioration of the spatial resolution of the ABI system. The important parameter of the analyser crystal is its angular sensitivity to analyse the phase gradient as was shown in Fig. 1(c). The steeper slope of the diffraction curve provides higher angular sensitivity of the phase gradient analysing. Calculation of the dynamical angular ranges of Ge(111) and Ge(400) analysers were done using the left and the right sides of the rocking curves for selected intensity points (0.3,0.5 and 0.8) and their related angles. Comparison of + and – values of the angular deviation $\Delta\alpha$ from central (FWHM) position shows that the Ge(400) analyser is approximately 2-times more sensitive than the Ge(111) analyser, see Tab. 1.

Tab. 1.*Dynamical angular ranges [arcsec (μrad)]of the diffraction curves for Ge(111) and Ge(400) analysers.*

Range of agular deviation arsec (μrad)	Ge(111)		Ge(400)	
	Left side	Right side	Left side	Right side
+Δα	0.79 (3.83)	0.94 (4.56)	0.33 (1.56)	0.46 (2.23)
-Δα	0.83 (4.02)	1.53 (7.42)	0.43 (2.08)	1.13 (5.48)

Comparison of intensity throughput using either Ge(111) or Ge(400) analyser in the proposed ABI system was done by setting the angular detector with perpendicular orientation to the diffraction plane using SKL simulation program [9].The simulation results are shown in Fig. 3. The first optical element, magnifier Ge(111) decreases the intensity to 30% of the initial source intensity. The second optical element, analyser Ge(111) causes the intensity reduction to10% of the initial source intensity. Simulation shows that using more sensitive Ge(400) analyser will result in a rapid decrease of the intensity to 4% of the initial source intensity.

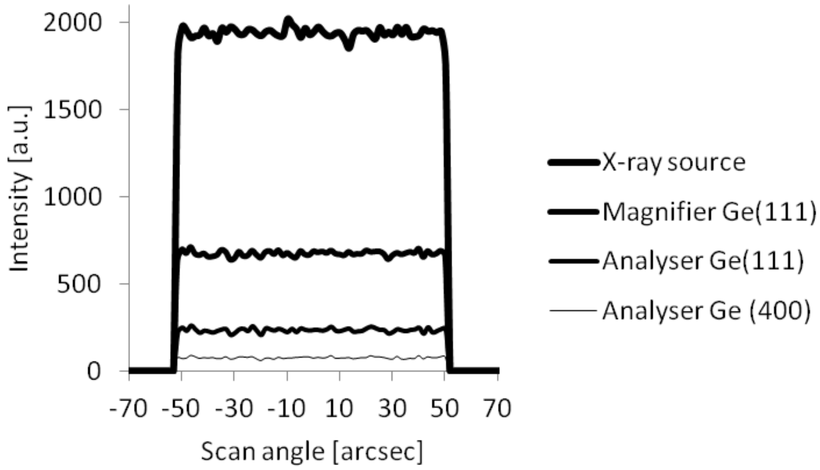

Fig.3:*Angular dependence of the intensity passing through the ABI X-ray system.*

5. Discussion and Conclusion

In this contribution it was shown that using Ge(111) crystals magnifier in ABI X-ray system allows submicron spatial resolution limitand in case of neglecting of other parameters down to 0.1 μm. The second optical elements serves as analyser of the X-ray wave-field, which carries an information about the sample. Sensitive analyser allows to image the phase gradient of the wave-field with a micro-radian angular resolution. In this contribution the symmetrically cut Ge(111) and Ge(400) analysers were compared. We showed that the Ge(400) analyser is approximately 2-times more sensitive than the Ge(111) analyser, using the same intensity range in both cases. Disadvantage of using Ge(400) analyser is a rapid decrease of the intensity to 4% of the initial source intensity. Although, using Ge(111) analyser allows only a slight increase of the intensity up to 10% of the initial source intensity.

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