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Beryllium, zinc and lead single crystals as a thermal neutron monochromators

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ABSTRACT

The monochromatic features of Be, Zn and Pb single crystals are discussed in terms of orientation, mosaic spread, and thickness within the wavelength band from 0.04 up to 0.5 nm. A computer program MONO written in "FORTRAN-77", has been adapted to carry out the required calculations. Calculations show that a 5 mm thick of beryllium (HCP structure) single crystal cut along its (002) plane having 0.6° FWHM are the optimum parameters when it is used as a monochromator with high reflected neutron intensity from a thermal neutron flux. Furthermore, at wavelengths shorter than 0.16 nm it is free from the accompanying higher order ones. Zinc (HCP structure) has the same parameters, with intensity much less than the latter.

The same features are seen with lead (FCC structure) cut along its (311) plane with less reflectivity than the former. However, Pb (311) is more preferable than others at neutron wavelengths $\leqslant 0.1$ nm, since the glancing angle ($\theta \sim 20°$) is more suitable to carry out diffraction experiments. For a cold neutron flux, the first-order neutrons reflected from beryllium is free from the higher orders up to 0.36 nm. While for Zn single crystal is up to 0.5 nm.

1. Introduction

Single crystal monochromators play a crucial role in neutron scattering instrumentation at continuous sources. Together with the source brightness and neutron beam properties, such as divergence, they determine the resolution in real and reciprocal space and the flux available for a neutron scattering experiment [1,2]. In most experiments, the full-width-at-half-maximum of the angular reflectivity distribution or rocking curve generated by neutron diffraction from an imperfect single crystal, commonly called neutron mosaic spread, should match with the beam divergence that ranges typically from 0.2° to 1°. Then intensity and resolution are said to be optimized. Neutron monochromators are typically 20 cm long and 20 cm wide. They are composed of smaller mosaic crystal slabs that are often oriented to achieve single or double focusing [3,4].

The materials most frequently used are highly oriented pyrolytic graphite (HOPG), copper, beryllium, zinc and germanium. Among these materials beryllium and zinc have the best properties. The atoms composing an efficient monochromator crystal should have high coherent scattering power and low incoherent and capture cross sections.

Heavy atoms like Pb (Lead) are favorable, because they are less affected by vibrations. Thermal vibrations decrease the monochromator efficiency in two ways. First, they diminish the coherent elastic Bragg scattering (Debye–Waller factor), and second, they increase the inelastically scattered intensity, which both contributes to a large extent to the neutron attenuation and adds unwanted background [1].

The use of large imperfect single-crystals of zinc and lead as a filter of thermal neutron beams have been measured by Adib et al. [5] in front of Egyptian-first Research Reactor "ET-RR1" beam port.

In the present work, a feasibility study of using Be, Zn and Pb single crystals cut along different planes is studied as a neutron monochromators. Their characteristics are discussed in terms of crystal mosaic spread and thickness. A computer code MONO has been developed to calculate the neutron wavelength distribution of reflecting power P^{θ}_{hkl} and reflected intensity I_{Ref} from the single crystal at both thermal and cold neutron fluxes. The MONO code is an adapted version of the computer code MONO-PG written by Adib et al. [6] and applied further by Adib et al. [7].

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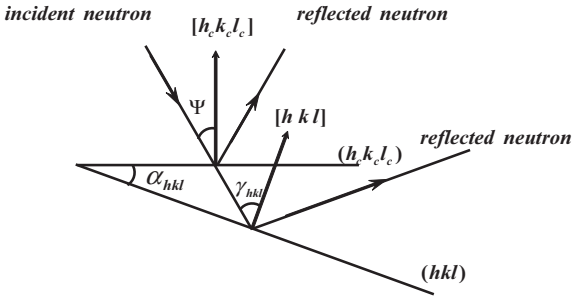

Fig. 1. A schematic diagram of the Bragg scattering from single crystal cut along ($h_c k_c l_c$) plane.

2. Theoretical treatment

The main parameters determining the quality of a single crystal as a neutron monochromator with reasonable resolution and sufficient reflected intensity are: the wavelength band of the reflected neutrons and the ratio of higher-order contaminations of the first one [8]. It is well known that the reflected neutrons from the (*hkl*) planes satisfy Bragg equation:

$$n\lambda = 2d_{hkl}\ \sin\theta_{hkl} \tag{1}$$

here n is the order of reflection and θ_{hkl} is the glancing angle to the (*hkl*) plane.

As shown by Naguib and Adib [9], the reflecting power P^{θ}_{hkl} for an imperfect single crystal depends upon the direction cosine of the diffracted beam γ_{hkl} and the inclination of the (hkl) plane to the crystal surface α_{hkl}. The schematic diagram of the Bragg scattering from single crystal cut along ($h_c k_c l_c$) plane and the reflected scattering from any (*hkl*) plane is shown in Fig. 1.

The reflected power of the (*hkl*) plane at glancing angle θ_{hkl} within $d\theta$ is given by Bacon [8] as:

$$P^{\theta}_{hkl}d\theta = \frac{ad\theta}{1+a+(1+2a)^{1/2}\ \coth[A(1+2a)^{1/2}]} \tag{2}$$

here $d\theta = d\lambda/2d_{hkl}\ \cos\theta_{hkl}$, $A = \mu t_o/\gamma_o$, $a = \frac{Q_{hkl}}{\mu}$ $W(\theta)$ and μ is the linear absorption coefficient. While t_o is the crystal thickness and γ_o is the direction cosine of the incident neutron beam relative to the inward normal crystal face. The crystallographic quantity (Q_{hkl}) is given by Bacon [8] as:

$$Q_{hkl} = \lambda^3 N_c^2 F^2/\sin 2\theta \tag{3}$$

$W(\theta)$ has a Gaussian distribution with standard deviation η on mosaic blocks of single crystal.

P^{θ}_{hkl} are calculated for planes that have Miller indices (*hkl*) the same as the cutting plane $h_c k_c l_c$ i.e., $\alpha_{hkl} = 0$ as well as $-h_c$, $-k_c$, $-l_c$ i.e., $\alpha_{hkl} = \pi$.

As shown by Bacon [8], the integrated reflectively $R^{\theta} = \int_{-\infty}^{+\infty} P^{\theta}_{hkl}d\theta$, from imperfect crystal of finite absorption reaches saturation for bulk crystal thickness of t_o.

A stationary monochromator crystal in a white neutron beam is totally reflecting over a wavelength range (R^{λ}) is given by Riste and Otnes [10] as:

$$R^{\lambda} = R^{\theta}\lambda\cot\theta_{hkl} \tag{4}$$

Also the peak reflectivity (R^p) is given by Shirane et al. [11] as:

$$R^p = \frac{R_o}{1+R_o} \tag{5}$$

where (R_o) is a constant given by:

$$R_o = \frac{Q_{hkl}t_o}{\sqrt{2\pi}\eta\sin\theta_{hkl}} \tag{6}$$

The reflected intensity I_{Ref} from crystals, when a neutron reactor beam having Maxwellian distribution $\Phi(\lambda)$ is given by:

$$I_{\mathrm{Ref}} = \Phi(\lambda) * P^{\theta}_{hkl} \tag{7}$$

where $\Phi(\lambda)$ for neutron gas temperature T is given by Gurevich and Tarasov [12] as:

$$\Phi(\lambda) = \frac{\text{constant}}{\lambda^5}\exp(-h^2/2mkT\lambda^2) \tag{8}$$

Table 1
Physical parameters of metal single crystals.

Physical property	Be	Zn	Pb
System and space group	(H.C.P.), P63mc[a]	(H.C.P.), P63mc[a]	(F.C.C.), Fm3m[a]
Atomic weight	9.012[c]	65.39[c]	207.21[c]
Lattice parameters (nm)	a_0 = 0.2275 c_0 = 0.3580[e]	a_0 = 0.2665 c_0 = 0.4947[b]	a_0 = 0.4950[d]
No. of molecules/unit cell	2[e]	2[b]	4[d]
No. of unit cells/m^3	6.18391E + 28[e]	3.28651E + 28[b]	0.824445E + 28[d]
Atomic positions	Be: (1/3,2/3,1/4) (2/3,1/3,3/4)[e]	Zn: (1/3,2/3,1/4) (2/3,1/3,3/4)[b]	Pb: (0,0,0)(1/2,1/2,0) (1/2,0,1/2) (0,1/2,1/2)
Coherent scattering lengths b (m)	0.7790E−14[c]	0.5680E−14[c]	0.9405E−14[c]
Total scattering cross section (barns)	7.631[c]	4.131[c]	11.118[c]
Absorption cross section at 0.025 eV (barns)	0.0076[c]	1.110[c]	0.171[c]

[a] Shirane et al. [11].
[b] Habib [15].
[c] Sears [18].
[d] Adib et al. [16].
[e] Wahba [17].

Table 2
Input parameters for reflecting power P^{θ}_{hkl}.

Crystal	Cutting plane (*hkl*)	d_{hkl} (nm)	Glancing angle (θ)°	t_o (mm)	$t_{eff.}$ (mm)	$\Delta\lambda$ (nm)
Be	002	0.1792	18.54	5.00	15.72	0.05E−2
Zn	002	0.2473	13.32	3.62	15.72	0.05E−2
Pb	311	0.1492	22.45	6.00	15.72	0.05E−2