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The effect of gravity on the resolution for time-of-flight specular neutron reflectivity

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ABSTRACT

The effect of gravity on neutron scattering is negligible if a thermal spectrum of up to 10 Å is used. Modern cold sources produce spectra with an ample quantity of cold neutrons. Gravity may play a crucial role for the cold part of the spectrum in neutron scattering experiments demanding high angle resolution. This mainly concerns the reflectometry method where a small deviation in the angle distribution may lead to visible effects. We present a theoretical model that takes into account the effect of gravity on the resolution function as well as the flux distribution for the specular neutron reflectometry. Theoretically calculated reflectivity curves convoluted with the model resolution function were compared with Monte-Carlo simulations, which imitated real measurements. The good agreement between the calculated and simulated curves allows one to apply the theoretical model to treat the real experimental data.

1. Introduction

Neutron reflectometry is a widely used method to study surface and interface structures [1,2]. The instrumental resolution function for zero-gravity specular reflectivity has been described in Ref. [3]. The analytical beam-analysis method coupling position, angle and wavelength of a neutron [4] has been applied previously. However, the angular resolution in a vertical scattering plane (horizontal sample plane) depends on gravity due to the bending of neutron trajectories. The effect of gravity is negligible if neutron spectra of up to 10 Å are used [5], which is typical for moderators without cold sources.

Reflectometry on the sources that generate spectra with a significant part of cold neutrons allows one to achieve low values of the scattering vector Q. The extended dynamical range provides considerably more detailed information on the scattering-length density profile perpendicular to the surface of fluids, membranes, polymers and biological objects. The gravity effect can be overcome if a monochromic incident neutron beam is used (steady-state reactors) and the center of the scattering pattern is corrected. In the case of the time-of-flight (TOF) technique (pulse neutron sources), the center of the scattering beam is smeared because neutrons with different wavelengths are deflected in the gravity field by different values.

Presently, the new multifunctional TOF reflectometer, GRAINS, is under construction at the modernized high flux pulsed reactor with the new cold moderator, IBR-2M, in Dubna (Russia) [6]. It is necessary to study the influence of gravity on the resolution function because the principal feature of this reflectometer is the horizontal sample plane. The main aim of this article is the development of the theoretical approach for the resolution function, which takes into account the effect of gravity. To test the approach, reflectivity curves smeared by the derived resolution function were compared with the reflectivity curves simulated by the VITESS Monte-Carlo software package [7]. The VITESS package allows users to carry out simulations of the neutron scattering with and without the influence of gravity and to identify the contribution of gravity on the reflectivity curves.

An ideal small-angle neutron spectrometer with perfect collimation was considered and an analytical form for the gravity resolution function was calculated in the paper dedicated to the effect of gravity [8]. It was shown that the total resolution function of a real spectrometer can be treated as a convolution of the gravity resolution function with the geometric and wavelength resolution functions. In the present paper, the influences of gravity and geometrical factors on the resolution of a TOF neutron specular reflectometer were not separated. In the present work, the instrumental angular resolution function for an idealized TOF reflectometer was deduced by extending the analytical beam-analysis method, which takes into account the influence of gravity. This function was obtained for the fixed neutron wavelength and was then convoluted with the wavelength resolution function. Thus, the total resolution function of the TOF reflectometer was represented in the integral form. We demonstrate that the effect of gravity is recognizable and has to be considered in real experiments.

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2. Theoretical expression for the resolution function

The general configuration of elements, which defines the reflectometry mode, was considered to estimate the effect of gravity on the reflectometer resolution. The source M, two slits $D1$ and $D2$ with widths w_1 and w_2, respectively, sample S of length L_S and a detector are shown in Fig. 1. The centers of the slits and the sample are on the line inclined at an angle θ to the horizontal plane. The distances between the corresponding elements are S_{MD1}, S_{D1D2}, S_{D2S} and L_0. Thus, the full neutron flight path can be calculated as $L=S_{MD1}+S_{D1D2}+S_{D2S}+L_0$. The coordinate system was chosen as shown in Fig. 1. The center of the coordinate system is at the center of the first slit.

The resolution function $R(\langle Q\rangle,Q)$ describes the distribution of the real scattering vectors Q around the measured value $\langle Q\rangle$, and the convolution of $R(\langle Q\rangle,Q)$ with the model reflectivity Int(Q) gives the experimentally measured reflectivity Int($\langle Q\rangle$) [4]

$$Int(\langle Q\rangle)=\int_0^{\infty} Int(Q)R(\langle Q\rangle,Q)\mathrm{d}Q. \quad (1)$$

The normalization of resolution function must be unity

$$\int_0^{\infty} R(\langle Q\rangle,Q)\mathrm{d}Q=1. \quad (2)$$

Let us consider neutrons with a wavelength λ. The distribution of the real scattering vector Q of these neutrons is determined by the angular divergence due to the finite collimation and the bending of the neutron trajectories in the gravity field. The analytical beam-line analysis method [4] has been employed to calculate the divergence at the sample position. In the original method, the distribution of neutrons is described as a function of the position, angle and corresponding wavelength. However, in our case, there was no crystal monochromator, and a white-beam pulsed-source instrument was considered. The position of any neutron with wavelength λ can be described by the distribution $I(z,z',\lambda)$, where z' is the angle of the wavevector with respect to the horizontal plane. Each element of the reflectometer transforms the distribution $I(z,z',\lambda)$. The transmission functions in each element of the instrument are approximated by Gaussian functions, which make it possible to calculate analytically the final neutron distribution $I(z,z',\lambda)$.

It was assumed that the neutron source radiates neutrons isotropically. This assumption is reasonable because the divergence of neutrons before the instrument was large in comparison with the divergence of the neutron beam after the slits. The first element of the instrument is the slit $D1$. The first slit passed only neutrons that fall into its aperture defined by width w_1. The transmission function is a box function, which can be approximated as a Gaussian function with standard deviation $\sigma_{z1}=w_1/\sqrt{12}$. Thus, the distribution right after the first slit can be written as:

$$I(z,z',\lambda)\propto \exp\left[-\frac{1}{2}\frac{z^2}{\sigma_{z1}^2}\right]. \quad (3)$$

The distribution of neutron positions in the beam changes along the flight path due to the divergence of the beam. A neutron with angle z' and position z will change its position after a distance S_{D1D2} to $z+z'S_{D1D2}+(g/2)(\lambda m/h)^2S_{D1D2}^2$, where g is the gravitational constant acceleration, h is the Planck constant and m is the neutron mass. The second slit $D2$ had the same transmission function as the first slit (3) with the standard deviation $\sigma_{z2}=w_2/\sqrt{12}$ and with the center of the distribution at $\theta\, S_{D1D2}$. Thus, the distribution after the second slit is given by the following expression:

$$I(z,z',\lambda)\propto \exp\left\{-\frac{1}{2}\left[\frac{z^2}{\sigma_{z1}^2}+\left(z+z'S_{D1D2}+\frac{g}{2}\left(\frac{\lambda m}{h}\right)^2S_{D1D2}^2-\theta S_{D1D2}\right)^2\Big/\sigma_{z2}^2\right]\right\}. \quad (4)$$

Let us consider the sample as a vertical slit of width $w_S=\theta\, L_S$ (the corresponding standard deviation of the transmission function is $\sigma_{zS}=w_S/\sqrt{12}$) at distance $S_{D1S}=S_{D1D2}+S_{D2S}$ from the first slit $D1$ (the corresponding center of the distribution is $\theta\, S_{D1S}$). Then, the distribution after the third slit is given by the following expression:

$$I(z,z',\lambda)\propto \exp\left\{-\frac{1}{2}\left[\frac{z^2}{\sigma_{z1}^2}+\frac{\left(z+z'S_{D1D2}+\frac{g}{2}\left(\frac{\lambda m}{h}\right)^2S_{D1D2}^2-\theta S_{D1D2}\right)^2}{\sigma_{z2}^2}+\frac{\left(z+z'S_{D1S}+\frac{g}{2}\left(\frac{\lambda m}{h}\right)^2S_{D1S}^2-\theta S_{D1S}\right)^2}{\sigma_{zS}^2}\right]\right\}. \quad (5)$$

The resulting distribution (5) consists of three Gaussian functions and has the following general form:

$$\exp\left\{-\frac{1}{2}\left[\frac{(z-A)^2}{\sigma_A^2}+\frac{(z-B)^2}{\sigma_B^2}+\frac{(z-C)^2}{\sigma_C^2}\right]\right\}. \quad (6)$$

The reduction of expression (6) to a form with one Gaussian function by extracting the perfect square within the exponent gives the following expression:

$$\exp\left[-\frac{1}{2}\frac{(z-\langle z\rangle)^2}{\sigma_z^2}\right]\exp\left[-\frac{1}{2}\frac{(A-B)^2\sigma_C^2+(A-C)^2\sigma_B^2+(B-C)^2\sigma_A^2}{\sigma_A^2\sigma_B^2+\sigma_A^2\sigma_C^2+\sigma_B^2\sigma_C^2}\right], \quad (7)$$

where

$$\langle z\rangle=\frac{A\sigma_B^2\sigma_C^2+B\sigma_A^2\sigma_C^2+C\sigma_A^2\sigma_B^2}{\sigma_A^2\sigma_B^2+\sigma_A^2\sigma_C^2+\sigma_B^2\sigma_C^2},\quad \sigma_z=\frac{\sigma_A\sigma_B\sigma_C}{\sqrt{\sigma_A^2\sigma_B^2+\sigma_A^2\sigma_C^2+\sigma_B^2\sigma_C^2}}. \quad (8)$$

Since the second exponent in expression (7) does not depend on z, the integration of expression (7) over z from $-\infty$ to $+\infty$ gives the constant from the first exponent multiplied by the unchanged second exponent. The resulting angular distribution for the neutrons in the first slit $D1$ that will eventually be reflected by the sample can be obtained by extracting the perfect square within the second exponent

$$I(z',\lambda)\propto \exp\left[-\frac{1}{2}\frac{(z'-\langle z'\rangle)^2}{\sigma_{z'}^2}\right]\times\exp\left[-\frac{1}{2}\frac{\kappa-\langle z'\rangle^2}{\sigma_{z'}^2}\right], \quad (9)$$

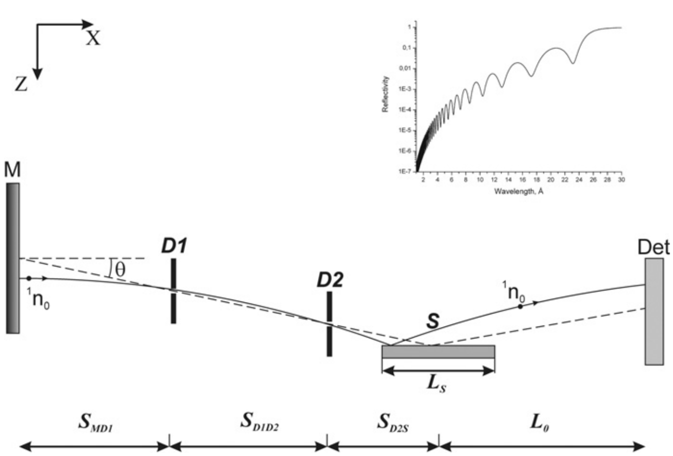

Fig. 1. Layout of reflectometer with a horizontal sample plane. The bent solid line demonstrates the real neutron trajectory in the gravity field. The dashed line depicts the axis passing through the centers of both slits and the sample center. The inset shows the ideal reflectivity as a function of neutron wavelengths from monolayer with a critical angle of 5.56×10^{-4} rad/Å and thickness of 1500 Å on a substrate with a critical angle of 4.17×10^{-4} rad/Å at a grazing angle of 15 mrad.