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Analysis and design of multilayer structures for neutron monochromators and supermirrors

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ABSTRACT

A relatively simple and accurate analytical model for studying the reflectivity of neutron multilayer monochromators and supermirrors is proposed. Design conditions that must be fulfilled in order to reach the maximum reflectivity are considered. The question of the narrowest bandwidth of a monochromator is discussed and the number of layers required to build such a monochromator is derived. Finally, we propose a new and efficient algorithm for synthesis of a supermirror with specified parameters and discuss some inherent restrictions on an attainable reflectivity.

1. Introduction

Multilayer structures have found a wide application in neutron instrumentation as monochromators, polarizes and supermirrors [1,2]. The latter ones, for instance, are commonly used nowadays at research reactors for construction of neutron guides with enhanced angular acceptance designed to transport neutrons over long distances. Multilayer supermirrors also find use in neutron focusing devices [3–5] opening a new way in neutron instrumentation.

Generally, a multilayer structure represents a thin film system composed of layers of two different materials alternatively and repeatedly deposited on a flat substrate (Fig. 1).

These materials are chosen to have high and low effective potentials for neutrons (also known as neutron optical potentials) and, therefore, a multilayer system can be considered as a sequence of one-dimensional square-well potentials. During propagation through the system a partial reflection and transmission of a neutron wave occurs at every interface resulting in appearance of multiple waves within the system (see Fig. 1). In the case of a periodic structure, the multiple wave interference leads to distinctive band structures in the energy spectrum of the beams reflected from or transmitted through the multilayer. Hence, with a proper selection of the layer materials and thicknesses one can, in principle, built a system with desired spectral properties. In the present paper we propose a relatively simple and accurate analytical method for studying the reflectivity, R, of multilayer mirrors and apply this method for design of two main systems which have an extensive application in neutron instrumentation: (a) a very narrow bandwidth system for a neutron monochromator and (b) a very wide bandwidth system for a neutron supermirror. We begin with the multilayer structure made up as a sequence of identical bilayers repeated many times in one direction where each bilayer consists of two thin films of different materials. Such systems are widely used as monochromators in neutron optics (see, e.g., [6–9]). We shall find conditions that must be fulfilled in order to attain the maximum reflectivity for neutrons with a fixed incident wave vector. We then evaluate the bandwidth and the number of bilayers required to build such a monochromator.

We next apply the obtained results for the synthesis of a neutron supermirror. In that system, successive bilayers vary gradually in thickness in such a way that the neutron reflectivity displays a very wide bandwidth [10–19]. We introduce a new and efficient algorithm for design of a supermirror with specified parameters and discuss some inherent limitations on an attainable reflectivity.

2. General remarks

For a given material an effective potential, U, is defined as

$$U = \frac{2\pi\hbar^2}{m_n} \sum_j N_j b_j, \tag{1}$$

where m_n is the neutron mass, b_j is the bound coherent scattering length and N_j is the number density of nuclei. The summation runs

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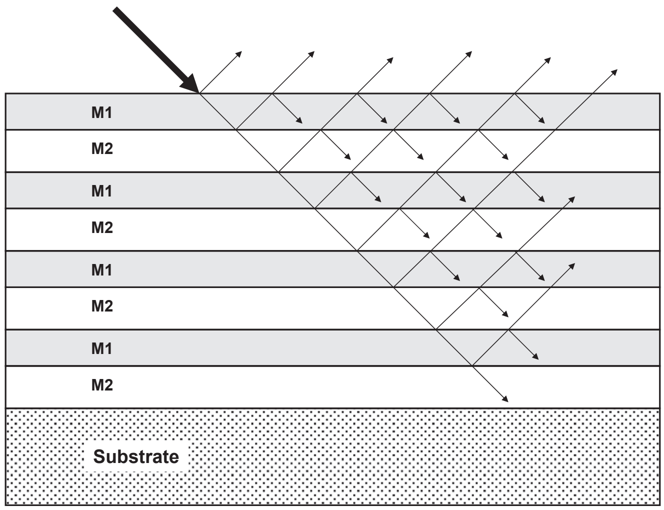

Fig. 1. View of the multilayer structure composed of layers of two different materials $M1$ and $M2$ deposited on a flat substrate. The multiple waves are shown schematically (see text).

over all elements and isotopes that constitute the layer. It is worth noting that in magnetic materials the effective potential will also include a magnetic interaction of neutrons with matter. This obviously opens a way for construction of polarizing devices. In the present paper we do not give a special consideration to that case since all formulae for polarizing systems can be obtained straightforward from our results derived for the general case of wave propagation in a one-dimensional potential.

It is evident that neutron waves propagating through a multilayer structure undergo multiple reflections at interfaces and the resulting reflectivity and transmittance of the system are determined by the interference of all the multiple reflected waves. The interference pattern depends apparently on the phases of summed waves and, thus, on the thicknesses of the layers and the magnitudes of the neutron wave vectors within the layers. The latter ones are defined by the following expression:

$$k=\sqrt{\frac{2m_n}{\hbar^2}(E_0-U)}, \tag{2}$$

where E_0 is the energy of an incident neutron in vacuum. Generally, in order to calculate the phase of the wave at a given point one needs to know the magnitude of the wave vector and the direction of the wave propagation. However, for a one-dimensional potential structure the problem can be simplified significantly. Indeed, in that case the components of the neutron momentum which are parallel to the multilayer surface do not vary when the neutron travels through the interface between two different media. Thus, these components of the neutron wave vector and the part of the neutron energy associated with those components are constant and they can be omitted from the subsequent consideration. As a result the wave propagation through the system can be characterized merely by the component normal to the multilayer surface (see, e.g., [13,17,20])

$$k_\perp=\sqrt{\frac{2m_n}{\hbar^2}(E_{0\perp}-U)} \tag{3}$$

with $E_{0\perp}$ being the part of the incident neutron energy that corresponds to this component. Therefore, we reduce the problem of finding the specular reflection coefficient of neutrons with the wave vector $\vec{k}=(\vec{k}_{||},\vec{k}_\perp)$ incident upon a multilayer to the problem of finding the specular reflection coefficient of neutrons with the incident wave vector $\vec{k}=\vec{k}_\perp$. For simplicity we shall omit the sub index "⊥" from our subsequent calculations keeping in mind that only components normal to the surfaces (interfaces) are considered.

3. Multilayer system composed of identical bilayers: neutron monochromator

We assume first that the multilayer system is composed of thin films of non-absorbing and non-scattering materials. This is a reasonably good approximation since in most cases absorption and scattering are very low and can be initially neglected. We shall discuss their effect on the reflectivity later when we present our results obtained for supermirrors. Next, we postulate that in the case of the total reflection (i.e., $R=1$) the neutron flux through any plane, which is located within the multilayer parallel to the surface, has to be equal zero. This postulate looks obvious and we apply it below to study the reflectivity from a multilayer system.

To find the flux within a multilayer we have to solve the quantum-mechanical problem of a neutron wave traveling though the system with one-dimensional periodical potential (see Fig. 2).

In quantum mechanics a flux, F, is defined as

$$F=\frac{ih}{2m}(\psi\cdot\nabla\psi^*-\psi^*\cdot\nabla\psi), \tag{4}$$

where ψ and $\nabla\psi$ are the neutron wave function and its gradient and the asterisk denotes the complex conjugate. In the particular case of a one-dimensional potential the gradient becomes merely a derivative along the normal to the interface. The wave function within the thickness of any layer can be written in a common way (see Fig. 2)

$$\psi=\psi(+)+\psi(-)\equiv A\exp(ikx)+B\exp(-ikx). \tag{5}$$

Here A is the amplitude of the wave $\psi(+)$ traveling in the direction of the incident neutron wave and B – the amplitude of the wave $\psi(-)$ traveling in the opposite direction; k is the magnitude of the wave vector within the layer. On substituting Eq. (5) into Eq. (4), we obtain

$$F=\frac{kh}{m}(|A|^2-|B|^2). \tag{6}$$

We define now a reflectance amplitude, r (a priori complex), within a layer as

$$r=\frac{B}{A}. \tag{7}$$

From Eqs. (6) and (7) it follows that the condition $F=0$ holds only if $|r|^2=1$. Thus, using the postulate mentioned above, one may conclude that $|r|^2=1$ is required in order that $R=1$. The evaluation of the parameters of the multilayer system that ensure $|r|^2=1$ constitutes the main subject of our subsequent calculations.

First we discuss the reflection of the neutron wave from a semi-infinite multilayer in which the number of layers is infinite in one direction. Let us consider three subsequent layers within the multilayer (Fig. 2) which have numbers s, $s+1$ and $s+2$. By analogy with Eq. (5) one can write the neutron wavefunction in each layer as a sum of the waves traveling to the right and to the left:

$$\psi_s=A_s\exp(ik_sx)+B_s\exp(-ik_sx) \tag{8a}$$

$$\psi_{s+1}=A_{s+1}\exp(ik_{s+1}x)+B_{s+1}\exp(-ik_{s+1}x) \tag{8b}$$

$$\psi_{s+2}=A_{s+2}\exp(ik_{s+2}x)+B_{s+2}\exp(-ik_{s+2}x). \tag{8c}$$

Here a subscript index was used to identify a layer. We chose the system of coordinates with $x=0$ at the interface between the layers s and $s+1$. The requirement of the continuity of the wave function and its derivative at the interfaces $x=0$ and $x=a$ (see Fig. 2) leads to four equations with six unknown parameters $A_{s,s+1,s+2}$ and $B_{s,s+1,s+2}$.

$$A_s+B_s=A_{s+1}+B_{s+1} \tag{9a}$$