JP0150565

JAERI-Conf 2001-002

ICANS-XV
15th Meeting of the International Collaboration on Advanced Neutron Sources
November 6-9, 2000
Tsukuba, Japan

14.9
Analyses of diffuse scattering of neutron from supermirror

Cao Bin and Kazuhiko Soyama

Japan Atomic Energy Research Institute, Tokai, Naka, Ibaraki, 319-11 Japan
Email: Cao@shield4.tokai.jaeri.go.jp

Abstract

The neutron diffuse scattering from single rough interface and supermirror has been investigated. We develop a code based on the Distorted-Wave Born Approximation for simulating diffuse neutron scattering. The calculating method uses perturbation theory on the exact solution of the wave equation for smooth surface to calculate the diffuse scattering produced by surface roughness. The rough surface of supermirror is characterized by the correlation function C which consist of the parameters of the rms roughness σ, the height-height correlation length ξ, and the roughness exponent h.

I . Introduction

The supermirrors are expected to use in many applied fields because of its larger critical angle. For example, a focusing small angle neutron scattering system of supermirror could increase the neutron density at a sample position in return for extending the angle of neutron divergence. On the side, the supermirrors are widely used for neutron guide tube, since the critical glancing angle of mirrors is larger than that of total reflection mirror and the intensity of neutrons from a guide tube could be increased in proportion to the square of the critical angle. However on account of objection of deposition technique, the supermirror is impossible to be made a pure smooth surface, the diffuse scattering will be occurred by the roughness of supermirror. It will effects the qualities of formation of image at a focal point for SANS system and decreases the intensities of neutrons from a guide tube. For this reason, it is important to have knowledge of the behavior for diffuse neutron scattering from supermirror.

Ⅱ. Theory

1. The diffuse neutron scattering from a single rough interface

Before analyzing diffuse neutron scattering from supermirror, let us first consider the diffuse neutron scattering from a single rough interface. Expression for the coherent and incoherent contributions to the differential cross section for neutron scattering by a rough surface have been derived by solving the schrödinger equation:

$$-\frac{\hbar^2}{2m}\left[\nabla^2\Psi(r)+k^2\Psi(r)\right]=V(r)\Psi(r) \qquad (1)$$

For the real rough interface, the interaction potential is separated into two parts: $V(r)=V_0(r)+V_1(r)$, $V_1(r)$ is small perturbation on $V_0(r)$.

Let us consider an incident $\exp(i\mathbf{k}_1\cdot\mathbf{r})$ plane wave on the surface from $z>0$. Putting $V(r)=V_0(r)$ in Eq.(1), it is found that

$$\Psi_1(r)=\begin{cases} e^{ik_1\cdot r}+r(k_1)e^{ik'_1\cdot r}, & z>0 \\ t(k_1)e^{ik^t_1\cdot r}, & z<0 \end{cases} \qquad (2)$$

$$\Psi_2(r)=\begin{cases} e^{ik_2\cdot r}+r^*(k'_2)e^{ik'_2\cdot r}, & z>0 \\ t^*(k_1)e^{ik^t_2\cdot r}, & z<0 \end{cases} \qquad (3)$$

where $\Psi_2(r)$ is a time reversed state for a beam incident on the surface with wave vector $-k'_2$. Using the distorted-wave Born approximation(DWBA), the expression for the diffuse scattering, integrated over the acceptance perpendicular to the scattering plane, is given as[1]

$$(I_2/I_1)_{\text{diff}} = \frac{k_1^3}{8\pi^2\theta_1}\left|1-n^2\right|^2\left|t_r(\theta_1)t_r(\phi'_1)\right|^2 S(q_z^t)\delta\phi'_1 \qquad (4)$$

$$S(q_z^t)=\frac{\exp\left\{-\left[(q_z^t)^2+(q_z^{t*})^2\right]\sigma^2/2\right\}}{\left|q_z^t\right|^2}\times\int_0^\infty dR\cos(q_rR)\left[\exp\left\{\left|q_z^t\right|^2\sigma^2C(R)\right\}-1\right] \qquad (5)$$

$$q_r=\frac{1}{2}k_1(\theta_1^2-\phi_1'^2) \qquad (6)$$

$$q_z^t=nk(\theta_2+\phi_2) \qquad (7)$$

Here q_r is the wave-vector transfer in air while q^z_t is the wave-vector transfer in the reflection medium.. The height-height correlation function C(R) which appears in Eq.(5) is the same as that introduction by Sinha et *al*[2]:

$$C(R)=\sigma^2\exp[-(R/\xi)^{2h}], \tag{8}$$

where σ is the mean−square roughness and exponent h which determines the texture of the roughness takes values between zero and one. The quantity ξ in the above equations plays the role of a length scale with in the rough surface as well as providing a cutoff. Diffuse scattering geometry is shown in Fig.1. θ_2, ϕ_2 are the refraction angle corresponding to the incident angle θ_1 and diffuse scattering angle ϕ_1'

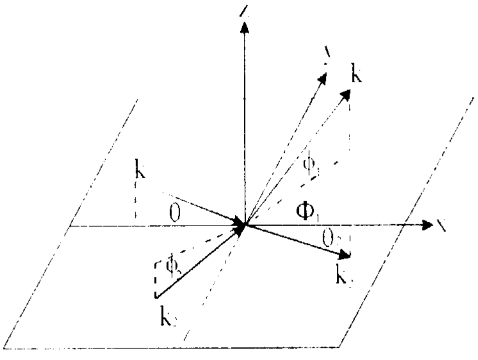

Fig. 1.A schematic view of diffuse scattering system showing the incidence angle θ_1 and reflection angle ϕ_1'.

2. The diffuse neutron scattering from the supermirror

Differing from the single rough interface, the supermirror is composed of a sequence of multilayer. According to the DWBA, the cross section for diffuse scattering from the multilayers is given by [3]

$$\left(\frac{d\sigma}{d\Omega}\right)=\frac{\rho k_1^2}{8\pi^2}\sum_{j,k=1}^{N}(n_j^2-n_{j+1}^2)(n_k^2-n_{k+1}^2)^*$$

$$\times\sum_{m,n=0}^{3}G_j^m G_k^n\exp\{-0.5[(q_{z,j}^m\sigma_j)^2+(q_{z,k}^{n*}\sigma_k)^2]\}S_{jk}^{mn}(q_x) \tag{9}$$

where n_j is the refractive index of the material beneath the jth interface, G_j^m represents the transmitted and reflected distorted wave at the jth interface, $q_{z,j}^m$ is the momentum transfer within each layer. The respective expressions for G_j^m and $q_{z,j}^m$ are given in Table1.

Table1. $k_{i,j}$ and $k_{f,j}$ denote the wave vector in the medium j for incidence angle a_i and exit angle a_f. The amplitudes of transmitted and reflected wave are T and R

$G_j^0=T_{i,j+1}T_{f,j+1}$	$\mathbf{q}_j^0=\mathbf{k}_{i,j+1}+\mathbf{k}_{f,j+1}$
$G_j^1=T_{i,j+1}R_{f,j+1}$	$\mathbf{q}_j^1=\mathbf{k}_{i,j+1}-\mathbf{k}_{f,j+1}$
$G_j^2=R_{i,j+1}T_{f,j+1}$	$\mathbf{q}_j^3=-\mathbf{q}_j^0$
$G_j^3=R_{i,j+1}R_{f,j+1}$	$\mathbf{q}_j^2=-\mathbf{q}_j^1$

The factor S is $$S_{jk}^{mn}(q_x)=\frac{1}{q_{z,j}^m q_{z,k}^{n*}}\int_0^\infty dX\{\exp[q_{z,j}^m q_{z,k}^{n*}C_{jk}(X)]-1\}\times\cos(q_xX). \tag{10}$$

with q_x given by $q_x=k_1(\cos\alpha_f-\cos\alpha_i)$. In Eq.(10) S_{jk}^{mn} denotes the Fourier transform of the correlation function $C_{jk}(X)$.

Correlation function $C_{jk}(X)$

In order to calculate the diffuse scattering from the supermirror, the correlation functions $C_{jk}(X)=<\phi_j(x)\,\phi_k(x+X)>x$ must be considered. $\phi_j(x)$ denotes the height of the interface j at the lateral position x with respect to the average interface z_j.
In the case of j=k, autocorrelation functions C_{jj} can be expressed as

$$C_{jj}(X)=C_j(X)=\sigma_j^2\exp[-(X/\xi_j)^{2h_j}] \qquad (11)$$

which is similar to the case of a single rough interface. In order to describe the $C_{jk}(X)(j\neq k)$ which is the roughness from interface j to k, we first determine the autocorrelation functions $C_j(X)$ and $C_k(X)$ of self-affine interface if the interface j and k would be isolated from each other. Therefore $C_{jk}(X)$ additionally depends on the relationship between the $C_j(X)$ and $C_j(X)$ of the Fourier components of the two interfaces. Finally the correlation functions can be written as

$$C_{jk}(X)=\sigma_j\,\sigma_k\{\exp[-(X/\xi_j)^{2h_j}]\exp[-(X/\xi_k)^{2h_k}]\}^{1/2}\exp(-d_{jk}/\xi_\perp) \qquad (12)$$

where d_{jk} is the distance between the jth and kth layer. ξ_j is the vertical distance over which the correlations between layers j and k are damped by a factor of 1/e.

Ⅲ. Result

1. The diffuse neutron scattering from a single rough interface

Figure 1, 2,3 are the simulation results based on the scanning mode in which the incidence angle θ_1 remains constant and the diffuse scattering angle ϕ'_1 is changed. Figure 1 shows the

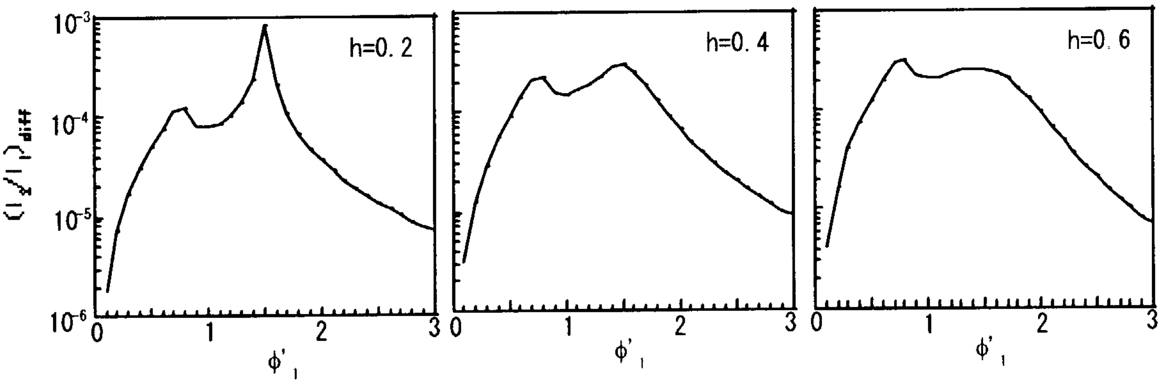

Fig.1. Diffuse neutron scattering from a nickel surface with roughness of standard deviation $\sigma=8\overset{0}{A}$, an incident angle $\theta_1=1.5^0$, ϕ'_1 is a diffuse scattering angle.

diffuse neutron scattering from a rough nickel surface varies with the roughness exponent h. There is a maximum in the diffuse scattering when the incident and reflection angles are equal, that is, at the specular condition[4] . The sharpness of this maximum depends on the value of the roughness exponent, h: small values of h, corresponding to surfaces that subjectively appear more "jagged", give sharper peaks in the diffuse scattering. In order to calculate the Fourier transform of correlation function C(R), the maximum period in the Fourier series

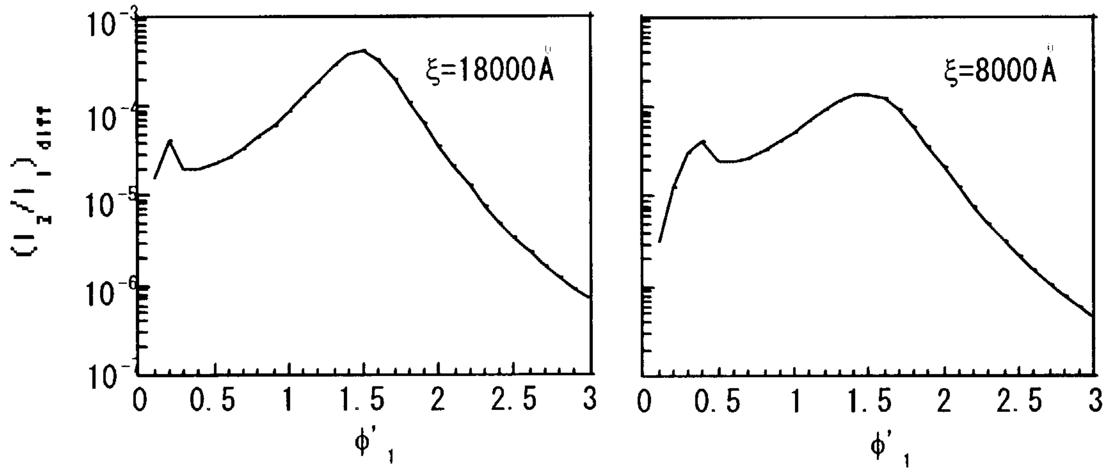

Fig.2. Diffuse neutron scattering from a nickel surface with roughness of standard deviation σ =10Å , a roughness exponent h=0.8 and neutron wavelength of 8Å .

must be known. Sinha *et al.* introduce a "cut-off" length ξ that is the scale at which the surface shows lateral correlation. At most ξ is equal to the finite lateral dimensions of the sample L. Figure .2 shows the intensities of diffuse scattering neutrons vary with the cut-off" length ξ . Similar to Figure. 1, larger values of ξ tend to give sharper diffuse

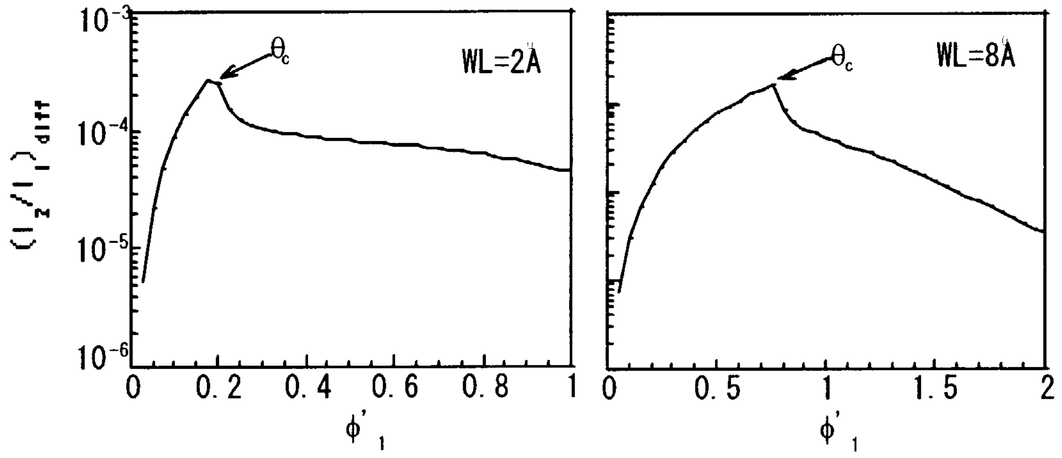

Fig.3. Diffuse neutron scattering from a nickel surface with roughness of standard deviation σ =12Å , a roughness exponent h=0.8 and correlation length ξ =3000Å .

scattering. Excepting for the specular peak, there is also small peak appearing in Figure.1, 2. That is called the Yoneda peak whenever incident angle or reflection angle is equal to the critical angle of materials. The proportional relationship between neutron wavelength and the critical angle is shown in Figure.3. Figure.4 presents the simulation data obtained from rocking mode which both the incidence angle θ_1 and the diffuse scattering angle ϕ'_1 are changed and their sum $\theta_1+\phi'_1$ is keep constant. The intensities of diffuse neutron scattering increase

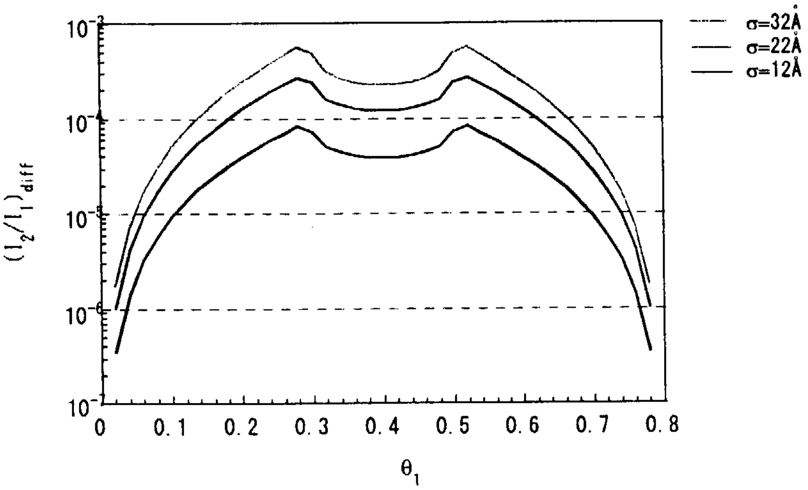

Fig.4. Diffuse neutron scattering from a nickel surface with a roughness exponent h=0.8 , correlation length ξ =3000Å and neutron wavelength of 8Å .

along with the increment of rms roughness as shown in Figure .4.

2. The diffuse neutron scattering from supermirror

Figure. 5 shows diffuse neutron scattering of sample1 from Ni/Ti multilayers consisting 3

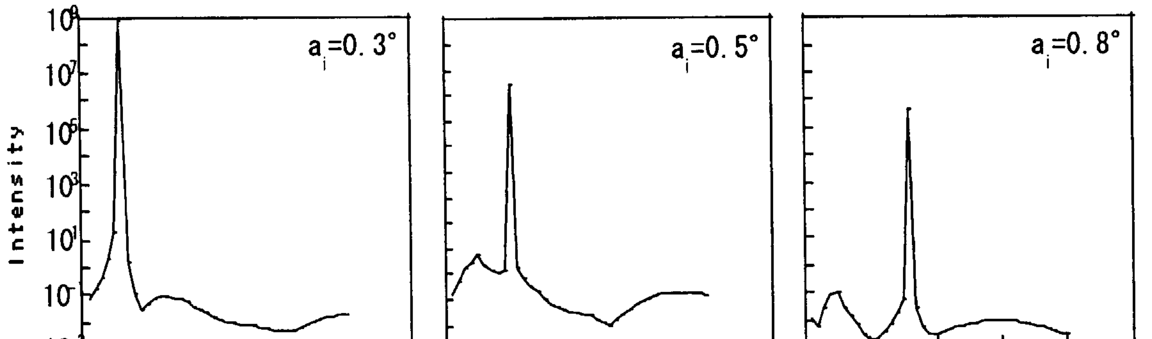

Fig.5. Scanning mode for simulating diffuse neutron scattering . The incidence angle and diffuse scattering angle are a_i and a_f .

bilayers with a d-space of 30Å . As the angle a_i is smaller than the critical angles of Ni, the penetration depth of neutron is small and the scattering mainly stems from the topmost interface[5]. In the incidence angle become larger, the neutrons be able to penetrate the supermirror deeply, all of the layers contribute to the diffuse scattering would be observed. However, only few layers in simple1, it is not easy to differentiate the contribution by the multiplayer as shown in Figure.5. Figure. 6 shows diffuse neutron scattering of from Ni/Ti multiplayer consisting 10 bilayers (20 layers) with a d-space of 50Å . It is evident to observe the peaks of diffuse scattering in Firure.6.

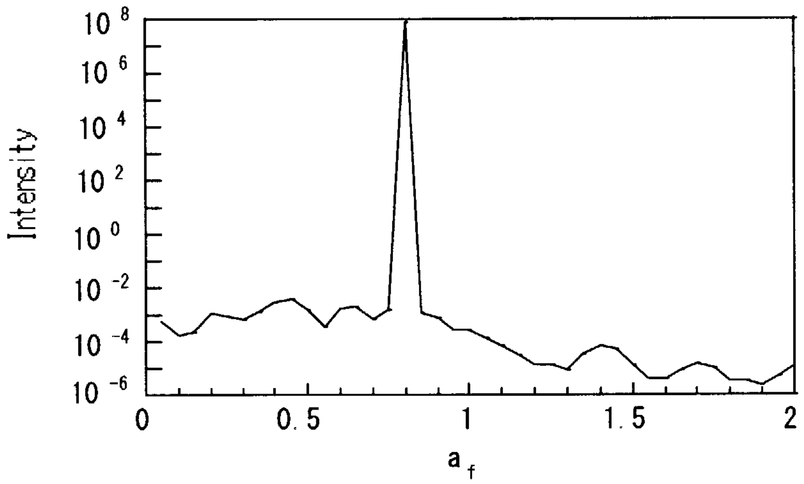

Fig. 6. The simulation for diffuse scattering from multiplayer consisting 10 bilayers with incidence angle $a_i = 0.8^0$.

IV. Conclusions

We developed the simulation code based on DWBA for calculating non-specular neutron scattering. The diffuse neutron scattering from a single rough interface and the multiplayer has been observed using this code. We have succeed to calculate the intensities of diffuse scattering varying with the parameters of roughness and express that the simulation code is very useful in qualitative analysis of the change of diffuse scattering for a single rough interface.

We have also studied the influence of the incidence angle on the scanning mode simulated for Ni/Ti multilayers. In the future work, we expect to investigate the particulars of off-specular neutron scattering varying with the performance of supermirror using this simulation code.

References

[1] Wolfgang Weber and Bruno Lengeler, Phys. Rev. B46, 7953(1992).

[2] S. K. Sinha, E. B. Sirota, S. Garoff and H. B. Stanley, Phys. Rev. B46, 2287(1988).

[3] J. Stettner, L. Schwalowsky, O. H. Seeck, M. Tolan and W. Press, Phys. Rev. B52, 1398(1996).

[4] Roger Pynn, Phys. Rev. B45, 602(1992).

[5] J.-P. Schlomka, M. Tolan, L. Schwalowsky, O. H. Seeck, J. Stettner, and W. Press, Phys. Rev. B51, 2311(1995).