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X-Ray Scattering Studies of Multilayer Interfaces

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Abstract. The results of specular and diffuse x-ray scattering studies of multilayers are discussed. We show here that such studies can yield detailed statistical information about the interfacial roughness and morphology. Results on a $GaAs/AlAs$ multilayer are presented and the data is analyzed within the Born approximation.

1. Introduction

In this paper we present results on the characterization of interfacial roughness of multilayers using the x-ray reflectivity technique. Although detailed characterization of a multilayer system requires analysis of both reflectivity data at small angles and data in the (wide angle) Bragg reflection regime, we shall restrict ourselves here to discussing only the small angle region. In the small angle limit here we neglect the crystal structure of the materials assuming only uniform electron densities in the layers separated by (rough) interfaces. This analysis gives us knowledge about the "*global*" interfacial roughness and its conformality over the entire multilayer. The analysis of the scattering data is done within the Born approximation.

2. The Model

It has been shown [1] that a knowledge of the height-height correlation function

$$C_0(R) = \langle \delta Z(0) \delta Z(R) \rangle. \tag{1}$$

can be used to derive the specular and diffuse scattering intensities for solid as well as liquid [2] surfaces using the Born approximation. Here $\delta Z(R)$ [assumed to be a single valued function] is the height fluctuation of the surface above the plane at a lateral position R. In the case of multilayers we have to generalize this function taking into account the possibility of correlation between height fluctuations of different interfaces and we assume the form

$$C_{ij} \equiv < \delta Z_i(0) \delta Z_j(R) > = C_0(R) * \exp(-|Z_i - Z_j|/\xi_\perp) + C_1(R)\delta_{ij} \tag{2}$$

$\xi_\perp$ is the correlation length for the roughness perpendicular to the interface and Z_i, Z_j are the mean positions of interfaces i and j respectively. The second term represents intrinsic (uncorrelated) fluctuations of a single interface and generally takes [1] the form $\sigma_i^2 \exp((-R/\xi_\parallel)^{2h})$ with $(0 < h < 1)$. The first term represents conformal height fluctuations of the interfaces i, j, and $C_0(R)$ can be taken to have the same form as $C_1(R)$ with amplitude σ_0^2. By using this height-height correlation function and also assuming same r.m.s random error δ in the deposition thickness of each layer one can derive the expression [3] for scattering intensity from N such interfaces as

$$
\begin{aligned}
I = \frac{I_0}{q_z^2} \frac{b^2}{K_0^2 \sin\alpha \sin\beta} \sum_{ij} \Delta\rho_i \Delta\rho_j \exp(-iq_z(Z_i - Z_j)) \\
X \exp[-q_z^2(\frac{1}{2}\sigma_i^2 + \frac{1}{2}\sigma_j^2 + \sigma_0^2 + \frac{1}{2}\delta^2 |i-j|)] \\
\int\int dx dy \exp(q_z^2 C_{ij}(R)) e^{-iq_\parallel \cdot R} \\
* R(q_\parallel, q_z).
\end{aligned}
\tag{3}
$$

In the equation (3) $\Delta\rho_i$ represents difference between electron densities of the medium above and below the ith interface, α and β are respectively grazing angle of incidence and scattering, b is the Thomson scattering length given by e^2/mc^2 and K_0 is the wave vector of the incident radiation. The last factor in Eq. (3) represents a convolution with the instrumental resolution functions in q-space. It should be noted here that the above expression is not valid near the critical angle and has to be modified according to the distorted wave Born approximation to explain the scattering in that region. The integral in Eq. (3) can be split into two parts. one of which yields the specular reflectivity and the other yields the diffuse scattering where the integral in Eq. (3) is replaced by

$$
F_{ij}(\vec{q}) = \int\int dx dy [\exp(q_z^2 \sigma^2 e^{-(R/\xi_\parallel)^{2h}} e^{-|Z_i - Z_j|/\xi_\perp}) - 1] e^{-iq_\parallel \cdot R} \tag{4}
$$

3. Results and Discussions

We shall present here the data for a multilayer, which has 77 bilayers of $GaAs$ and $AlAs$, to demonstrate the use of the above expressions. The experiment was performed at the X-22B beamline of NSLS at Brookhaven National Laboratory. While taking the data the resolution in the direction normal to the scattering plane was kept wide open. This effectively performed one integration and we thus have to deal with only a one dimensional integral to evaluate Eq. (4). In Fig. 1. we show the specular and longitudinal diffuse scattering (i.e. parallel to but displaced from the specular ridge) as a function of q_z. The presence of peaks in the longitudinal diffuse scattering clearly demonstrates the conformality of the interfaces. It should be mentioned here that to obtain the "*true*" specular component of the scattering, one has to subtract the diffuse component from the measured specular data and correct it for the variation of the resolution function. Unless the above procedure is followed one can grossly underestimate the "*global*" roughness, since one is measuring only the "*local*" roughness determined by the instrumental resolution. The true specular component (away from the critical angle) and a fit with the curve calculated from Eq. (3) are shown in Fig. 2. For our fit, we assume all the σ_i^2 to be equal. One may note that there is a small "*hump*" in the experimentally observed specular reflectivity in the vicinity of $q_z = 0.3 Å^{-1}$. This may be due to the effect of increasing roughness as we move towards the surface of the multilayer, but was not accounted for in the present model. The total bilayer thickness and the thickness ratio between the layers are obtained to be 122.86Å and 0.684 respectively; "*global*" roughness σ and cumulative roughness δ are found to be 2.1Å and 1.07Å respectively. In Fig. 3 we show analysis of a typical transverse diffuse scan. The specular component of the scan is assumed to be a Gaussian function with the

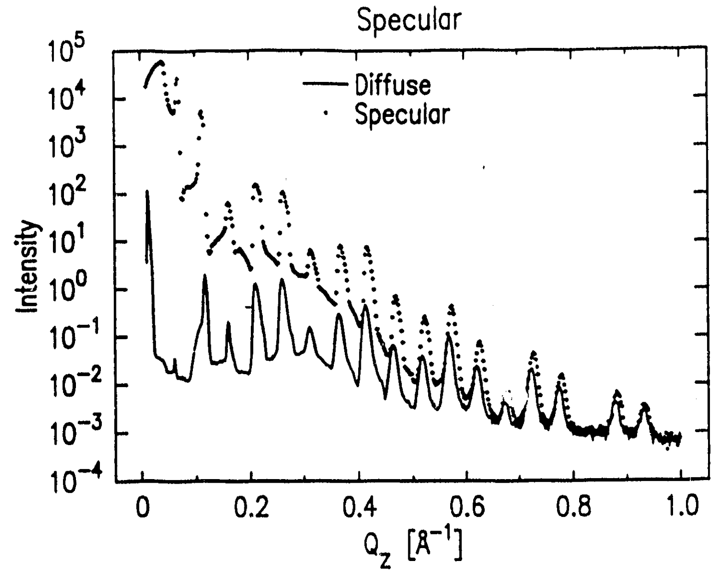

Fig. 1. As measured specular reflectivity and longitudinal diffuse scattering data for GaAs/AlAs multilayer.

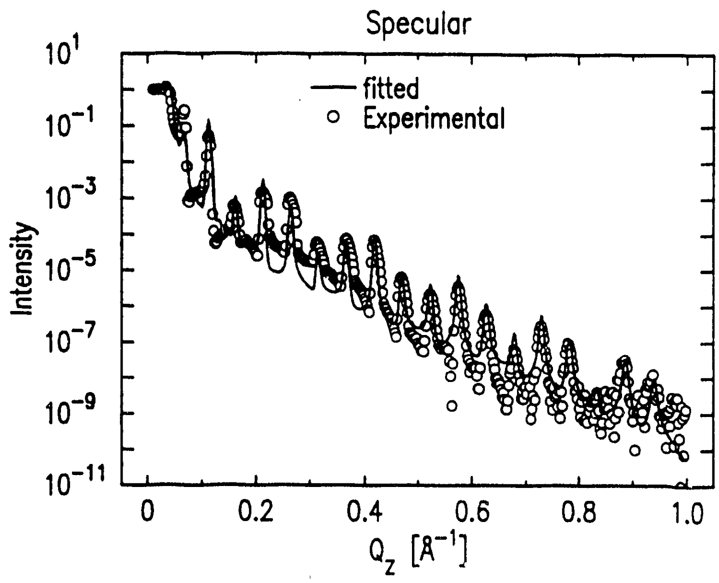

Fig. 2. Specular reflectivity data and the fitted curve as described in the text.

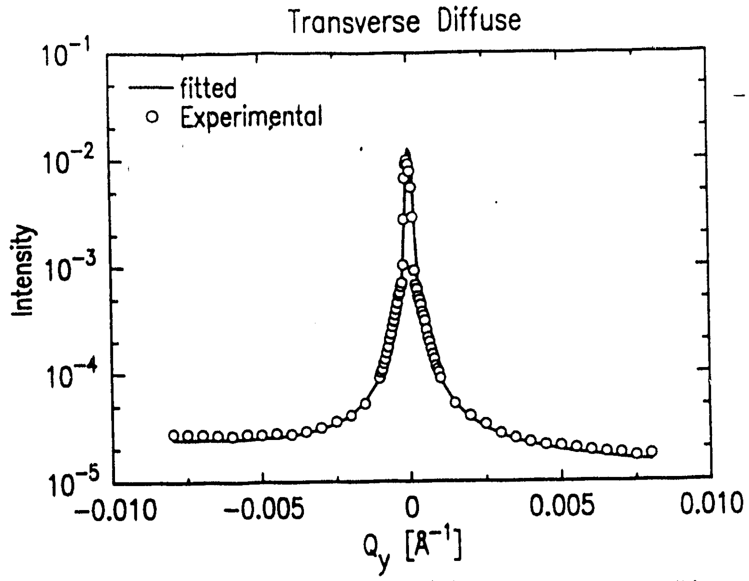

Fig. 3. Transverse diffuse scattering data across the fifth Bragg peaks. The solid curves represent the calculated scattering. The central portion represents the calculated Gaussian shaped specular component which was added to the diffuse scattering.

the width of the resolution function at that position. The diffuse component is calculated using Eq. (4) with a further assumption that correlation length $\xi_\perp$ is much larger than the multilayer thickness. The solid line in Fig. 3 shows the fitted curve generated by numerical integration of equation (4) and the obtained values of the parameters h and $\xi_\parallel$ are found to be 0.4 and 7000 Å respectively. The small value of h, which contains information regarding the texture of the roughness, indicates that the interface is not a smooth one although it has a large in plane correlation length. In the limit that $\xi_\perp \to \infty$, Eq. (3) shows that the q_z dependence of the ratio of the diffuse comoonent I_D to the specular component I_s is given by

$$I_D = C I_s q_z F(q_z) \tag{5}$$

where C is a constant and $F(q_z)$ is the integral in Eq. (4) which is now independent of i, j and evaluated at $q_\parallel = 0.001 \mathring{A}^{-1}$. Fig. (4) shows I_D calculated using Eq. (5) and I_s as given the experimentally observed specular reflectivity (i.e. including the small hump at $q_z = 0.3\mathring{A}^{-1}$ which was not accounted for in the model). It can be seen that the agreement is good, showing a high degree of conformality for the multilayers.

We have shown here that analysis of small angle specular reflectivity and diffuse scattering data of multilayer systems can generate information regarding the interfacial roughness, its conformality and texture. This in turn provides us valuable hints regarding the growth process for multilayers. Detail analysis of the specular and diffuse scattering data is beyond the scope of this short communication and will be presented in a future publication.

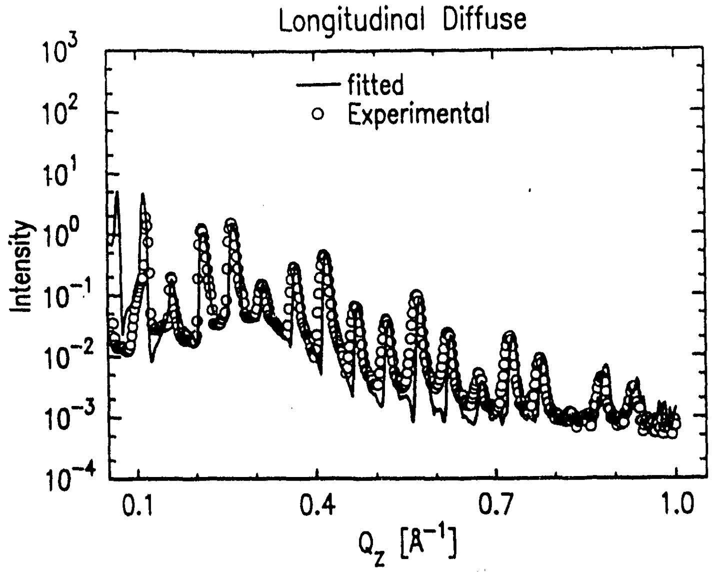

Fig. 4. Longitudinal diffuse scattering data and the fitted curve as described in the text.

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