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THE CHARACTERIZATION OF INTERFACE ROUGHNESS AND OTHER DEFECTS IN MULTILAYERS BY X-RAY SCATTERING

S.K. Sinha, M.K. Sanyal, and A. Gibaud,*
Physics Department, Brookhaven National Laboratory
Upton, New York 11973 U.S.A.

S.K. Satija, C.F. Majkrzak
National Institute for Standards and Technology
Gaithersburg, Maryland 20899 U.S.A.

H. Homma
Physics Department, Brooklyn College of CUNY
Brooklyn, New York 11210 U.S.A.

INTRODUCTION

In this paper we present some theoretical and experimental results on the characterization of roughness in thin films and multilayers by scattering techniques. Particular attention is focussed on the difference between specular and diffuse scattering and on correlated roughness between interfaces.

SPECULAR VS. DIFFUSE SCATTERING

There are two components to the scattering cross-section from a rough surface. One is a true specular component which is restricted to the specular ridge (chosen as the q_z axis in reciprocal space) and which contains the factors $\delta(q_x)\ \delta(q_y)$ and is a function of q_z. This component is thus limited only by the resolution width of the spectrometer in a transverse scan (rocking curve) across the specular ridge in q-space. The other is a diffuse component due to the height-height fluctuations of the interface. It is centered at $q_x=q_y=0$ but is in general broader than the instrumental resolution and gives "tails" to the rocking curves, as well as being a function of q_z. The specular reflectivity is obtained from the true specular component as [1,2]

$$R = R_F \exp\left(-q_z \tilde{q}_z \sigma^2\right) \tag{1}$$

where R_F is the usual Fresnel reflectivity for a smooth surface of the same material, $\tilde{q}_z$ is the value of q_z inside the medium $(=\sqrt{q_z^2 - q_c^2}$, where q_c is the critical normal wavevector transfer for total reflection), nd σ is the rms surface roughness. To obtain a true estimate of the <u>global</u> surface roughness one must subtract from the measured intensity the estimated diffuse scattering under the specular ridge, i.e. one must separate the two components (else one is measuring only a (smaller) <u>local</u> roughness over a region inversely proportional to the instrumental acceptance width in q-space). In practice, this can usually be done by measuring the diffuse scattering on either side of the specular ridge by slightly missetting the reflecting surface off the specular angle, although if the diffuse scattering is sharply peaked around the specular ridge (i.e. if the surface height-height correlations are long ranged) one may need very tight

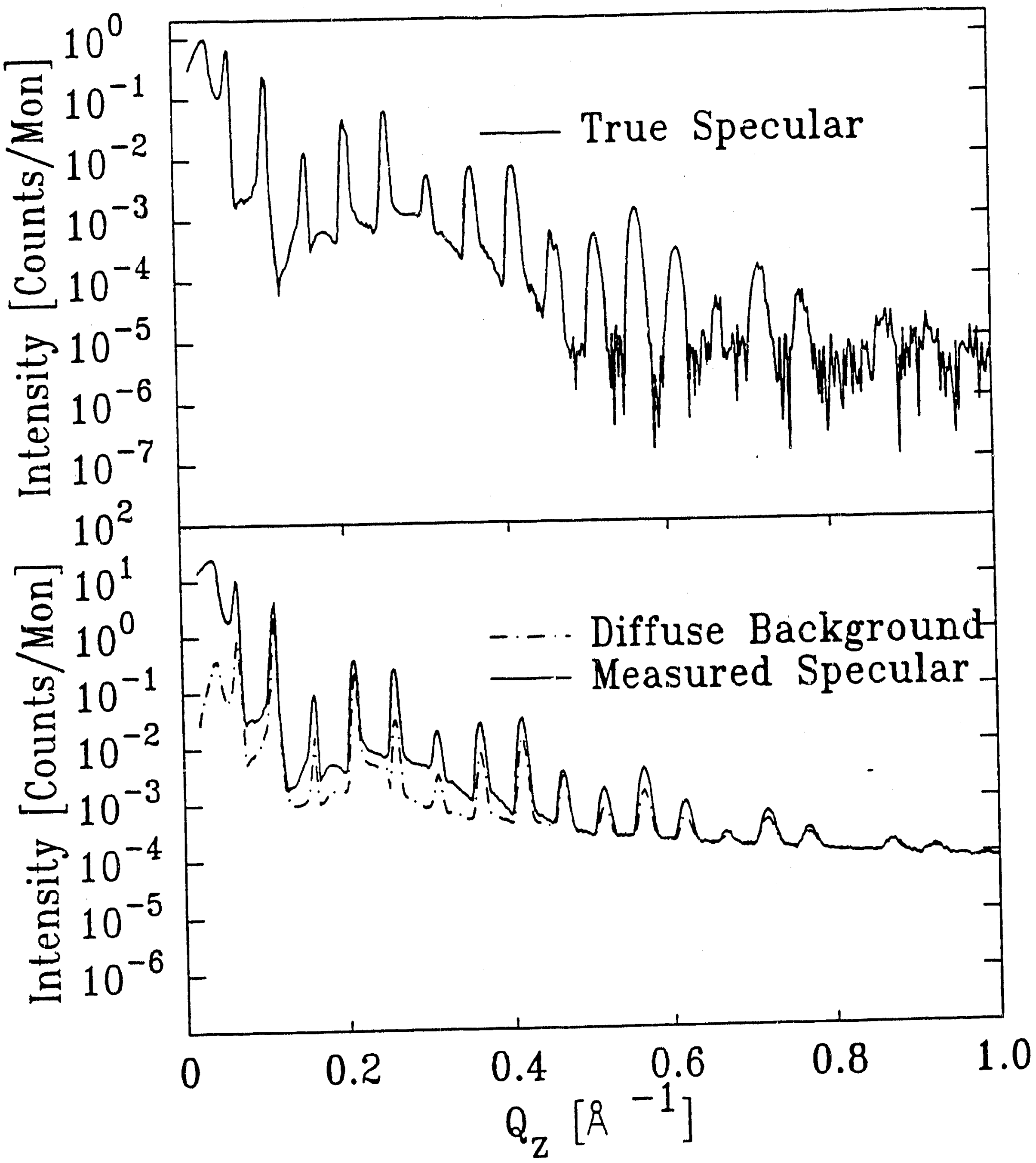

Fig. 1 (Lower) On-ridge nominal specular scattering (solid curve) and diffuse background (dotted curve) for a GaAs/AlAs multilayer at small angles. (Upper) The true (background subtracted) specular reflectivity.

resolution settings. One must also integrate over the width of the true specular peak in the rocking curve, noting that the resolution width changes continuously with q_z. Such procedures have generally not always been followed in reflectivity measurements from multilayers, resulting in probably considerable underestimates of surface roughness. As an example, we show in Fig. 1 the specular and diffuse scattering (i.e. off-specular scattering) from a GaAs/AlAs multilayer in the small angle region as measured at the National Synchrotron Light Source at Brookhaven[3]. Note that the difference which is the true amplitude of the specular scattering decreases much more rapidly with q_z than the "raw" intensity yielding a larger value of the roughness. Note also that the diffuse scattering also shows multilayer low angle Bragg peaks. This is due to correlated interface roughness and is discussed in the next section.

CONFORMAL INTERFACE ROUGHNESS

We now discuss the general results for scattering from a multilayer where the interfaces possess correlated or conformal roughness, in the sense illustrated in Fig. 2. We work here in the small angle limit, i.e. we neglect the crystal structure of the materials assuming only uniform electron densities in the layers separated by (rough) interfaces. This may be expressed mathematically in the following manner. If $\delta z_i(\mathbf{r})$ is the height fluctuation of interface i above its <u>average</u> value at lateral position $\mathbf{r}$ in the plane, we write

$$\left\langle \delta z_i(0)\delta z_j(\vec{r})\right\rangle = c_{ij}(\vec{r}) \tag{2}$$

If the roughness of the interfaces is truly uncorrelated, $c_{ij}(\mathbf{r})=\delta_{ij}c(\mathbf{r})$ where $c(\mathbf{r})$ can be generally taken to be of the form $\sigma^2 \exp(-r/\xi_{||})^h)$ $(o<h<1)$[1], and the diffuse scattering will be the incoherent sum of the diffuse scattering from each interface. If on the other hand, there is a degree of conformal roughness (as in Fig. 2), we may write

$$c_{ij}(\vec{r}) = c_o(\vec{r}) + \sigma^2 \exp\left(-\left|z_i - z_j\right|/\xi_\perp\right)\ c(\vec{r}) \tag{3}$$

where z_i, z_j are the mean positions of interfaces i.j respectively, and $\xi_\perp$ is a conformal correlation length along the z-direction. (We have assumed, for simplicity, that the mean square roughness of each interface is the same) $C_o(\mathbf{r})$ represents a short-wavelength fluctuation on each interface which is independent of the others. Then the expression for the diffuse scattering intensity from the N interfaces in the multilayer can be shown to be given in the Born approximation by[3]

$$I = \frac{I_o}{q_z^2}\frac{1}{k_o^2 Sin\alpha Sin\beta}\sum_{ij}\Delta\rho_i\Delta\rho_j\ \ e^{-iq_z(z_i-z_j)}\ \exp\left[-q_z^2\left(\sigma^2+\delta^2|i-j|\right)\right]\ F_{ij}(\vec{q}_{//}) \tag{4}$$

while the expression for the integrated specular reflectivity in the Born approximation is given by

$$R = \frac{16\pi^2}{q_z^4}\sum_{ij}\Delta\rho_i\Delta\rho_j^{\ -iq_z(z_i-z_j)}\exp\left[-q_z^2\left(\sigma^2+\delta^2|i-j|\right)\right] \tag{5}$$

In Eqs. (4) and (5), I is the detector counts per second, I_o the incident beam intensity (we assume the sample completely intercepts the beam), k_o the wavevector of the incident radiation, α and β the angles which the incident and scattered beams respectively make with the surface,

$$\Delta\rho_i = \frac{e^2}{mc^2}\left(n_i^- - n_i^+\right) \tag{6}$$

where $n_i^\pm$ denotes the electron density of the medium above or below the interface i, δ is the root-mean-square random error in the mean thickness of each layer compared to its nominal mean thickness, and

$$F_{ij}(q_{//}) = \iint dxdy\left[e^{q_z^2 c_{ij}(\vec{r})} - 1\right]\ e^{-i\vec{q}_{//}\cdot\vec{r}} \tag{7}$$

$q_{||}$ being the component of the set momentum transfer parallel to the surface. These expressions are only valid for $q_z >> q_c$ while near or below

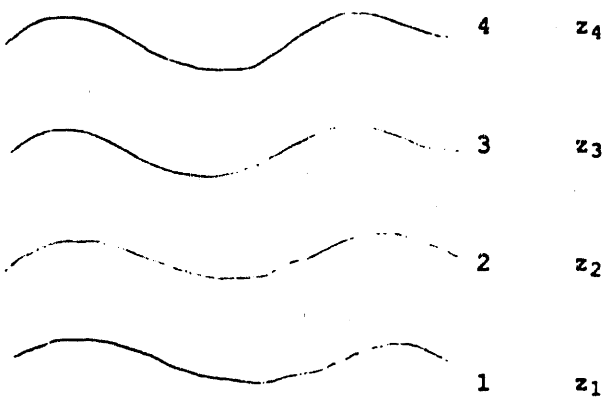

Fig. 2 Schematic showing conformally rough interfaces in a multilayer. The interfaces are denoted by 1,2,...etc. with average heights z_1, z_2,... above a reference $z=0$ plane.

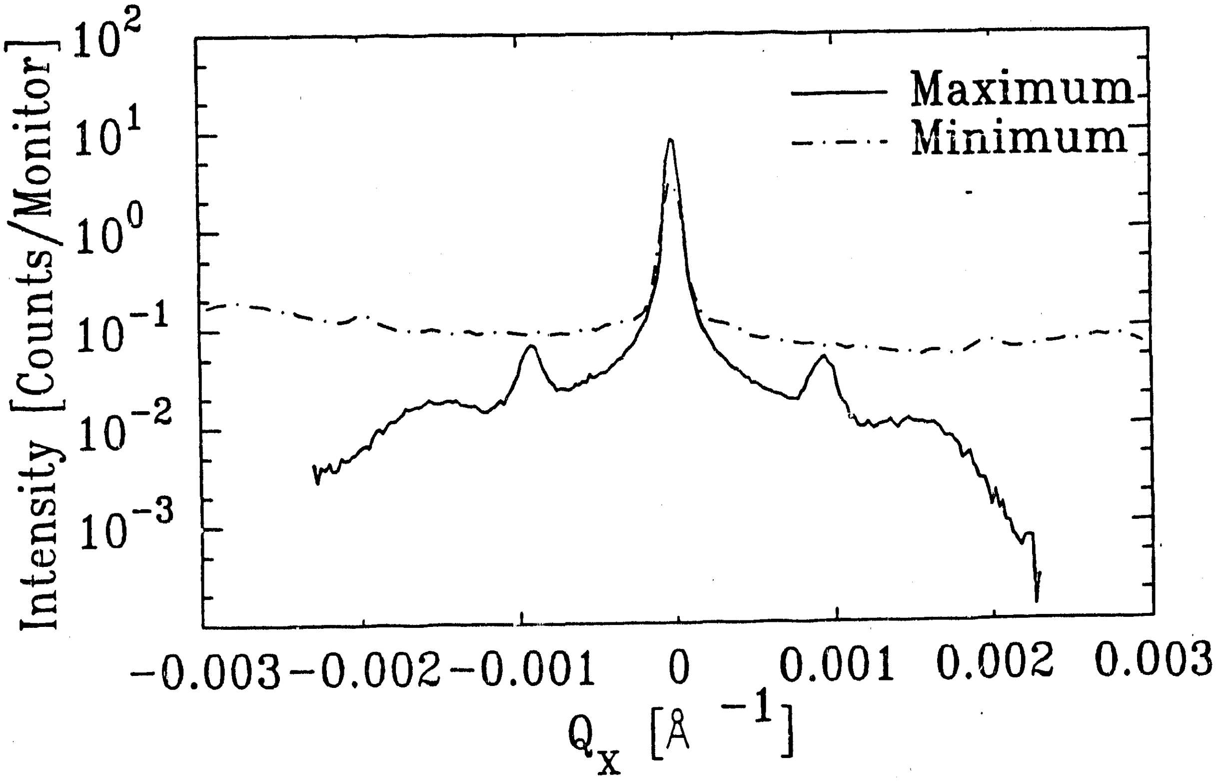

Fig. 3 Transverse scans of the diffuse scattering across the specular ridge for a Pb/Ge multilayer at a specular maximum and at a minimum.

the critical angle they have to be modified according to the Distorted Wave Born Approximation[2] in a manner which we shall not have space to discuss here. Eq. (6) must of course also be convolved with the instrumental resolution in order to reproduce the observed counts.

We now discuss qualitatively the structure of the scattering. The factor $e^{-q_z^2\delta^2|i-j|}$ arising from the cumulative deposition error δ will produce a "smearing out" along q_z of both the specular (Bragg) peaks and the diffuse scattering peaks. (In the limit of an infinite number of bilayers, the Bragg peaks would become delta functions in q_z but are broadened to Lorentzians by this factor). If $\xi_\perp$ is very large, i.e. the conformal roughness persists over all the interfaces, so that $c_{ij}(r)$ becomes more or less independent of i.j, then the factor $e^{-iq_z(z_i-z_j)}$in the diffuse scattering will produce constructive and destructive interference between the scattering from the various interfaces, resulting in the peaks in the diffuse scattering seen in Fig. 1. Thus a transverse scan (rocking curve) across the specular ridge will show a different line shape when q_z is at a Bragg peak and when it is at a minimum between peaks. This is illustrated in Fig. 3 for a Pb/Ge multilayer[4]. The transverse scan across a q_z-minimum is fairly flat, corresponding to rather short-length scale height-height correlations which are not conformal between interfaces, while that across a Bragg peak is peaked strongly at the specular ridge, implying conformal long length-scale height fluctuations across the interfaces. The additional peaks at transverse q-values do not imply periodic order along the surfaces, but are rather a interesting manifestation of what we may call "generalized Yoneida scattering[2,5] (due to multiple Bragg and diffuse scattering whenever either the incident or scattered beams make an angle with the surface corresponding to total reflection or Bragg scattering).

It should be borne in mind, for crystalline multilayers, that the roughness of the interfaces is a manifestation of the height and orientation distribution of the microcrystalline grains at the interface. Thus a combination of small and wide angle data is needed for a complete micro-characterization of the grain morphology in multilayers. Detailed results will be given elsewhere[3].

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*Permanent address - Universite du Maine, Faculte des Sciences, Route de LAVAL, 72017 Le Mans, Cedex, France.

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