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Grading effects in X-ray specular reflectivity analysis

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Introduction

Grazing incidence X-ray reflectometry is a powerful tool for surface analysis [1,2]. Specular reflectivity permits the analysis of density profile and roughness. However, our recent experiments [3] at BL14A have revealed the significance of considering grading at the surface and interfaces. Conventional models based on stacking uniform layers with interface roughness can sometimes lead to the wrong conclusion. This report describes some calculations.

Results and Discussion

Calculations were based on Parratt's theory [4] and assumed that the density gradient can be treated as a multilayered structure composed of extremely thin slices with different densities. Fig.1 shows the results for synthtic quartz substrate, the surface of which has linear and Gaussian grading, respectively, in the top 2 nm region. It is possible to analyze the reflectivity curve obtained by conventional procedures, i.e., curve fitting to the model taking into consideration homogenous layers and interface roughness. In this case, it was necessary to assume 2 thin layers on the substrate (i.e., 3-layer model) in order to obtain a good fit. The obtained parameters are summarized in Table 1. The corresponding reflectivity curves are plotted as dashed lines in Fig.1 as well.

The fit is quite good, and the differences in the reflectivity curves are small. However, one can see that the density for the 2nd intermediate layer is high for both grading cases, and even higher than that of the bulk (2.65 g/cm^3). Also, the roughness of the interface between the 1st and 2nd layers is quite big compared with other interfaces. Those unnatural features frequently appear when analysing practical samples, which usually have some grading due to chemical diffusion and/or near-surface damages during polishing etc. Even so, the present calculation requires further extension. It is probably not practical to treat roughness simply as a part of the density gradient

References

[1] J.Daillant, A.Gibaud, "X-Ray and Neutron Reflectivity: Principles and Applications", Springer,(1999).
[2] M.Tolan, "X-Ray Scattering from Soft-Matter Thin Films", Springer, (1999).
[3] M. Mizusawa and K.Sakurai, this report
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Table 1. The parameters obtained by the model neglecting grading effects for synthetic quartz

	Linear grading			Gaussian grading		
	Thickness (nm)	Roughness (nm)	Density (g/cm^3)	Thickness (nm)	Roughness (nm)	Density (g/cm^3)
Layer 1	1.24	0.10	0.93	1.56	0.1	0.93
Layer 2	1.07	0.83	2.95	0.56	0.39	3.13
Substrate	-	0.21	2.65	-	0.21	2.65
R value	Normal	1.56×10^{-6}		Normal	1.87×10^{-7}	
	Log	9.51×10^{-5}		Log	1.35×10^{-4}	

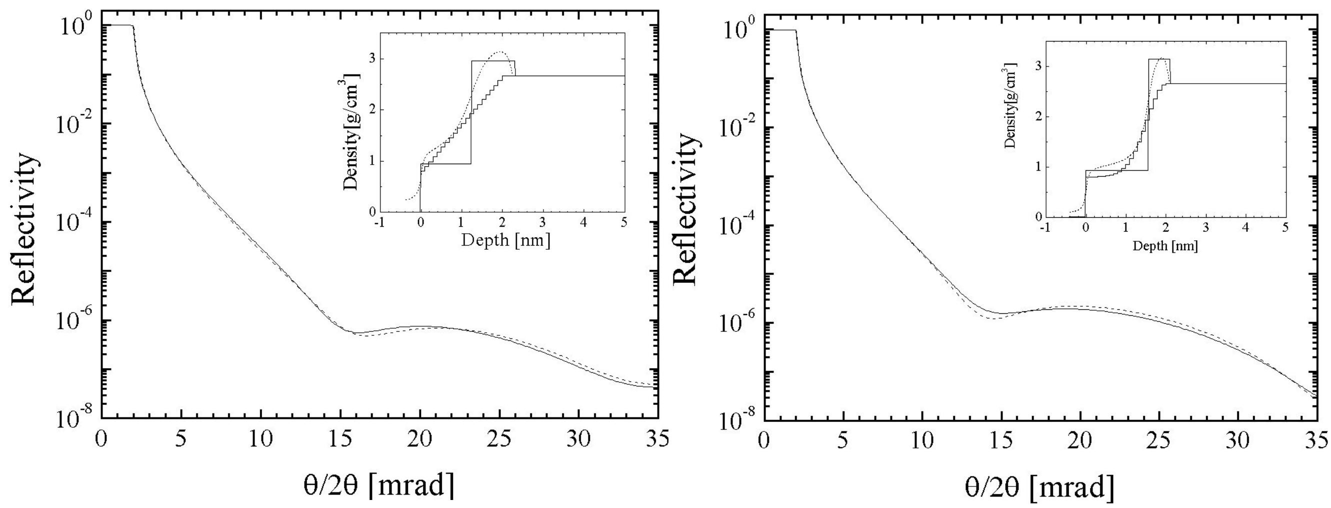

Figure 1. Calculated results for synthetic quartz with graded surface using a density grading model (solid line) and fitting results using a model with 3 homogeneous layers (dashed line). The models are shown as insets (the dashed line is the electron density profile obtained from the fitting to the 3-layer model). Linear grading c (left), Gaussian grading (right). The fitting results are shown in Table 1.