The Failure of Conventional Wisdom: Multilayer Roughness and Reflectivity

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There are two approaches that are conventionally used to incorporate the effects of interfacial roughness in the calculation of the specular reflectivity of a multilayer film. The first, which we will call the Debye-Waller (DW) method, is to simply multiply the reflectivity calculated in the absence of roughness with a factor $\exp[-16\pi^2\sigma^2/\lambda^2]$, where σ is some weighted average of the root-mean-square roughness of the interfaces. The second, more common method we will call the "modified Fresnel coefficient" (MFC) method. In this approach the interfacial roughness is assumed to modify the Fresnel coefficients that describe the specular reflectance (and transmission) at each interface, and these modified Fresnel coefficients are applied to the matrix or iteration methods used to calculate the reflectivity of the multilayer film. The purpose of this paper is to demonstrate that both of these conventional methods fail to accurately estimate the specular reflectivity of multilayer films.

We show with specific examples that, for interfacial roughness characteristic of realistic multilayer films, *the DW method systematically overestimates, and the MFC method systematically underestimates, the <u>decrease</u> in reflectivity due to the roughness*. The reason for this problem is that the phase coherence of the fields scattered by the different interfaces is of critical importance. The nonspecular scattering will be coherent if the roughness of the different interfaces is correlated (i.e. conformal). The DW method treats the scattering from the interfaces as perfectly coherent, as would be the case if the multilayer roughness was purely conformal. In contrast, the MFC method treats the scattering from the interfaces as completely incoherent, as would be the case if the roughness of the different interfaces was completely uncorrelated. Hence the decrease in the reflectivity predicted by the two methods can differ by a factor as large as N_{eff}, the effective number of bilayers contributing to the reflectivity.

In reality the interfacial roughness of multilayer films is partially correlated; low spatial frequencies tend to be replicated from layer to layer while high spatial frequencies are uncorrelated. Consequently the nonspecular scattering is partially coherent, varying from stronger to weaker coherence as the scattering angle increases. The DW and MFC methods place lower and upper bounds on the specular reflectivity, respectively. To accurately calculate the decrease in specular reflectivity due to roughness, one must perform the laborious task of integrating the nonspecular scattering.

The failure of the conventional methods of calculating reflectivity has serious implications for those using x-ray scattering as a tool for characterizing roughness in multilayer structures; the error incumbent in the reflectivity calculation can invalidate the structural characterization of the film. For example, consider the common practice of using the MFC method to model an x-ray reflectivity measurement. Typically the interfacial roughness σ is treated as a fitting parameter when there is no independent measurement of roughness available. In this case the value of σ inferred by modeling the reflectivity data will be overestimated. Similarly, if σ is independently determined and used in the MFC calculation, the calculated reflectivity will exceed the measured value, and the disparity will be (incorrectly) attributed to other unknown parameters such as contamination of the top surface.