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Analysis of X-ray reflectivity from sputtered carbon thin films (2) Wavelet transform analysis

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Introduction

The recent pioneering application of wavelet transform for analysing X-ray reflectivity data [1] is quite significant because it can enhance information on the specific interface. This report describes the wavelet transform of X-ray reflectivity data from a carbon thin film sputtered on a Si wafer [2].

Theoretical Background

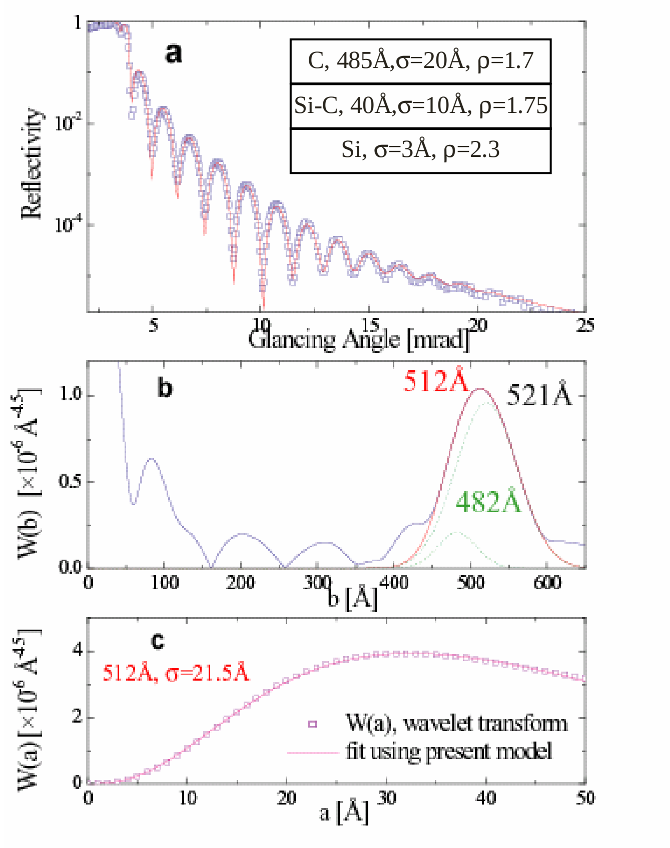
The wavelet coefficients $W_{a,b}$ for X-ray reflectivity, taking the Mexican Hat wavelet as the mother wavelet, can be written using two parameters *a* and *b*.

$$W_{a,b} = \sqrt{2\pi a}\int_{q_1}^{q_2} q'^4 \left|R_N(q')\right|^2 \Phi_a(q' - q_{\min}) \exp(iq'b)\, dq'$$

where $q' = 2k_0\sqrt{\sin^2(\theta_0) - \sin^2(\alpha_c)}$,

$$\Phi_a(q') = (q'a)^2 \exp\left[-(q'a)^2/2\right] ,$$

For specific *a* value, this is essentially the same as a conventional Fourier transform and exhibits maxima at, $b=z_{ij}$ where z_{ij} is the thickness of the layer between interfaces *i* and *j*. On the other hand, *W(a)* for a particular layer ($b=z_{ij}$) can give information on the specific interface.



Data Analysis

Figure 1a shows the experimental reflectivity obtained from a carbon thin film for 8.04 keV X-rays. The details of the sample preparation were described elsewhere [2]. The thicknesses of the particular layers were determined from the dependence of wavelet coefficients on the position parameter *b*, where each peak represents the response from a particular layer as shown in Fig.1b. The asymmetric peak at 512Å is the superposition of the responses from the C layer and total film. Decomposition of this peak gave two Gaussian curves centered at 482Å and 521Å, giving the thickness of the intermediate Si-C layer as 39Å. The approximate roughness of the film can be determined from the fit of W(a) for the peak at 512Å in Fig.1b, and the results are shown in Fig.1c. Here, it is not easy to determine the roughness for each interface, because of the extremely thin Si-C layer in the present case. The technique can give good initial values for further optimization. The obtained values are listed in the table in Fig.1a.

This approach allows the thickness and roughness of each layer in the studied system to be obtained from the wavelet transform of the reflectivity curve without assumption of a particular film structure. The advantage of this method in comparison to conventional fitting of the reflectivity curve is that, when estimating roughness, the number of simultaneously fitting parameters is reduced to one. The method can be applied to the analysis of thin films with unknown chemical and physical properties. It is useful for the characterization of structures with a complex composition, particularly oxide or diffuse layers. The authors would like to thank Dr. S. Takahashi (NIMS) for preparing the samples.

References

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Figure 1. Analysis of X-ray reflectivity of carbon thin film sputtered on a silicon substrate.
a Reflectivity curve. Closed circle, experimental data. Solid line, calculation using parameters listed in the table.
b Wavelet transform of X-ray reflectivity (*b* dependence)
c Wavelet transform of X-ray reflectivity (*a* dependence)