

Multiparameter Characterization of subnanometer Cr/Sc-Multilayers

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Problem: Limited Reflectivity



Cr/Sc Mirrors show only a fraction of theoretically possible reflectivity at an AOI 1.5°



Interface Properties



Roughness (diffuse scattering)



Interdiffusion (diminished reflectivity)

Binary Model





Parameters:

- Multilayer period D
- Sc and Cr layer thicknesses
- Nevot/Croce factor (roughness and interdiffusion)

Can the experiment be described with this model?

Binary Layer Approach





Binary Model with only Nevot/Croce factor fails



Graded interface model needed?

Graded Interface Model





Graded interface model with explicit gradual changes at the interfaces and interdiffusion

Parameter	Definition
$\overline{D / \mathrm{nm}}$	$= d_{\rm Sc} + d_{\rm Cr}$
Γ_{Sc}	$= d_{ m Sc}/D$
s_d / nm	$= s_{ m Sc} + s_{ m Cr}$
Γ_s	$= s_{ m Sc}/s_d$
η	layer intermixing
σ_r / nm	r.m.s. roughness
$ ho_{Sc}$	Sc density w.r.t. bulk density
$ ho_{Cr}$	Cr density w.r.t. bulk density

Analysis Strategy

Parameters:

- Multilayer period D
- Sc and Cr layer thicknesses
- Interdiffusion/mixing of the two materials
- Interface properties/shape
- Nevot/Croce factor (roughness)



➡ fit based on particle swarm optimization followed by MCMC sampling



Analysis Strategy

Parameters:

- Multilayer period D
- Sc and Cr layer thicknesses
- Interdiffusion/mixing of the two materials
- Interface properties/shape
- Nevot/Croce factor (roughness)

Combination of complementary methods:

- EUV reflectivity (EUV)
- Cu K-*α* XRR
- Resonant EUV reflectivity (across Sc L-edge) (REUV)
- X-ray fluorescence analysis (X-ray standing wave, **XSW**)

Combined fit based on particle swarm optimization





Complementary Experiments





Resonant EUV reflectivity (across Sc L-edge) X-ray fluorescence analysis (X-ray standing (REUV)



Combined Analysis





Consistent Model





- The two layers interdiffuse strongly (50-60 %)
- Asymmetric interface gradients

Confidence Intervals





DWBA Modelling



$$\begin{pmatrix} \frac{d\sigma}{d\Omega} \\ \frac{d\sigma}{diffuse} \end{pmatrix} = \frac{A\pi^2}{\lambda^4} \sum_{j=1}^N \sum_{i=1}^N (n_j^2 - n_{j+1}^2)^* (n_i^2 - n_{i+1}^2) \left((T_j^{(1)} + R_j^{(1)})^* (T_j^{(2)} + R_j^{(2)})^* \right) \\ \times (T_i^{(1)} + R_i^{(1)}) (T_i^{(2)} + R_i^{(2)}) c_{\perp}^{ij}(q_x) C(q_x) \longleftarrow \frac{\text{Power Spectral Density (PSD)}}{\text{Density (PSD)}}$$

$$Multilayer Factor$$

$$C(q_x) = \frac{4\pi H \sigma^2 \xi_{\parallel}^2}{(1 + ||q_x||^2 \xi_x^2) (1 + H)} \quad c_{ij}^{\perp}(q_x) = \exp\left(-\sum_{j=1}^{\max(i,j)} \frac{d_n}{\xi_{\perp}(q_x)}\right)$$

$$C(q_x) = \frac{4\pi HO |\zeta_{\parallel}|}{(1 + |q_x|^2 \xi_{\parallel}^2)^{1+H}} \quad c_{ij}^{\perp}(q_x) = \exp\left(-\sum_{n=\min(i,j)}^{\infty} d_n/\xi_{\perp}\right)$$

Integral PSD:

$$\sigma_r = \frac{1}{2\pi} \sqrt{\int_0^\infty q_{\parallel} C(q_{\parallel}) \, dq_{\parallel}}$$

Haase et al.: Appl. Optics 53, No. 14, 3019-3027 (2014)

Diffuse scattering





Integral PSD: $\sigma_r = \frac{1}{2\pi} \sqrt{\int_0^\infty q_{\parallel} C(q_{\parallel}) \, dq_{\parallel}}$

Root mean square roughness: $\sigma_r = 0.17 \pm 0.02$



Summary and Outlook



- The combination of several complementary methods is required to deduct a consistent model
- Ultra-thin multilayer systems require explicit modeling of the interfaces showing strong interdiffusion
- Roughness and interdiffusion can be distinguished by DWBA simulations based on the explicit model found above

A. Haase, S. Bajt, P. Hönicke, V. Soltwisch and F. Scholze: J. Appl. Cryst. **49**, No. 6, p. 2161-2171 (2016))