• Designing a multilayer

- Designing a multilayer
- Reflection from a graded index

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Homework Assignment #02: Problems on Blackboard due Tuesday, February 18, 2020

Materials for multilayer monochromator chosen to reflect 12 keV x-rays at  $\sim 2$  degrees with 0.5% and 1.0% bandwidth

A. Khounsary et al., "A dual-bandwidth multilayer monochromator system," *Proc. SPIE* **10760**, 107600j (2018).

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Common design parameters include bilayer filler fraction  $\Gamma = 0.5$ , roughness  $\sigma = 0.35$  nm, and number of bilayers N = 300

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Common design parameters include bilayer filler fraction  $\Gamma = 0.5$ , roughness  $\sigma = 0.35$  nm, and number of bilayers N = 300

 $MoSi_2/B_4C$  and  $Mo/B_4C$ were selected for the 0.5% and 1.0% bandwidth coatings, respectively

C. Segre (IIT)

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# Multilayer fabrication & testing

The 0.5% and 1.0% bandwidth layers were deposited side-by-side on a monolithic 20 mm  $\times$  30 mm  $\times$  100 mm polished silicon block



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#### Multilayer fabrication & testing

The 0.5% and 1.0% bandwidth layers were deposited side-by-side on a monolithic 20 mm  $\times$  30 mm  $\times$  100 mm polished silicon block

When illuminated with 12 keV xrays the two multilayers showed diffraction peaks at nearly the same angle. The reflectivities were both over 75% and the bandwidths were 0.52% and 0.86%, respectively.

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# Multilayer spectrum



A. Khounsary et al., "A dual-bandwidth multilayer monochromator system," Proc. SPIE 10760, 107600j (2018).

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The density profile of the interface can be described by the function f(z) which approaches 1 as  $z \to \infty$ .

The reflectivity can be computed as the superposition of the reflectivity of a series of infinitesmal slabs of thickness dz at a depth z.

The differential reflectivity from a slab of thickness dz at depth z is:

$$\delta r(Q) = -i\frac{Q_c^2}{4Q}f(z)dz$$

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Calculating the full reflection coefficient relative to the Fresnel reflection coefficient

$$\frac{R(Q)}{R_F(Q)} = \left| \int_{-\infty}^{\infty} \left( \frac{df}{dz} \right) e^{iQz} dz \right|^2$$

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The error function is often chosen as a model for the density gradient

$$f(z) = erf(rac{z}{\sqrt{2}\sigma}) = rac{1}{\sqrt{\pi}}\int_0^{z/\sqrt{2}\sigma} e^{-t^2}dt$$

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$$Q = k \sin \theta, \quad Q' = k' \sin \theta'$$

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# Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.
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$$\begin{aligned} r_{V} &= -r_{0}\rho \int_{V} e^{i\vec{Q}\cdot\vec{r}}d\vec{r} \\ &= -r_{0}\rho \int_{V} \vec{\nabla}\cdot\left(\hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_{z}}\right)\cdot d\vec{r} \\ r_{5} &= -r_{0}\rho \int_{S}\left(\hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_{z}}\right)\cdot d\vec{S} \end{aligned}$$

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The actual scattering cross section is the square of this integral

$$\frac{d\sigma}{d\Omega} = \left(\frac{r_0\rho}{Q_z}\right)^2 \int_S \int_{S'} e^{iQ_z(h(x,y) - h(x',y'))} e^{iQ_x(x-x')} e^{iQ_y(y-y')} dxdydx'dy'$$

If we assume that h(x, y) - h(x', y') depends only on the relative difference in position, x - x' and y - y' the four dimensional integral collapses to the product of two two dimensional integrals

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$$= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int \left\langle e^{iQ_z(h(0,0) - h(x,y))} \right\rangle e^{iQ_x x} e^{iQ_y y} dx dy$$

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where  $A_0 / \sin \theta_1$  is just the illuminated surface area

If we assume that h(x, y) - h(x', y') depends only on the relative difference in position, x - x' and y - y' the four dimensional integral collapses to the product of two two dimensional integrals

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Finally, it is assumed that the statistics of the height variation are Gaussian and

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2 \left\langle \left[h(0,0) - h(x,y)\right]^2 \right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Define a function  $g(x, y) = \langle [h(0, 0) - h(x, y)]^2 \rangle$  which can be modeled in various ways.

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by the definition of a delta function

 $2\pi\delta(q) = \int e^{iqx} dx$ 

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this leads to a rapid drop in reflectivity as the surface roughness increases



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Gaussian with variance  $\mathcal{A}Q_z^2$ 

16+08 0.08 1e+07 0.06 ď 1e+06 0.04 100000 0.02 10000 1000 -0.01 -0.005 0 0.005 0.01 ď,



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1e+09

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And the scattering exhibits both a specular peak, reduced by uncorrelated roughness, and diffuse scattering from the correlated portion of the surface

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TEHOS, tetrakis–(2ethylhexoxy)–silane, a non-polar, roughly spherical molecule, was deposited on Si(111) single crystals

C.-J. Yu et al., "Observation of molecular layering in thin liquid films using x-ray reflectivity", Phys. Rev. Lett. 82, 2326–2329 (1999).

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Deviations from uniform density are used to fit experimental reflectivity

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There are always peaks between 10-20Å and 20-30Åand a broad peak at the free surface showing the presence of ordered layers of molecules.

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# Layering in liquid films



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There are always peaks between 10-20Å and 20-30Åand a broad peak at the free surface showing the presence of ordered layers of molecules.

The authors conclude that the presence of a hard smooth surface is required for ordering and therefore deviations from an ideal, isotropic liquid.

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The sample was flipped to a downward facing position and silver atoms deposited for a period of time, then flipped to an upward facing position for the reflectivity measurements

C. Thompson et al., "X-ray-reflectivity study of the growth kinetics of vapor-deposited silver films," Phys. Rev. B 49, 4902–4907 (1994).

The goal of this project was to understand the evolution of surface roughness during the growth of a silver thin film.

The question is whether there is surface diffusion of the deposited atoms during the growth

In order to study this question, a silicon substrate was placed in the growth chamber and illuminated with x-rays after a period of deposition

The sample was flipped to a downward facing position and silver atoms deposited for a period of time, then flipped to an upward facing position for the reflectivity measurements

5 deposition with thicknesses varying from 10 nm to 150 nm were studies

C. Thompson et al., "X-ray-reflectivity study of the growth kinetics of vapor-deposited silver films," Phys. Rev. B 49, 4902–4907 (1994).

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Ag/Si films: 10nm (A), 18nm (B), 37nm (C), 73nm (D), 150nm (E)

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-Distribution 10<sup>1</sup>  $g(R) (nm^2)$ 5 Δ -10 z (nm) 100 100 200 300 (nm)  $10^{-1}$ 101 R (nm)

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C. Segre (IIT)

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High vapor pressure and thermal excitations limit the number of pure metals which can be studied but alloy eutectics provide many possibilities

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surface layer is rich in Bi (95%), second layer is deficient (25%), and third layer is rich in Bi (53%) once again



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 $F_1B = F_2B = a$ 

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A cost effective way to focus in both directions is a toroidal mirror which has a fixed bend in the transverse direction but which can be bent longitudinally to change the vertical focus.







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- Refractive lenses good final focus, focus moves with energy, significant attenuation and hard to change focal length

Rh Pt 50 cm glass x-rays



Ultra low expansion glass polished to a few Å roughness



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One platinum stripe and one rhodium stripe deposited along the length of the mirror on top of a chromium buffer layer



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A bending mechanism to permit vertical focusing of the beam to  $\sim$  60  $\mu m$ 

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### Mirror performance (cont.)



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As energy rises, the Pt layer begins to show the reflectivity of a thin slab.