Today's outline - September 18, 2024

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- Multilayer monchromator

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- Graded interfaces

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Reading Assignment: Chapter 3.9–3.10

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Reading Assignment: Chapter 3.9–3.10

Homework Assignment #03:
Chapter 3: 1,3,4,6,8
due Monday, September 30, 2024

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- Multilayer monchromator
- Graded interfaces
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Reading Assignment: Chapter 3.9–3.10

Homework Assignment #03:
Chapter 3: 1,3,4,6,8
due Monday, September 30, 2024

Homework Assignment #04:
Chapter 4: 2,4,6,7,10
due Monday, October 14, 2024

Parratt's method review

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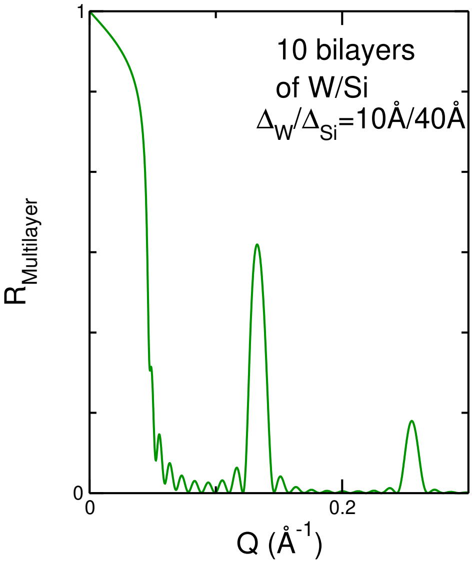

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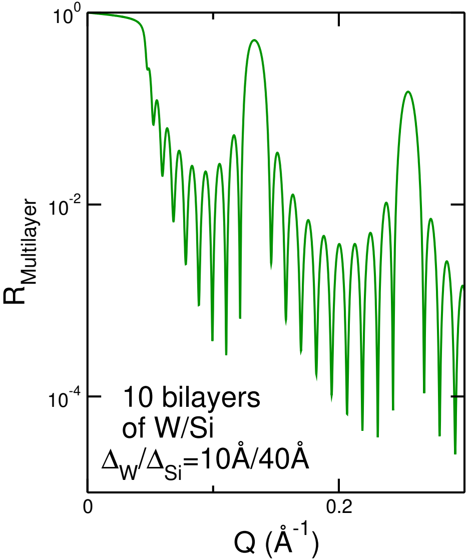

Multilayer design

Materials for multilayer monochromator chosen to reflect 12 keV x-rays at ~ 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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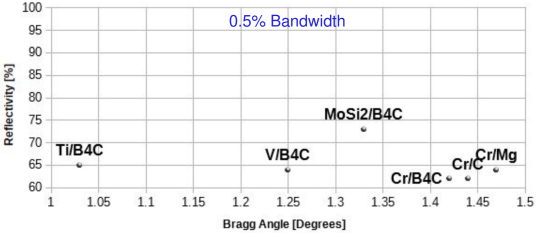

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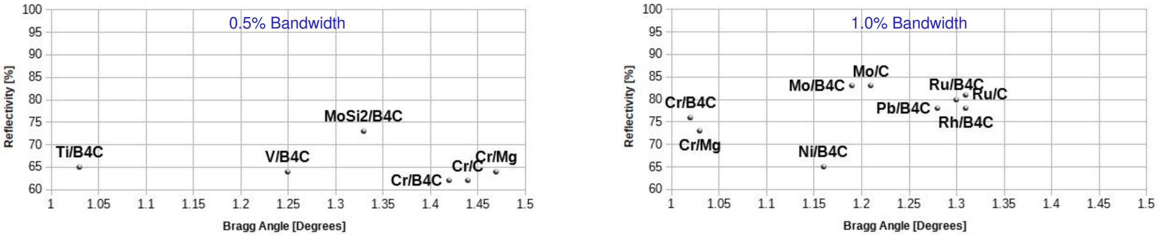

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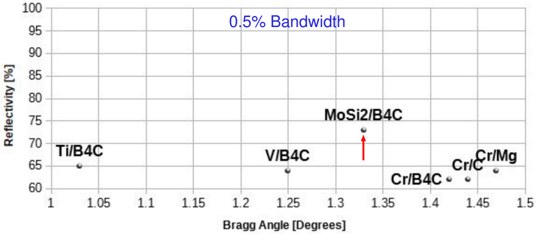
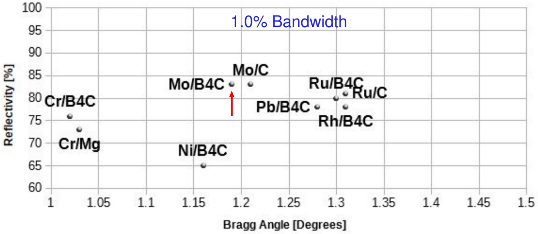
$MoSi_2/B_4C$ and Mo/B_4C were selected for the 0.5% and 1.0% bandwidth coatings, respectively





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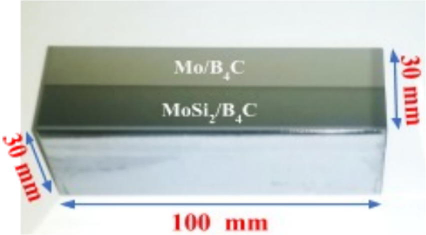
Multilayer fabrication & testing

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



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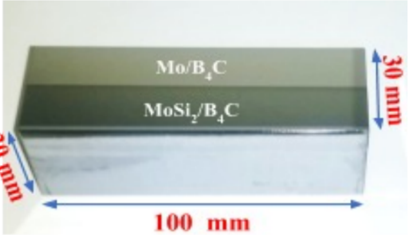

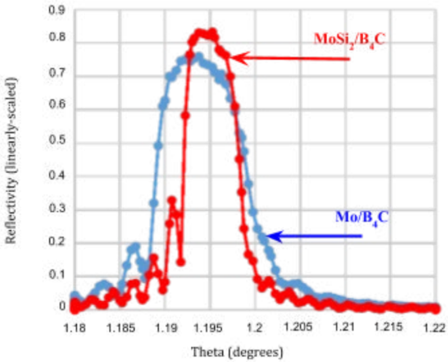

When illuminated with 12 keV x-rays the two multilayers showed diffraction peaks at nearly the same angle. The reflectivities were both over 75% and the bandwidths were 0.52% and 0.86%, respectively.

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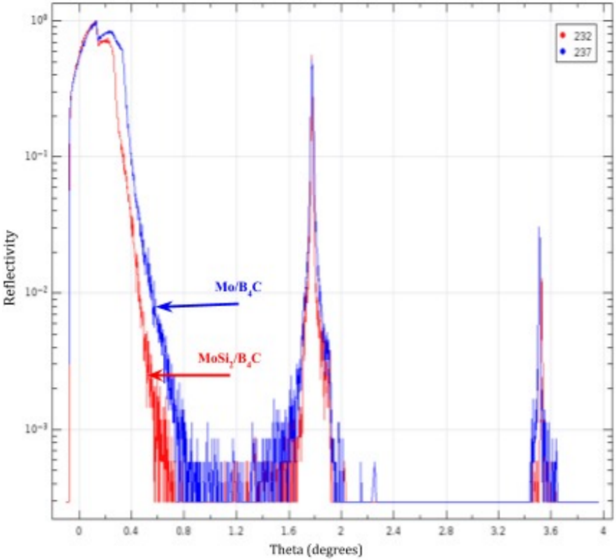
Multilayer spectrum



The reflectivity over a wide range of angles at 8 keV shows total external reflection at low angles with cutoff at zero degrees

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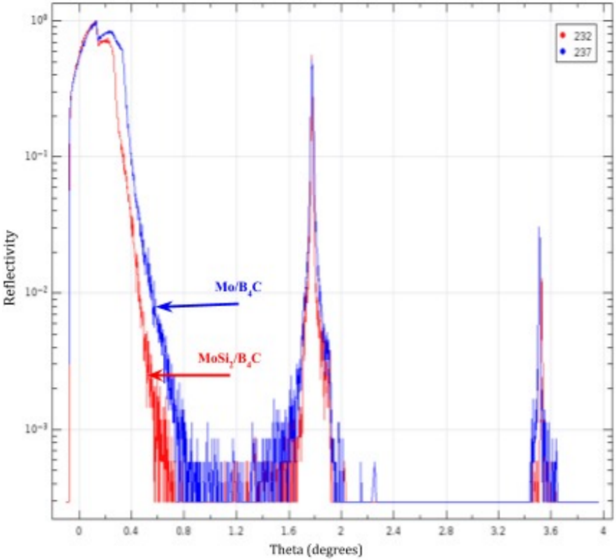

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First and second order multilayer diffraction peaks appear at higher angles

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Graded interfaces

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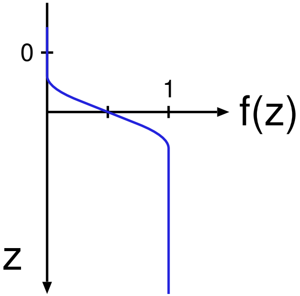

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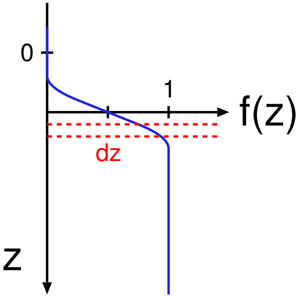

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The reflectivity can be computed as the superposition of the reflectivity of a series of infinitesmal slabs of thickness dz at a depth z.

Reflectivity of a graded interface

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

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Calculating the full reflection coefficient relative to the Fresnel reflection coefficient

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

The error function - a specific case

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

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

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whose Fourier transform is also a Gaussian, which when squared to obtain the reflection coefficient, gives.

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

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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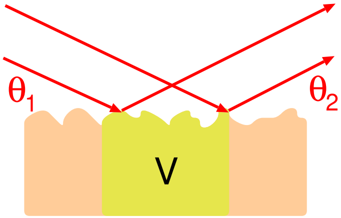

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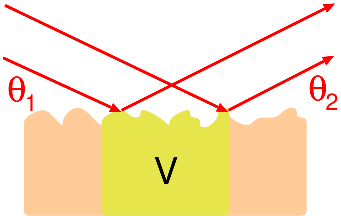

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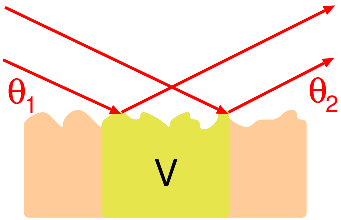

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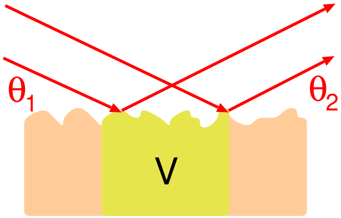

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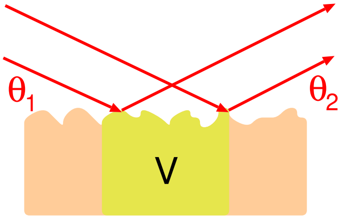

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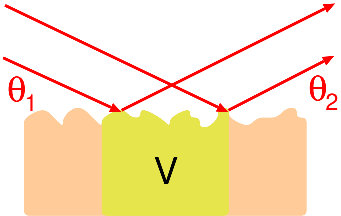

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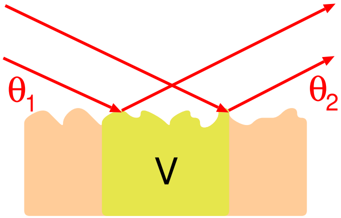

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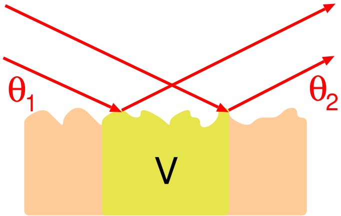

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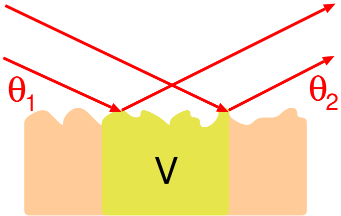

The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

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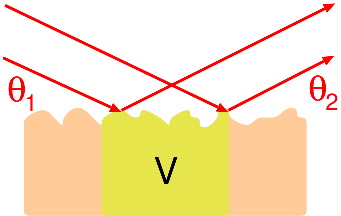

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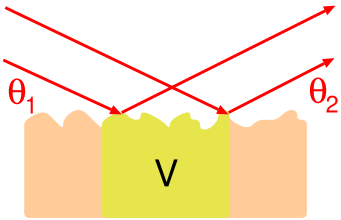

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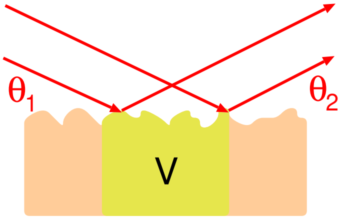

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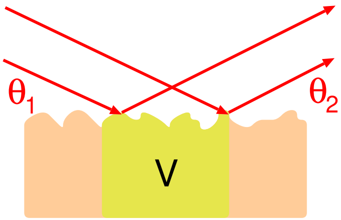

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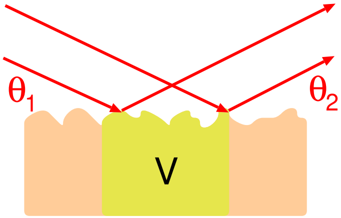

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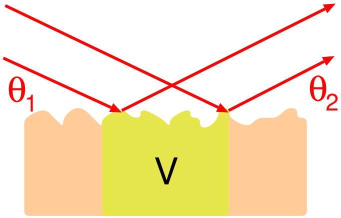

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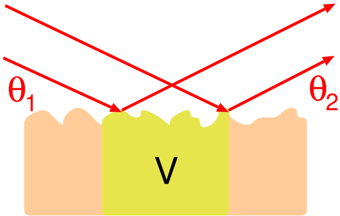

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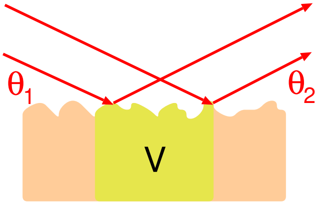
Reflection from a rough surface leads to some amount of diffuse scattering on top of the specular reflection from a flat surface. The scattering from an illuminated volume is given by V.



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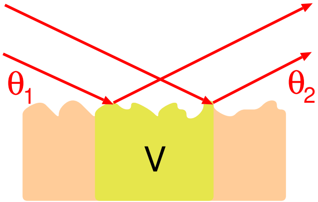

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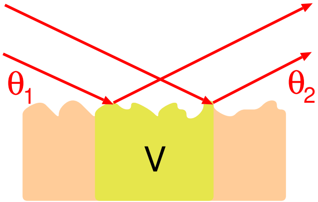

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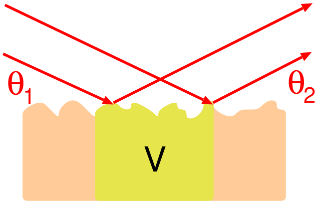

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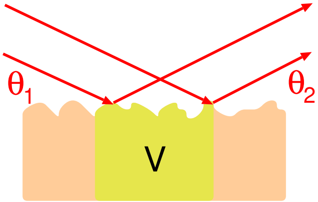

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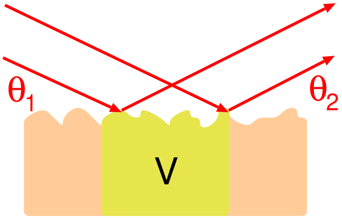
This integral is highly model dependent and can now be evaluated for a number of different cases.

Evaluation of surface integral

The side surfaces of the volume do not contribute to this integral as they are along the $\hat{z}$ direction, and we can also choose the thickness of the slab sufficiently large such that the lower surface will not contribute.



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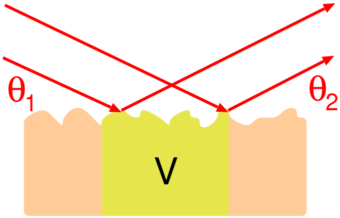

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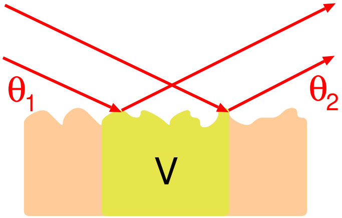

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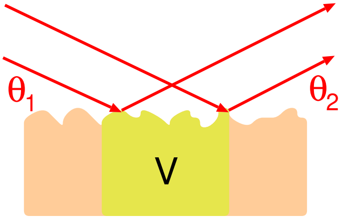

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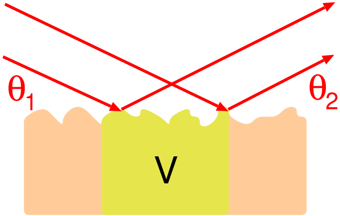

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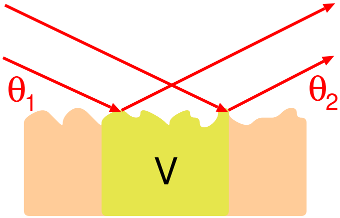

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$$\frac{d\sigma}{d\Omega} = r_S^2 = \left(\frac{r_0 \rho}{Q_z}\right)^2 \int_S \int_{S'} e^{iQ_z(h(x,y)-h(x',y'))} e^{iQ_x(x-x')} e^{iQ_y(y-y')} dxdydx'dy'$$

Scattering cross section

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

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

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For a perfectly flat surface, $h(x,y) = 0$ for all x and y.

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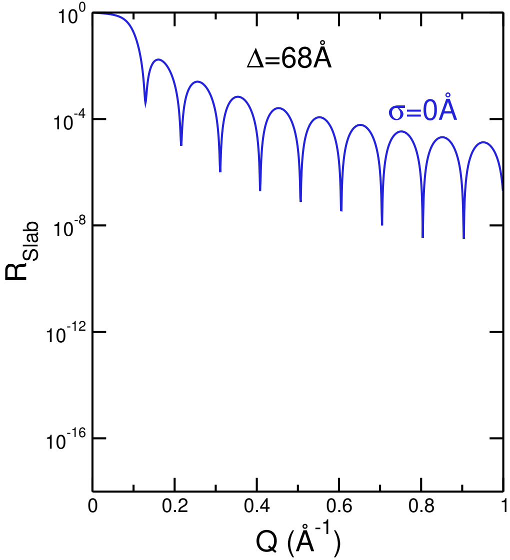

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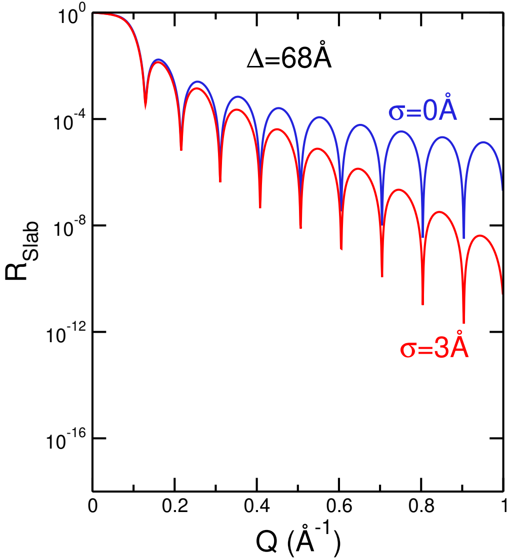

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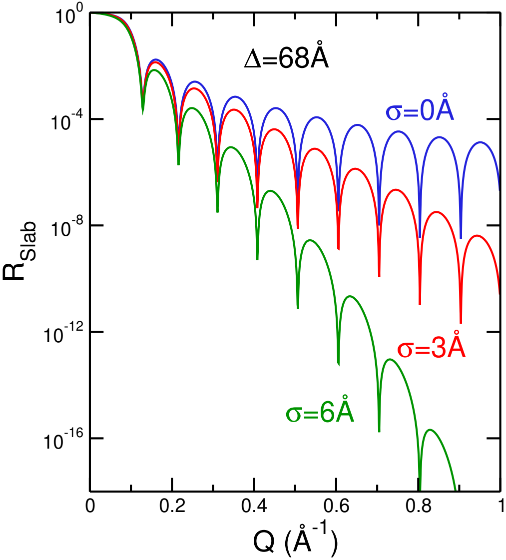

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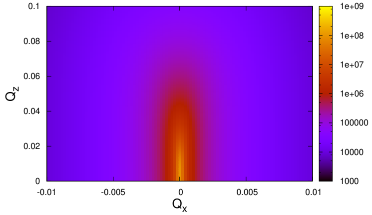
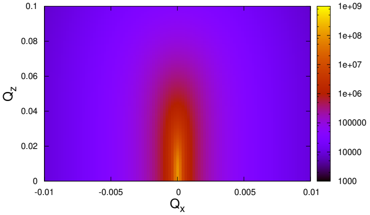


Unbounded correlations - limiting cases

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-\mathcal{A}Q_z^2|x|^{2h}/2} \cos(Q_x x)dx$$

This integral can be evaluated in closed form for two special cases, both having a broad diffuse scattering and no specular peak.



$h = 1/2$: Lorentzian with half-width $\mathcal{A}Q_z^2/2$

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{A_0 r_0^2\rho^2}{2\sin\theta_1}\right) \frac{\mathcal{A}}{(Q_x^2 + (\mathcal{A}/2)^2 Q_z^4)}$$

$h = 1$:

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{2\sqrt{\pi}A_0 r_0^2\rho^2}{2\sin\theta_1}\right) \frac{1}{Q_z^4} e^{-\frac{1}{2}\left(\frac{Q_x^2}{\mathcal{A}Q_z^2}\right)}$$

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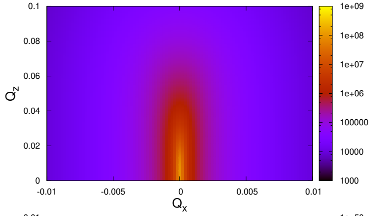

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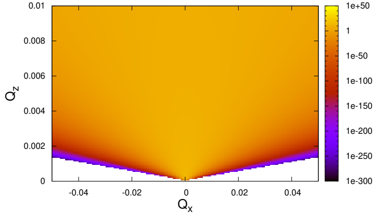

$h = 1$: Gaussian with variance $\mathcal{A}Q_z^2$

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Bounded correlations

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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

Layering in liquid films

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

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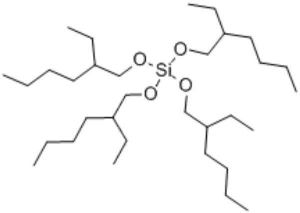

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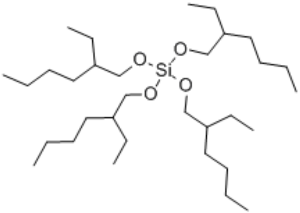

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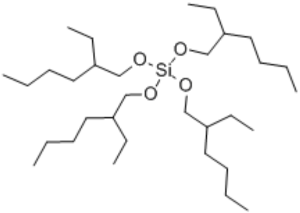

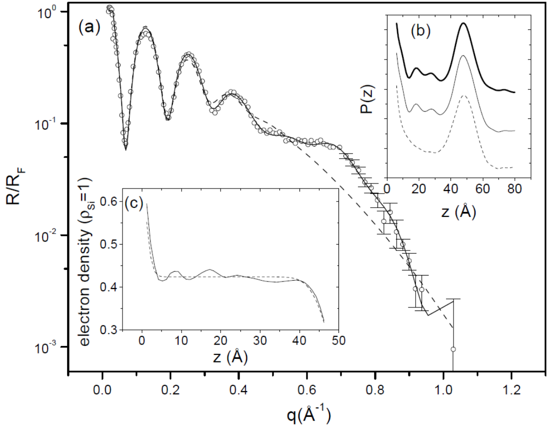

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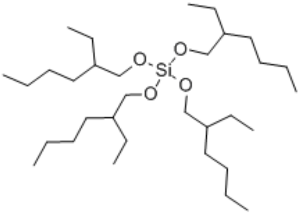

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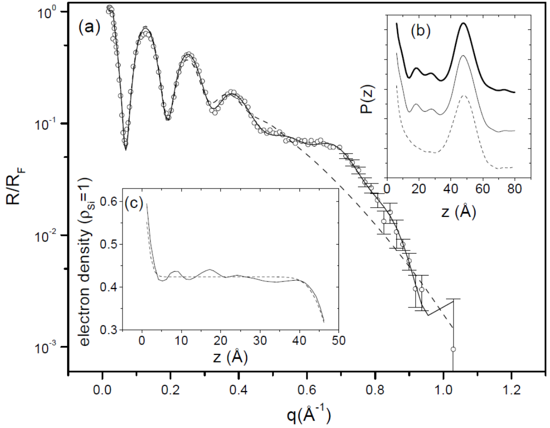

Deviations from uniform density are used to fit experimental reflectivity

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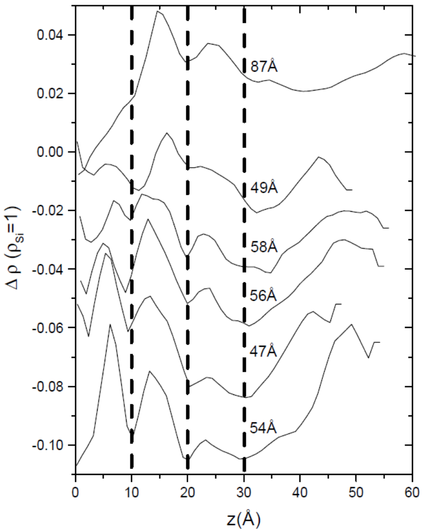

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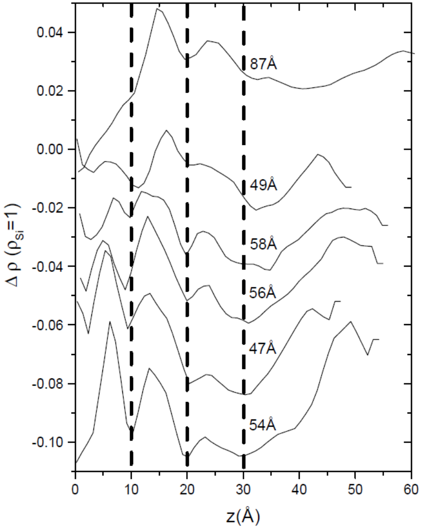

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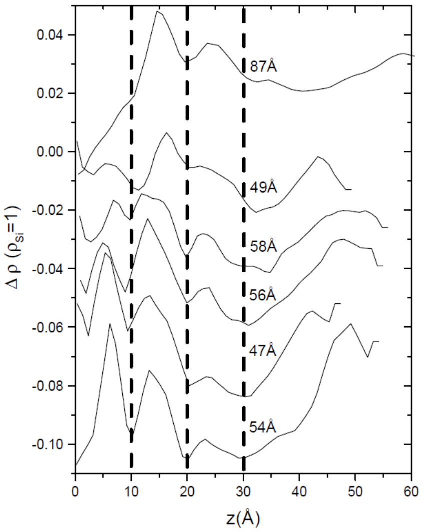

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There are always peaks between 10-20Å and 20-30Å and a broad peak at the free surface showing the presence of ordered layers of molecules.

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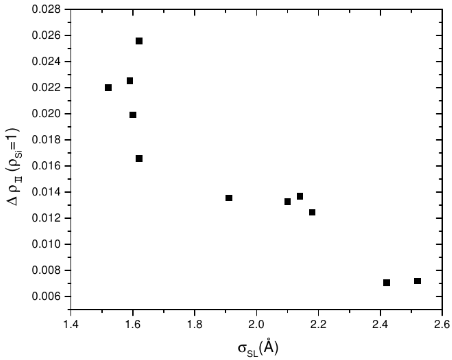

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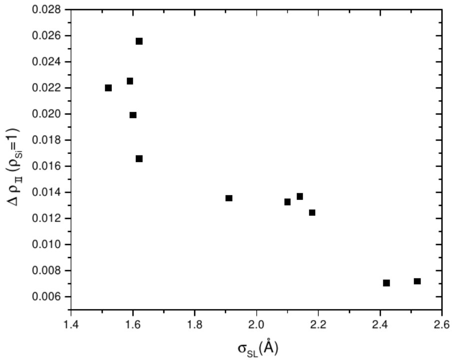

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Film growth kinetics

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

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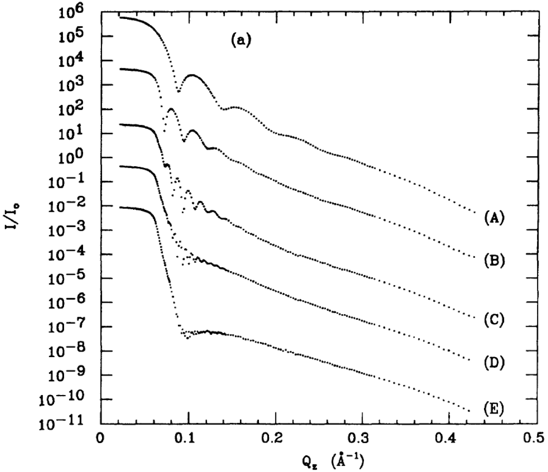

C. Thompson et al., "X-ray-reflectivity study of the growth kinetics of vapor-deposited silver films," *Phys. Rev. B* **49**, 4902–4907 (1994).

Film growth kinetics

Gaussian roughness profile with a "roughness" exponent $0 < h < 1$. As the film is grown by vapor deposition, the rms width σ, grows with a "growth exponent" β and the correlation length in the plane of the surface, ξ evolves with the "dynamic" scaling exponent, $z_s = h/\beta$.

$$g(r) \propto r^{2h} \qquad \sigma \propto t^{\beta}$$

$$\xi \propto t^{1/z_s} \qquad \langle h \rangle \propto t$$

$h \approx 0.33$, $\beta \approx 0.25$ for no diffusion.

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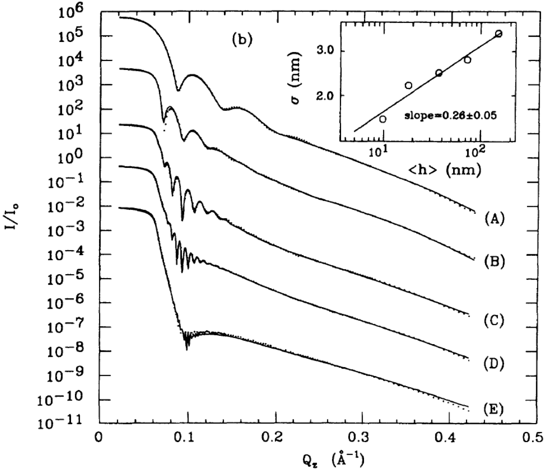

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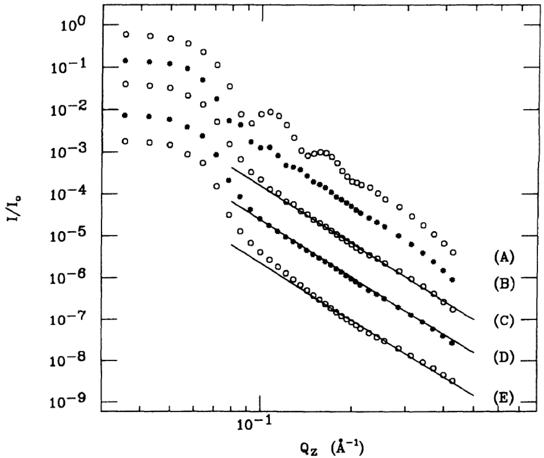

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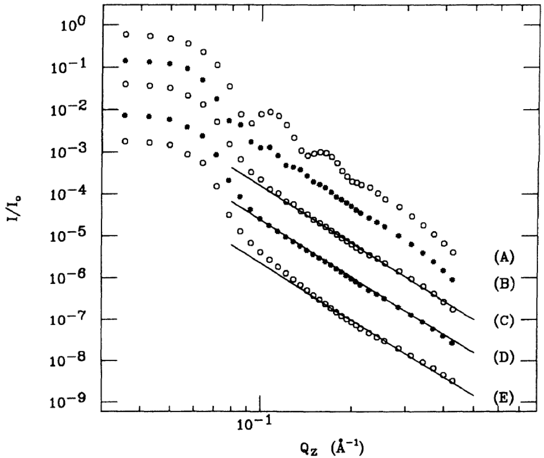

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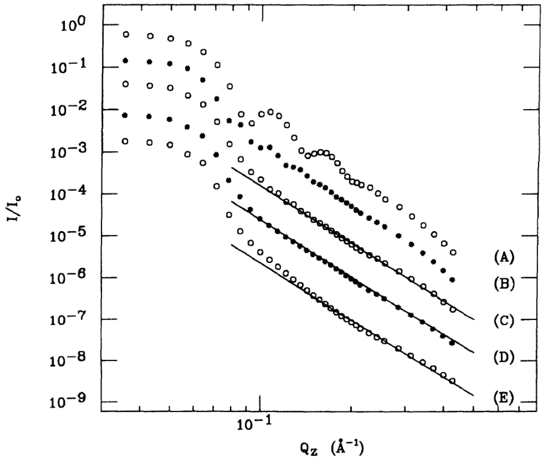
This gives $h = 0.63$ but is this correct?



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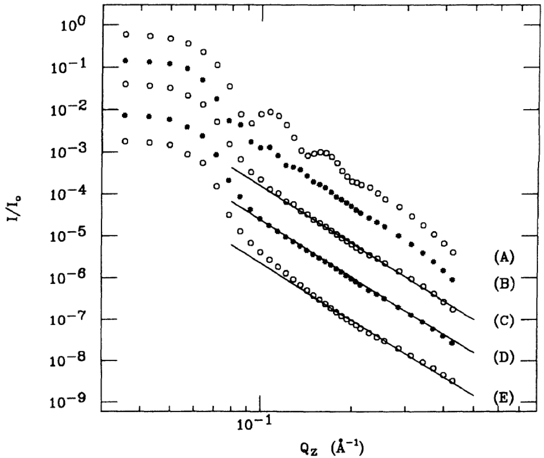

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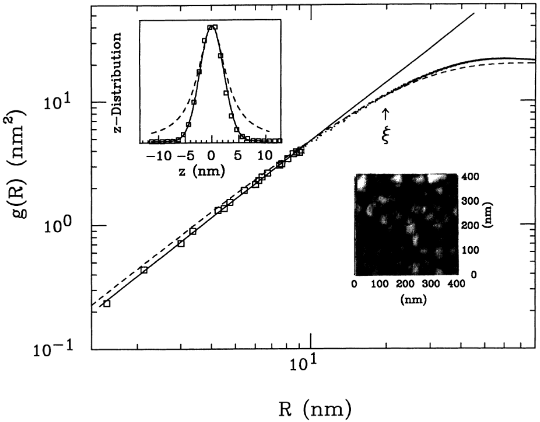

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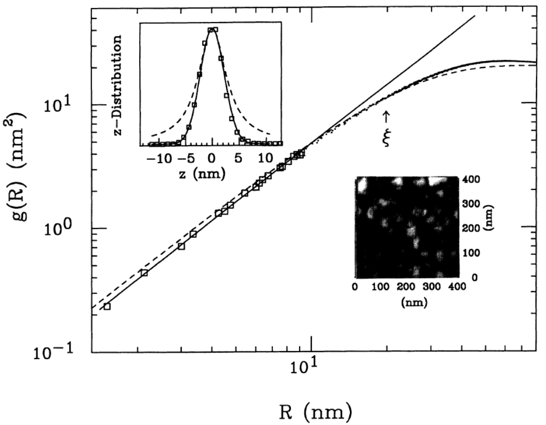

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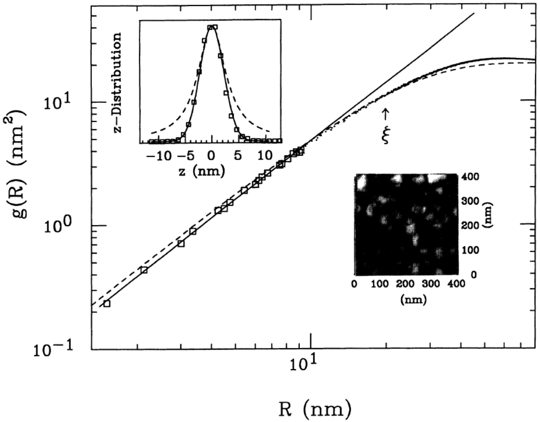
$$h = 0.78, \quad \xi = 23\text{nm}, \quad \sigma = 3.2\text{nm}$$

Thus $h = 0.70, \beta = 0.26$



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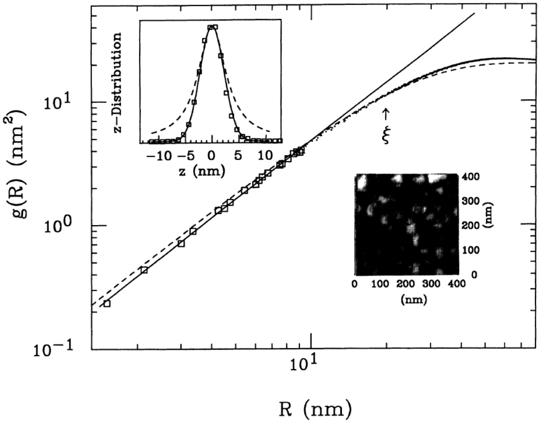

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Liquid metal surfaces

X-ray reflectivity using synchrotron radiation has made possible the study of the surface of liquid metals

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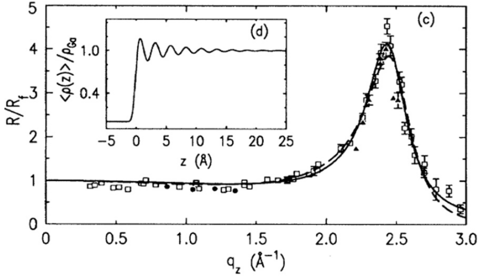

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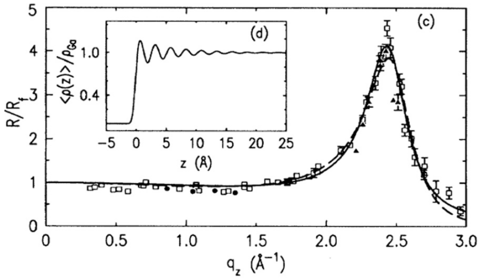

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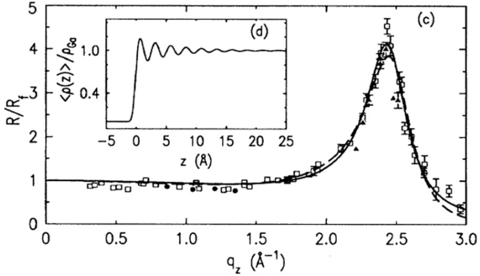

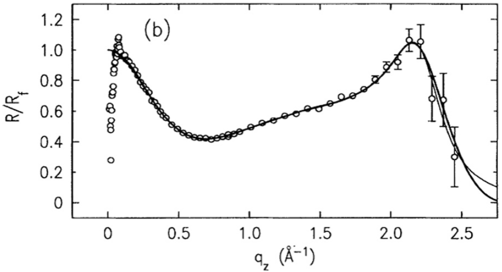

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High vapor pressure and thermal excitations limit the number of pure metals which can be studied but alloy eutectics provide many possibilities

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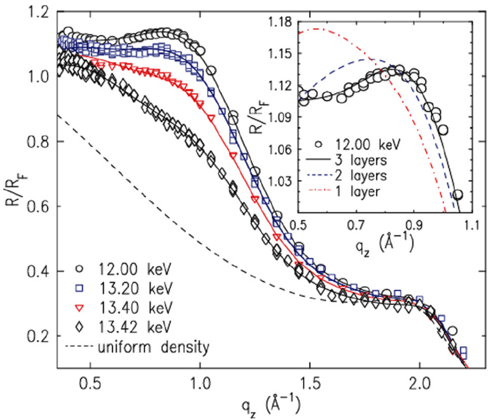

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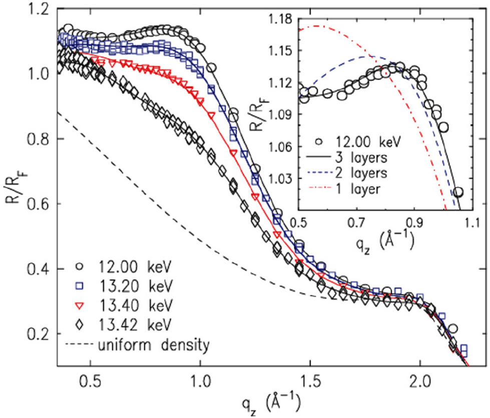
surface layer is rich in Bi (95%), second layer is deficient (25%), and third layer is rich in Bi (53%) once again



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