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Homework Assignment #03:
Chapter3: 1, 3, 4, 6, 8
due Wednesday, October 05, 2016

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Two days have been set aside for our class to be at Sector 10 MRCAT at the Advanced Photon Source

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I will try to get BioCAT time as well for those interested

Writing a General User Proposal

1. Log into the APS site
2. Start a general user proposal
3. Add an Abstract
4. Choose a beam line
5. Answer the 6 questions

Parratt's recursive method

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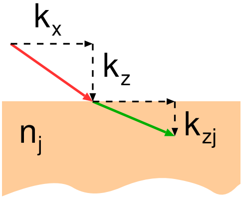
Because of continuity, $k_{xj} = k_x$ and therefore, we can compute the z-component of $\vec{k}_j$



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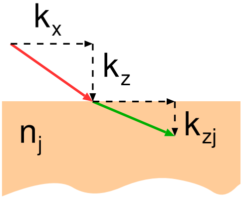
$$k_{zj}^2 = (n_j k)^2 - k_x^2$$



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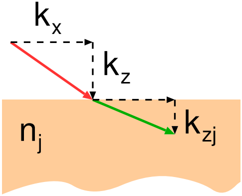

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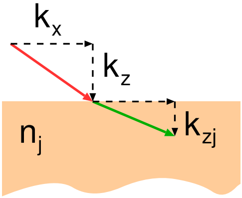

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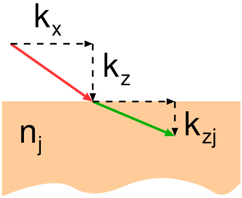

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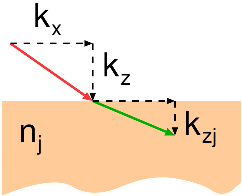

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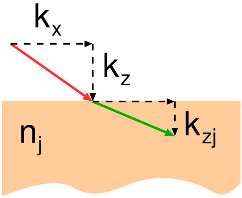

$$\begin{aligned} Q_j &= 2k_j \sin\alpha_j = 2k_{zj} \\ &= \sqrt{Q^2 - 8k^2\delta_j + 8ik^2\beta_j} \end{aligned}$$

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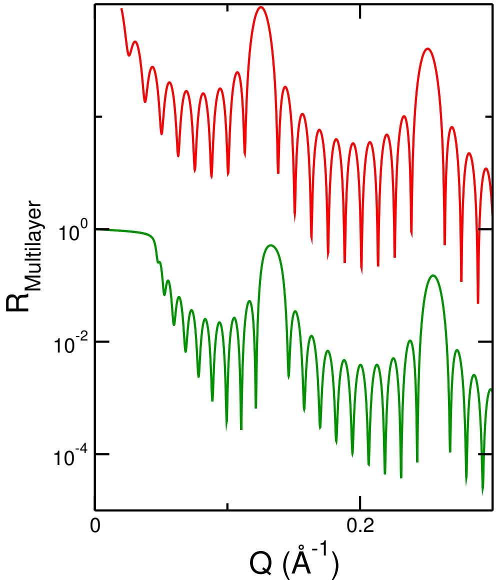
The recursive relation can be seen from the calculation of reflectivity of the next layer up

$$r_{N-2,N-1} = \frac{r'_{N-2,N-1} + r_{N-1,N} p_{N-1}^2}{1 + r'_{N-2,N-1} r_{N-1,N} p_{N-1}^2}$$

Kinematical - Parratt comparison



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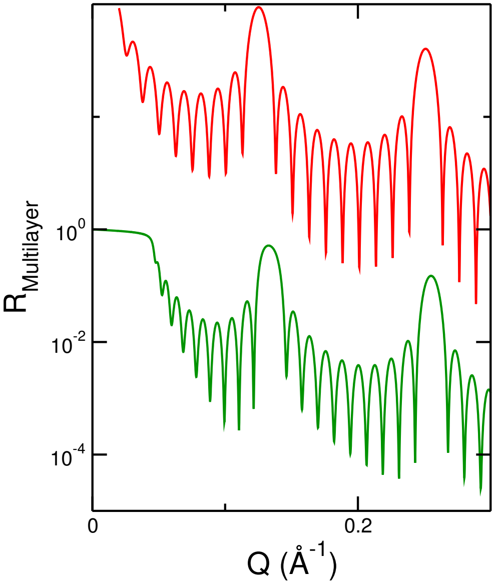

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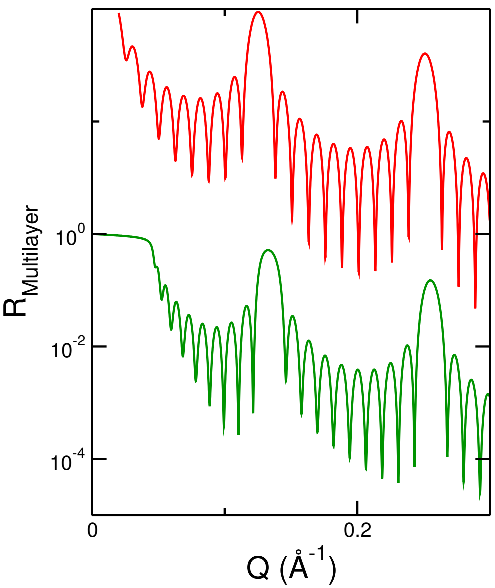

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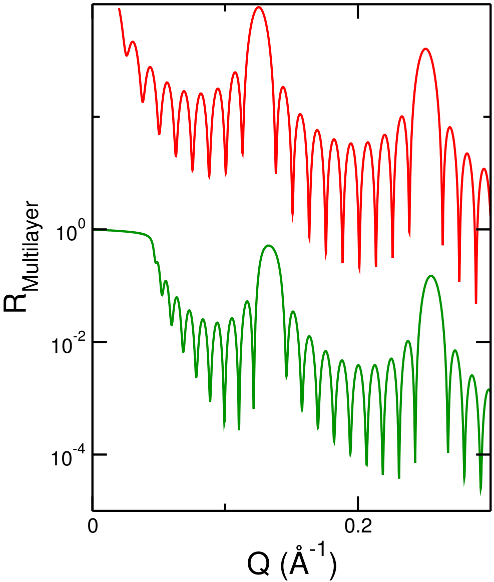

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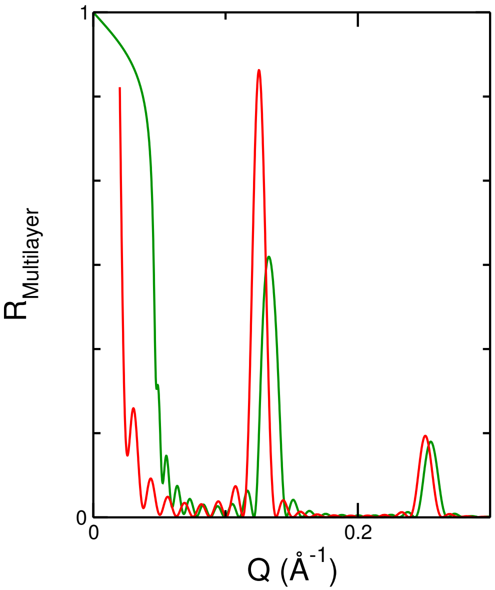

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Peaks in kinematical calculation are somewhat higher reflectivity than true value.

Graded interfaces

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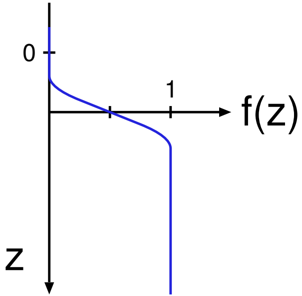

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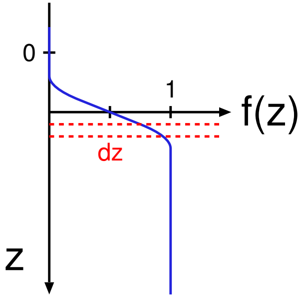

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The density profile of the interface can be described by the function $f(z)$ which approaches 1 as $z \to \infty$.

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

Reflectivity of a graded interface

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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

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

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

Rough surfaces

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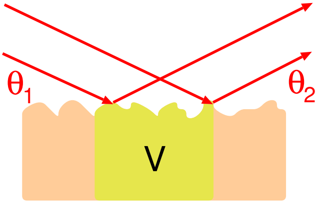

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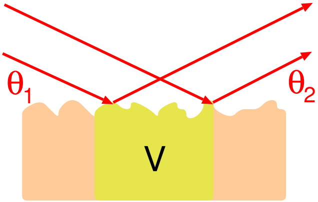

The incident and scattered angles are no longer the same, the x-rays illuminate the volume V.

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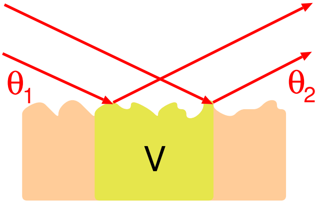

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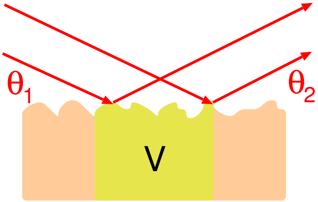

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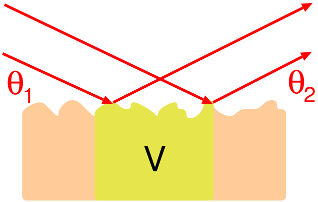

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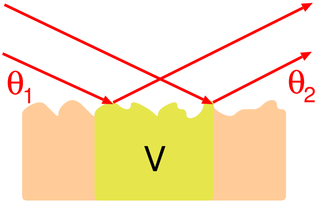

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The actual scattering cross section is the square of this integral

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

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

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$$R(Q_z) = \frac{I_{sc}}{I_0} = \left(\frac{Q_c^2/8}{Q_z}\right)^2 \left(\frac{1}{Q_z/2}\right)^2 = \left(\frac{Q_c}{2Q_z}\right)^4$$

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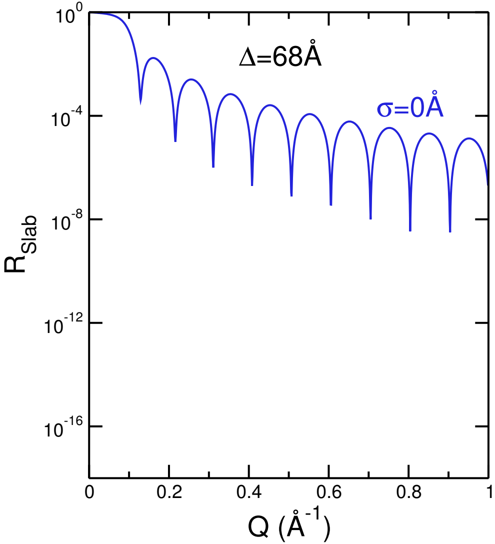

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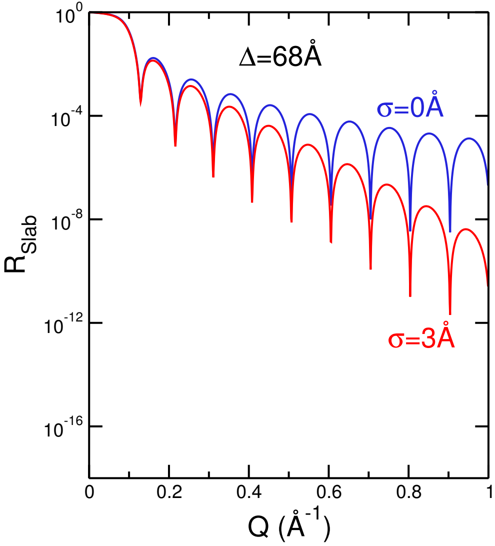

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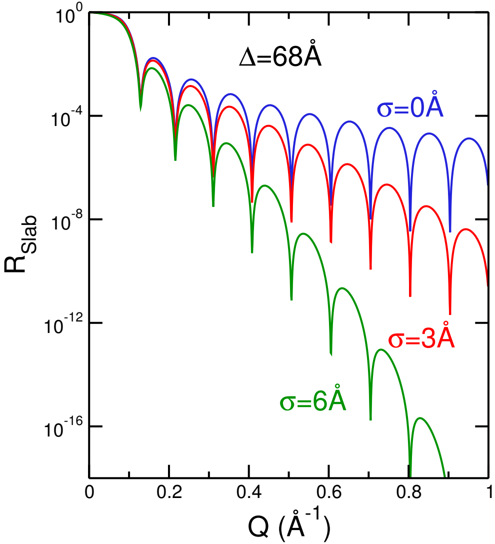

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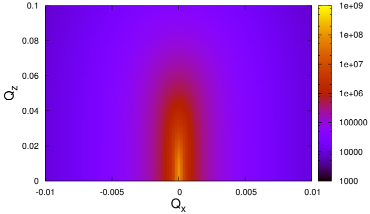

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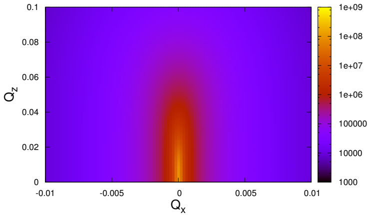

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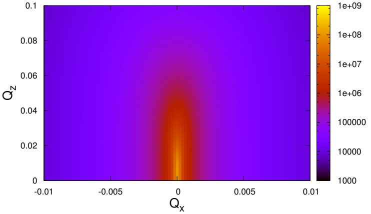

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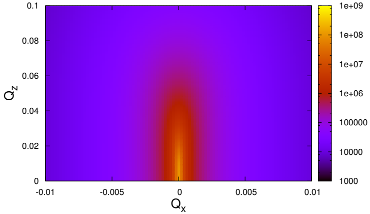

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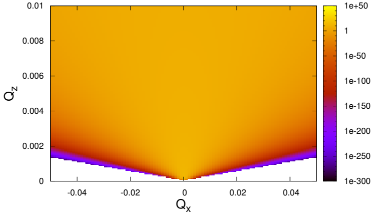
Gaussian with variance $\mathcal{A}Q_z^2$



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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