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Today’s Outline - February 08, 2018

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Homework Assignment #02: Problems on Blackboard due Tuesday, February 13, 2018

APS Visits: 10-ID: Friday, March 23, 2018
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Rough surfaces

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 \( V \).

\[
V = -r_0 \rho \int V e^{i \vec{Q} \cdot \vec{r}} d^3r
\]

Using Gauss' theorem, this volume integral can be converted to an integral over the surface of the illuminated volume. This integral is highly model dependent and can now be evaluated for a number of different cases.
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\[ r_V = -r_0 \rho \int_V e^{i\vec{Q} \cdot \vec{r}} d^3r \]
\[ r_S = -r_0 \rho \frac{1}{iQ_z} \int_S e^{i\vec{Q} \cdot \vec{r}} dxdy \]
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Using Gauss’ theorem, this volume integral can be converted to an integral over the surface of the illuminated volume.

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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Thus, the integral need only be evaluated over the top, rough surface whose variation we characterize by the function \( h(x, y) \)

\[
\vec{Q} \cdot \vec{r} = Q_z h(x, y) + Q_x x + Q_y y
\]

The actual scattering cross section is the square of this integral

\[
d\sigma d\Omega = (r_0 \rho Q_z)^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'
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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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where $A_0/\sin \theta_1$ is just the illuminated surface area and the term in the angled brackets is an ensemble average over all possible choices of the origin within the illuminated area.
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where $A_0 / \sin \theta_1$ is just the illuminated surface area and the term in the angled brackets is an ensemble average over all possible choices of the origin within the illuminated area.

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

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

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

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

For a perfectly flat surface, \( h(x, y) = 0 \) for all \( x \) and \( y \).
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by the definition of a delta function

\[
2\pi \delta(q) = \int e^{iqx} \, dx
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the expression for the scattered intensity in terms of the momentum transfer wave vectors is

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$$I_{sc} = \left( \frac{l_0}{A_0} \right) \left( \frac{d\sigma}{d\Omega} \right) \frac{\Delta Q_x \Delta Q_y}{k^2 \sin \theta_2}$$
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$$R(Q_z) = \frac{I_{sc}}{I_0} = \left( \frac{Q_c^2/8}{Q_z} \right)^4 \left( \frac{1}{Q_z/2} \right)^2 = \left( \frac{Q_c}{2Q_z} \right)^4$$
Uncorrelated surfaces

For a totally uncorrelated surface, $h(x, y)$ is independent from $h(x', y')$ and
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This quantity is simply related to the rms roughness, $\sigma$ by $\sigma^2 = \langle h^2 \rangle$ and the cross-section is given by

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Which, apart from the term containing $\sigma$ is simply the Fresnel cross-section for a flat surface
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This quantity is simply related to the rms roughness, \( \sigma \) by \( \sigma^2 = \left< h^2 \right> \) and the cross-section is given by

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\left( \frac{d\sigma}{d\Omega} \right) = \left( \frac{d\sigma}{d\Omega} \right)_{\text{Fresnel}} e^{-Q_z^2 \sigma^2}
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for a perfectly flat surface, we get the Fresnel reflectivity derived for a thin slab.
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For an uncorrelated rough surface, the reflectivity is reduced by an exponential factor controlled by the rms surface roughness \( \sigma \).

![Graph showing reflectivity vs. Q](image-url)

- \( \Delta = 68\text{Å} \)
- \( \sigma = 0\text{Å} \)
- \( \sigma = 3\text{Å} \)
- \( \sigma = 6\text{Å} \)
Assume that height fluctuations are isotropically correlated in the $x$-$y$ plane. Therefore, $g(x, y) = g(r) = g(\sqrt{x^2 + y^2})$. 

In the limit that the correlations are unbounded as $r \to \infty$, $g(x, y)$ is given by 

$$g(x, y) = A r^2 h$$

where $h$ is a fractal parameter which defines the shape of the surface.

- Jagged surface for $h \ll 1$
- Smoother surface for $h \to 1$

If the resolution in the $y$ direction is very broad (typical for a synchrotron), we can eliminate the $y$-integral and have 

$$\frac{d\sigma}{d\Omega} = r_0 \rho Q z^2 A_0 \sin \theta \int e^{-A Q^2 z |x|/2} \cos(Q x) dx$$
Correlated surfaces

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$$\left( \frac{d\sigma}{d\Omega} \right) = \left( \frac{r_0 \rho}{Q_z} \right)^2 \frac{A_0}{\sin \theta_1} \int e^{-AQ_z^2|x|^2h/2} \cos(Q_xx) dx$$
Unbounded correlations - limiting cases

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Gaussian with variance \( \mathcal{A}Q_z^2 \)
Bounded correlations

If the correlations remain bounded as $r \to \infty$
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$$g(x, y) = 2 \langle h^2 \rangle - 2 \langle h(0, 0)h(x, y) \rangle = 2\sigma^2 - 2C(x, y)$$

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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

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

Specular reflection measurements were made at MRCAT (Sector 10 at APS) and at X18A (at NSLS).

Deviations from uniform density are used to fit experimental reflectivity.


C. Segre (IIT)
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$h$ can be obtained from the diffuse off-specular reflection which should vary as

\[ I(q) \propto \sigma^{-(3+1)/h} q \]

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

Measure it directly using STM

\[ g(r) = 2\sigma^2 \left[ 1 - e^{(r/\xi)^2} \right] \]

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

Thus $z_s = h/\beta = 2.7\,\text{˚A}$ and diffraction data confirm $\xi = 19.9\,\text{˚A}$.
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The MRCAT mirror

- Ultra low expansion glass polished to a few Å roughness
- One platinum stripe and one rhodium stripe deposited along the length of the mirror on top of a chromium buffer layer
- A mounting system which permits angular positioning to less than 1/100 of a degree as well as horizontal and vertical motions
- A bending mechanism to permit vertical focusing of the beam to $\sim 60 \, \mu m$
The MRCAT mirror

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50 cm
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When illuminated with 12 keV x-rays on the glass “stripe”, the reflectivity is measured as:

- With the Rh stripe, the thin slab reflection is evident and the critical angle is significantly higher.
- The Pt stripe gives a higher critical angle still but a lower reflectivity and it looks like an infinite slab.

Why?

![Graph showing reflectivity vs. angle for glass and different materials](image-url)

**Reflectivity**

- **12 keV**
- **glass**
- **Rh**
- **Pt**

**α (degrees)**

- 0.0
- 0.2
- 0.4
- 0.6
- 0.8
- 1.0

**Reflectivity**

- 1.0
- 0.8
- 0.6
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Mirror performance

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As we move up in energy the critical angle for the Pt stripe drops. The reflectivity at low angles improves as we are well away from the Pt absorption edges at 11,565 eV, 13,273 eV, and 13,880 eV. As energy rises, the Pt layer begins to show the reflectivity of a thin slab.
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Tangential focusing mirror

The shape of an ideal mirror is an ellipse, where any ray coming from one focus will be projected to the second focus. Consider a 1:1 focusing mirror. For an ellipse the sum of the distances from any point on the ellipse to the foci is a constant.

\[ F_1P + F_2P = 2a \]
Tangential focusing mirror

The shape of an ideal mirror is an ellipse, where any ray coming from one focus will be projected to the second focus. Consider a 1:1 focusing mirror. For an ellipse the sum of the distances from any point on the ellipse to the foci is a constant.

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Types of focusing mirrors

A simple mirror such as the one at MRCAT consists of a polished glass slab with two “legs”.

A force is applied mechanically to push the legs apart and bend the mirror to a radius as small as $R = 500\text{m}$.

The bimorph mirror is designed to obtain a smaller form error than a simple bender through the use of multiple actuators tuned experimentally.

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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[Diagram of a simple mirror with two legs being pushed apart]

[Diagram of a bimorph mirror with multiple actuators applying force]
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Dual focusing options

• Toroidal mirror — simple, moderate focus, good for initial focusing element, easy to distort beam
• Saggittal focusing crystal & vertical focusing mirror — adjustable in both directions, good for initial focusing element
• Kirkpatrick-Baez mirror pair — in combination with an initial focusing element, good for final small focal spot and variable energy
• Zone plates — in combination with an initial focusing element, gives smallest focal spot, but hard to vary energy
• Refractive lenses — good final focus, focus moves with energy, significant attenuation and hard to change focal length
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