Introduction of X-ray Reflectivity
In GISAXS, the angle $\alpha_i$ is very small (<0.5°) for GISAXS, X-ray penetrates the sample and reflection is very strong, beam stopper is required to protect detector.

In our experiment, $\alpha_i = 1.8^\circ$, beam intensity is reduced dramatically, no stopper.
Simple Explanation - consider as diffraction of scattered x-ray

\[ AB = AO \cdot \sin \alpha_i, \ AC = AO \cdot \sin \alpha_f \]

In order to get interference pattern,

\[ AB + AC = m\lambda (m = 1, 2, 3...) \]

\[ d \sin \alpha_i + d \sin \alpha_f = m\lambda \]

\[ \frac{\sin \alpha_i + \sin \alpha_f}{\lambda} = \frac{m}{d} \]

Given wave-vector transfer

\[ q_z = \frac{2\pi}{\lambda} (\sin \alpha_i + \sin \alpha_f) \]

\[ q_z = \frac{2\pi m}{d} \]

\[ q_{z,1} = \frac{2\pi}{d} \]

\[ q_{z,2} = \frac{2\pi \times 2}{d} \]

\[ \Delta q_z = \frac{2\pi}{d} \]

\[ d = \frac{2\pi}{\Delta q_z} \]
Reflection and Transmission at Single Surface

n: refractive index

\[ n = 1 - \delta + i\beta \]

\[ \delta = \frac{\lambda}{2\pi} r_0 \rho \approx 10^{-4} \text{ to } 10^{-6} \]

\[ \beta = \frac{\lambda}{4\pi} \mu \approx 10^{-6} \text{ to } 10^{-9} \]

Snell-Descartes law: \( \cos \alpha_i = n \cos \alpha_t \)

\[ \exists \text{ transmitted wave only if } \cos(\alpha_t) \leq 1, \text{ i.e. } \alpha_i \geq \alpha_c \]

If \( \alpha_i \leq \alpha_c \),
- Incident wave totally externally reflected.
- Transmitted wave exponentially damped with \( z \).

\( \alpha_c \): critical angle for total external reflection of X-rays

\[ \alpha_c = \sqrt{2\delta} = \sqrt{\frac{r_0}{\pi}} \times \lambda \times \sqrt{\rho} \approx 0.1 \text{ to } 0.5^\circ \]
Reflection and Transmission at Single Surface

- Fresnel equations:

$R = \frac{E_r}{E_0} = \frac{q_z - \sqrt{q_z^2 - q_c^2}}{q_z + \sqrt{q_z^2 - q_c^2}}$

$T = \frac{E_t}{E_0} = \frac{2q_z}{q_z + \sqrt{q_z^2 - q_c^2}}$

$R = rr^* = |r|^2 = \left|\frac{E_r}{E_0}\right|^2$

$T = tt^* = |t|^2 = \left|\frac{E_t}{E_0}\right|^2$

Relationships between the amplitudes of incident, transmitted and reflected beam.

Wave-vector transfer

$q_z = \frac{2\pi}{\lambda} (\sin \alpha_i + \sin \alpha_f)$

Amplitude

Intensity
Reflectivity from Multiple Layers

\[ q_{z,j} = \sqrt{q_z^2 - q_{c,j}^2} \]
\[ r_{j,j+1} = \frac{q_{z,j} - q_{z,j+1}}{q_{z,j} + q_{z,j+1}} \]

\[ r = r_{0,1} + r_{1,2} e^{iq_{z,1}d_1} + r_{2,3} e^{i(q_{z,1}d_1+q_{z,2}d_2)} + \cdots + r_{j,j+1} e^{i \sum_{k=0}^{i-1} q_{z,k} d_k} + \cdots \]

\( q_{c,j} \) is the wave-vector transfer in medium \( j \) at critical angle.
Approximation

\[ r = r_{0,1} + r_{1,2} e^{i q_z d_1} + r_{2,3} e^{i (q_z d_1 + q_z d_2)} + \cdots + r_{j,j+1} e^{i \sum_{k=0}^{j} q_z d_k} + \cdots \]  

(1)

\[ R(q_z) = \left| \sum_{j=0}^{n} r_{j,j+1} e^{i q_z z_j} \right|^2 \text{ with } r_{j,j+1} = \frac{q_{z,j} - q_{z,j+1}}{q_{z,j} + q_{z,j+1}}. \]

A further approximation consists in neglecting the refraction and the absorption in the material in the phase factor in Eq. (1):

\[ r = \sum_{j=0}^{n} r_{j,j+1} e^{i q_z \sum_{m=0}^{j} d_m}. \]

A final approximation consists in assuming that the wave vector \( q_z \) does not change significantly from one medium to the next so that the sum in the denominator of \( r_{j,j+1} \) may be simplified:

\[ r_{j,j+1} = \frac{q_{z,j}^2 - q_{z,j+1}^2}{(q_{z,j} + q_{z,j+1})^2} = \frac{q_{c,j+1}^2 - q_{c,j}^2}{4 q_z^2} = \frac{4 \pi r_e (\rho_{j+1} - \rho_j)}{q_z^2} \]

(2)

Where \( q_{c,j} = \sqrt{16 \pi r_e \rho_j} \) \( r_e \) is the classical radius of the electron \( \rho_j \) is the electron density of layer \( j \)
Thus, if the origin of the \( z \) axis is chosen to be at the upper surface (medium 0 at a depth of \( z_1 = 0 \)), consider that the material is made of an infinite number of thin layers, the sum may then be transformed into an integral over \( z \), and the reflection coefficient becomes:

\[
r = 4\pi r_e \sum_{j=1}^{n} \frac{(\rho_{j+1} - \rho_j)}{q_z^2} e^{iq_z \sum_{m=0}^{j} d_m}.
\]

Replacing \( (4\pi r_e \rho_s)^2/q_z^4 \) by \( R_F(q_z) \):

\[
R(q_z) = r_r^* = R_F(q_z) \left| \frac{1}{\rho_s} \int_{-\infty}^{+\infty} \frac{d\rho(z)}{dz} e^{iq_z z} d_z \right|^2
\]

and

\[
\frac{R(q_z)}{R_F(q_z)} = \frac{1}{\rho_s^2} T F \left[ \rho'(z) \otimes \rho'(z) \right]
\]
Examples

The data inversion gives the autocorrelation function of the first derivative of the electron density

\[
\frac{R(q_z)}{R_F(q_z)} = \frac{1}{\rho_s^2} TF \left[ \rho'(z) \otimes \rho'(z) \right]
\]

\(R_F\): Fresnel reflectivity of the substrate

Ref: X-ray and neutron reflectivity principles and applications, 2009
**Examples**

**Grazing Incidence Small Angle X-ray Scattering (GISAXS)**

**Principle**

- 2D image around direct beam: Fourier transform of objects

**Morphology**
- Shape
- Sizes
- Size distributions
- Particle-particle pair correlation function

**Standard 3D growth (Volmer-Weber)**

Example: 20 Å Ag/MgO(001) 500K

Anisotropic islands: truncated square pyramids with (111) facets

Examples

Self-organized growth of magnetic cobalt dots on an interfacial dislocation network: Co/Ag/MgO(100)

All the pictures, the center scatter rod is blocked to protect detector, due to small angle, strong intensity

Interferences
Co islands are ordered

F. Leroy et al, PRL 95, 185501 (2005)
**Pilatus 100K Detector System**

<table>
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<tr>
<th>Parameter</th>
<th>Value</th>
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<tr>
<td>Framing rate</td>
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</tbody>
</table>

\( K_i \) is the direction of incident X-ray, pointing to sample. The recorded image is the reflected beam intensity image.
Sample: spec_start_S144_00190

\[
\frac{R(q_z)}{R_F(q_z)} = \frac{1}{\rho_0^2} \text{TF} \left[ \rho'(z) \otimes \rho'(z) \right]
\]

FFT vs. thickness

Abs(FFT) vs. thickness (Å)
Local Average

\[ \frac{R(q_z)}{R_F(q_z)} = \frac{1}{\rho_s^2} TF \left[ \rho'(z) \otimes \rho'(z) \right] \]

\[ \log[I_0 \bullet R(q_z)] - \log[I_0 \bullet R_F(q_z)/\rho_s^2] = \log[TF[\rho'(z) \otimes \rho'(z)]] \]

Local average (Green curve) is defined as:

\[ \log[R_F(q_z)/\rho_s^2] \approx \frac{1}{N} \sum_{q_z=\Delta q_z}^{q_{z2}} \log[R(q_z)] \]

\[ \Delta q_z = q_{z2} - q_{z1} > \text{oscillation period} \]
Sb film only deposited on Si (100).

Two methods get the similar result for Sb deposition on Si (100).