X-ray and Neutron Scattering from Crystalline Surfaces and Interfaces

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Buried Interface Structure
to understand the growth and function of materials

Crystal growth from a vapor

- Nucleation
- Edge diffusion
- Step-Edge Barrier
- Terrace diffusion
Morphology $\rightarrow$ atomic scale mechanisms

Cu/Cu(001)

Zuo & Wendelken
Interplay between two regimes of **Length Scales**

- Interatomic distances
  → Structure, physics, chemistry → Mechanisms

- “Mesoscale” – Nanoscale
  → Morphology → Mechanisms
Unique Advantages of X-ray Scattering:

- Atomic-scale structure at a buried interface
- Morphological structure at buried interfaces
- Subsurface phenomena
  Strains and defects near a surface
- Accurate statistics of distributions
  (eg. Island size distributions)

Neutrons: low intensity- limited to reflectivity

- Soft Matter and Bio materials; H₂O & D₂O
- Magnetic materials
Example:
Rotation of graphene planes affect electronic properties

Graphene made from SiC
Morphology $\rightarrow$ atomic scale mechanisms

- Nanoclusters
- Atomic interfacial structure
- Interface roughness
- Nucleation/growth/coarsening at interfaces
- Crystalline morphology
- Vacancy clusters
Objective

- An introduction to surface scattering techniques
  Build a conceptual framework

- Reciprocal Space is a large place: where do we look?
Scattering of X-rays and Neutrons: Helmholtz Equation

\[ \nabla^2 \vec{E} + k^2 n^2(\vec{r})\vec{E} = 0 \]

\[ \nabla^2 \Psi + \frac{2m}{\hbar^2} [E - V(\vec{r})] \Psi = 0 \]

\[ n(\vec{r}) = \text{inhomogeneous refractive index} \]

Refractive Index for neutron:
\[ n(\vec{r}) = \sqrt{1 - \frac{2m}{\hbar^2 k^2} V(\vec{r})} = \sqrt{1 - \frac{\lambda^2 \rho_b(\vec{r})}{\pi}} \]

Scattering length density:
\[ \rho_b(\vec{r}) \xrightarrow{\text{monoatomic}} \rho_N(\vec{r})b \]

number density \rightarrow scattering length:
\[ b = \begin{cases} \rho_e f(Q) & \text{x-rays} \\ \text{tabulated - neutrons} & \end{cases} \]

One language for both x-rays and neutrons
Wavevector Transfer:

\[ \vec{Q} = \vec{k}_f - \vec{k}_i \]

\[ |\vec{Q}| = \frac{4\pi}{\lambda} \sin \theta \sim \frac{2\pi}{d} \]

Probing Length Scale
Regimes of Scattering

(Consider specular reflection)

1. Grazing angle reflectivity: strong scattering \( d \gg \) interatomic distances
   
   Exact solution required. Neglect atomic positions: homogeneous medium

2. Bragg region: strong scattering; \( d \sim \) interatomic distances = \( a \)
   
   Exact solution required. Atomic positions needed. Similar to e\(^-\) band theory.

3. Everywhere else: weak scattering

   Born approximation \( \rightarrow \) simplification. Atomic positions required.

\[
|\vec{Q}| = \frac{4\pi}{\lambda} \sin \theta
\]

Surface information \( \rightarrow \) “3”

3D: surface info is everywhere except at Bragg points
Grazing Angles: Refraction and Total Reflection

\( d >> a \): consider homogeneous medium

Use average refractive index:

\[
n = \sqrt{1 - \frac{\lambda^2 \rho_b}{\pi}} \equiv 1 - \delta \quad \delta = \frac{\lambda^2 \rho_b}{2\pi} \ll 1 \quad (\sim 10^{-5})
\]

With absorption: \( n = 1 - \delta - i\beta \)

Snell’s Law:

\[
\sin^2 \theta' = \sin^2 \theta - 2\delta
\]

Critical Angle for Total Reflection:

\[
\theta_c = \sqrt{2\delta}
\]

Wavevector transfer:

\[
Q'^2 = Q^2 - Q_c^2
\]

\[
Q_c^2 = 16\pi\rho_b
\]

Only \( k_z \) component is affected by the surface. \( k_x \) is unchanged.
Total Reflection

\[ \sin^2(\theta') = 0 = \sin^2(\theta_c) - 2\delta \]

Critical Angle for Total External Reflection:

\[ \theta_c = \sqrt{2\delta} \]

\[ Q_c = \frac{4\pi}{\lambda} \theta_c \]

Beam does not transmit below \( \theta_c \)
Frenel Reflectivity for a Single Interface

Exact Result for
A Single Interface

\[ R = \left| \frac{Q - Q'}{Q + Q'} \right|^2 \]

Critical angle for
Total External Reflection

\[ R = \frac{\text{refl power}}{\text{inc power}} \]
Transmission Amplitude

\[ T_i = \frac{2 \sin \alpha_i}{\sin \alpha_i + (\sin^2 \alpha_i - 2 \delta)^{1/2}} \]

H. Dosch, PRB 35, 2137 (1987)

FIG. 1. Fresnel transmissivity \( |T_i|^2 \) as a function of \( \alpha_i/\alpha_c \) for a transparent medium and the real systems Fe₃Al and Pb.
Penetration Length

\[ \Lambda = \frac{1}{\text{Im } Q'_z} \]

\[ l_{i,f} = \frac{1}{2} \sqrt{2 \{ (2\delta - \sin^2 \alpha_{i,f}) + [(\sin^2 \alpha_{i,f} - 2\delta)^2 + (2\beta)^2]^{1/2} \}^{1/2} } \]

H. Dosch, PRB 35, 2137 (1987)
Calculation of reflectivity

Reflectivity, $R$, can be calculated, exactly, by matching boundary conditions at the interfaces.

Multi-slice method:
Numerical simulations

L.G. Parratt, Phys Rev 95, 359 (1954)
M-layer

http://www.ncnr.nist.gov/reflpak/
Soft Matter: Neutron Reflectivity

- Thin film interfaces
- Light elements
- Isotopic substitutions
- Polymers

D. J. McGillivray and M. Lösche
D. J. Vanderah and J. J. Kasianowicz
G. Valincius

Biophysical Journal Volume 95 November 2008 4845–4861
Magnetic Films: Neutron Reflectivity

- Magnetic thin films
  Spin-polarized neutrons

FeCo/GaAs

Vortices in Thin-Film Superconductors
Studied by Spin-Polarized Neutron Reflectivity (SPNR)

S-W. Han, J.F. Ankner, H. Kaiser, P.F. Miceli, E. Paraoanu, L.H. Greene, PRB 59, 14692 (1999)
Regimes of Scattering

(Consider specular reflection)

1. Grazing angle reflectivity: strong scattering \( d \gg \text{interatomic distances} \)
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   Born approximation \( \rightarrow \) simplification. Atomic positions required.

\[
|\mathbf{Q}| = \frac{4\pi}{\lambda} \sin \theta
\]

\[
d \sim \frac{2\pi}{Q}
\]

\[
d \sim \frac{2\pi}{|Q - G|}
\]

Surface information \( \rightarrow \) “3”
Differential Scattering Cross Section

Weak Scattering
“Born Approximation” or “Kinematic Approximation”

\[ \frac{d\sigma}{d\Omega} = P S(\vec{Q}) = P |A(\vec{Q})|^2 \]

P is the polarization factor (x-ray case)
S(Q) is the structure factor
A(Q) is the scattering amplitude
f(Q) is the atomic form factor
\( \rho_b \) is the scattering length density

Reflectivity:
\[ R = \frac{1}{A_{inc}} \int d\Omega \frac{d\sigma}{d\Omega} \]

\[ d\Omega = \frac{d^2 \vec{Q}_p}{k^2 \sin(\alpha_f)} \]
Born Approximation: simple sum over atomic positions

\[ A(\vec{Q}) = \int d^3 \vec{r} \rho_b(\vec{r}) e^{i\vec{Q} \cdot \vec{r}} = \sum_{\vec{r}} b_{\vec{r}} e^{i\vec{Q} \cdot \vec{r}} \]

Sum over all atomic positions

\[ b = r_e f(Q) \text{ for x-rays or tabulated for neutrons} \]
Born Approximation works if the reflectivity is not too large.

\[ R = \left| \frac{Q - Q'}{Q + Q'} \right|^2 \] Exact

\[ R \approx \left( \frac{Q}{2Q_c} \right)^4 \] Born approx.

Specular Reflection
General Case: non-specular scattering

Grazing Incidence Effects

3D Scattering

$\vec{Q} = \vec{k}_f - \vec{k}_i$

If $\vec{k}_i$ or $\vec{k}_f$ are near grazing:

- refraction of both beams
- internal wavevector transfer: $\vec{Q}'$
- transmission of both beams: $T_i, T_f$
Perpendicular to Surface: internal $Q'$ and external $Q$ are different

$$Q_z = k_z^{(f)} - k_z^{(i)} = (2\pi/\lambda) \left[ \sin\alpha_f + \sin\alpha_i \right].$$

$$Q_z' = k_z^{(f)'} - k_z^{(i)'} = (2\pi/\lambda) \left[ (\sin^2\alpha_f - 2\delta - 2i\beta)^{1/2} + (\sin^2\alpha_i - 2\delta - 2i\beta)^{1/2} \right].$$

Parallel to Surface: internal $Q'$ and external $Q$ are same

$$Q'_x = Q_x = k_x^{(f)} - k_x^{(i)}$$

$$Q'_y = Q_y = k_y^{(f)} - k_y^{(i)}$$

H. Dosch, B.W. Batterman and D. C. Wack, PRL 56, 1144 (1986)
Penetration Length

\[ \Lambda = \frac{\lambda}{2\pi(l_i + l_f)} \]

\[ l_{i,f} = \frac{1}{2} \sqrt{2 \left( 2\delta - \sin^2 \alpha_{i,f} \right) + \left( \sin^2 \alpha_{i,f} - 2\delta \right)^2 + (2\beta)^2}^{1/2} \]

\[ \Lambda = \frac{1}{\text{Im} Q'_z} \]

H. Dosch, PRB 35, 2137 (1987)
Fe$_3$Al

H. Dosch, PRB 35, 2137 (1987)

**Distorted Wave Born Approximation**

\[ I_{\text{GID}}(Q') \propto \left| T_i \right|^2 S(Q') \left| T_f \right|^2 \]

- refraction
- transmission

\[ S(\tilde{Q}') \] is the structure factor using the internal wavevector transfer

(a) $\alpha_i/\alpha_c = 0.64$
\[ \Lambda_c = 40 \text{ Å} \]

(b) $\alpha_i/\alpha_c = 0.89$
\[ \Lambda_c = 60 \text{ Å} \]

(c) $\alpha_i/\alpha_c = 1.13$
\[ \Lambda_c = 150 \text{ Å} \]
A Six-Circle Diffractometer

- Extra Angles give flexibility
- Constraints are needed
- Common working modes:
  \[ \alpha_i = \text{fixed} \]
  \[ \alpha_f = \text{fixed} \]
  \[ \alpha_i = \alpha_f \]

Detector angles

X-ray beam

UHV Growth and Analysis Chamber
At Sector 6 at Advanced Photon Source

- UHV 10^{-10} Torr
- Evaporation/deposition
- Ion Sputtering
- LEED
- Auger
- Low Temp: 55K
- High Temp: 1500 °C
- Load Lock/sample transfer
Liquid Surface Diffractometer

The Effect of a Crystalline Boundary
What is a crystal truncation rod?

First consider:
- Large crystals; rough and irregular boundaries
- Boundaries neglected

\[ S(\vec{Q}) = \left| \sum_{n_x=0}^{N-1} e^{iQ_xa_n x} \sum_{n_y=0}^{N-1} e^{iQ_yb_n y} \sum_{n_z=0}^{N-1} e^{iQ_zc_n z} \right|^2 = \frac{\sin^2 \left( \frac{NQ_xa}{2} \right)}{\sin^2 \left( \frac{Q_xa}{2} \right)} \frac{\sin^2 \left( \frac{NQ_yb}{2} \right)}{\sin^2 \left( \frac{Q_yb}{2} \right)} \frac{\sin^2 \left( \frac{NQ_zc}{2} \right)}{\sin^2 \left( \frac{Q_zc}{2} \right)} \]

\[ \propto \sum_{\vec{G}} \delta(\vec{Q} - \vec{G}) \]

\( \vec{G} \) is a reciprocal lattice vector

**Real space**

**Reciprocal space**

Bragg points
Now consider a crystal with one atomically flat boundary...

Real space

• Large crystal; flat boundary \( z = 0 \)
• Neglect boundary at \( z = -\infty \)

\[ S(\vec{Q}) = b^2 \left| \sum_{n_z=0}^{N-1} \varepsilon^{n_z} e^{-iQ_z c n_z} \right|^2 \sum_{\vec{R}_p} \sum_{\vec{R}'_p} e^{i\vec{Q}_p \cdot (\vec{R}_p - \vec{R}'_p)} \]

Very small attenuation \( \varepsilon \ll 1 \)

Reflected wave vanishes

\[ \lim_{\varepsilon \to 1} \lim_{N \to \infty} \left| \frac{1 - \varepsilon^N e^{-iQ_z c N}}{1 - e^{-iQ_z c}} \right|^2 = \frac{1}{4 \sin^2 \left( \frac{Q_z c}{2} \right)} \approx \frac{1}{c^2 (Q_z - G_z)^2} \]
By neglecting the lateral boundaries:

\[ \sum_{\tilde{R}_p} \sum_{\tilde{R}'_p} e^{i\tilde{Q}_p \cdot (\tilde{R}_p - \tilde{R}'_p)} = N_{irr} \sum_{\tilde{R}_p} e^{i\tilde{Q}_p \cdot \tilde{R}_p} \]

and

\[ \sum_{\tilde{R}_p} e^{i\tilde{Q}_p \cdot \tilde{R}_p} = \left(\frac{2\pi}{S_c}\right)^2 \sum_{\tilde{G}_p} \delta(\tilde{Q}_p - \tilde{G}_p) \]

\[ N_{irr} \] = the number of irradiated atoms at the surface
\[ S_c \] = area per surface atom
\[ \tilde{G}_p \] = an in-plane reciprocal lattice vector

\[ S(\tilde{Q}) = \frac{(2\pi)^2 N_{irr} b^2}{S_c} \frac{1}{4\sin^2\left(\frac{Q_z c}{2}\right)} \sum_{\tilde{G}_p} \delta(\tilde{Q}_p - \tilde{G}_p) \]

CTR

Narrow reflection in-plane

Intensity falls slowly
Crystal Truncation Rods

Reciprocal Space

Specular rod \((Q_p=0)\)

Crystal Surface

Real Space
Crystal Truncation Rod Scattering for Specular Reflection from the Ag(111) Surface

\[ \propto \frac{1}{Q_z^2} \frac{1}{Q_z^2} \]

\[ \tilde{G} = 0 \]

\[ \tilde{G} = (111) \]

At atomically smooth

Rough, 3Å

Elliott et. al. PRB 54, 17938 (1996)
Miscut Surfaces

Tilted Rods

\[ \hat{n}_s \]

\[ \eta \]

Step ordering (typically semiconductors)

Step bunching (e.g. noble metals)
Angular Width of Specular Decreases with $Q_z$

$\Delta Q_p$ decreases with $Q_z$

$L \approx 9000 \text{Å}$

Can determine terrace size, $L$

$$\Delta Q_p = \frac{2\pi}{L}$$

$\Delta \omega = \frac{\Delta Q_p}{Q_z}$
Specular Reflection from the Ag(111) Surface
Correct Crystal Truncation Rod Scattering for Terrace Size

Elliott et. al. PRB 54, 17938 (1996)
The Effect of a Rough Surface
Sharper interface (real space) gives “broader” scattering

Elliott et. al. PRB 54, 17938 (1996)
Special location along CTR: anti-Bragg

**Bragg Position:**

$$Q_z c = 2\pi m$$

$$I = \left| \sum_{n_z=0}^{N-1} e^{-i2\pi n_z} \right|^2 \rightarrow N^2$$

**Anti-Bragg Position:**

$$Q_z c = \pi m \ (m \text{ odd})$$

$$I = \left| \sum_{n_z=0}^{N-1} e^{-i\pi n_z} \right|^2 \rightarrow 1$$

For a smooth surface

Anti-Bragg Positions

$I = 0$

out of phase

1 atomic layer
In situ vapor deposition in UHV

Synchrotron X-ray Beam

evaporator
Nucleation and Growth

Specular Anti-Bragg Intensity

Diffuse Scattering
Caused by lateral structure

\[ |A(\hat{Q})|^2 = \]

\[ = |b|^2 \sum_{\vec{R}_p} \sum_{\vec{R}'} R_{\text{irr}} |b|^2 \]

\[ = \frac{N_{\text{irr}} |b|^2}{|1 - e^{iQ_zc}|} \]

- Neglect lateral boundaries

\[ \text{CTR factor} \]

\[ \text{FT of average phase difference due to lateral height-differences} \]

\[ = S_T(Q_p) \]
Transverse Lineshape

Far regions of surface $R_p \rightarrow \infty$

Uncorrelated heights

$$\langle e^{iQ_z(h(\vec{R}_p + \vec{R}_p') - h(\vec{R}_p'))} \rangle_{\vec{R}_p'} \quad \rightarrow \quad \left| \langle e^{iQ_z h} \rangle \right|^2$$

Uncorrelated Roughness @ Large Distance Gives Bragg:

$$S_T^{Bragg}(\vec{Q}_p) = \left( \frac{2\pi}{S_c} \right)^2 \delta(\vec{Q}_p - \vec{G}_p) \left| \langle e^{iQ_z h} \rangle \right|^2$$

Short-Range Correlations Give Diffuse Scattering:

$$S_T^{Diffuse}(\vec{Q}_p) = \sum_{\vec{R}_p} e^{i\vec{Q}_p \cdot \vec{R}_p} \left\{ \left| \langle e^{iQ_z(h(\vec{R}_p + \vec{R}_p') - h(\vec{R}_p'))} \rangle_{\vec{R}_p'} \right|^2 - \left| \langle e^{iQ_z h} \rangle \right|^2 \right\}$$
Two Component Line Shape: Bragg + Diffuse

\[ S_T(\vec{Q}_p) = S^\text{Bragg}_T(\vec{Q}_p) + S^\text{Diffuse}_T(\vec{Q}_p) \]

- Bragg due to laterally uncorrelated disorder at long distances
- Diffuse due to short-range correlations
Layer-by-layer growth

- Specular Bragg Rod: intensity changes with roughness
- Strong inter-island correlations seen in the diffuse

Attenuation of the Bragg Rod and Surface Roughness

If height fluctuations are Gaussian: $\sigma$ is rms roughness

$$\left| \left\langle e^{iQ_z h} \right\rangle \right|^2 \rightarrow e^{-Q_z^2 \sigma^2}$$

But crystal heights are discrete for a rough crystal:

$$\left| \left\langle e^{iQ_z h} \right\rangle \right|^2 \rightarrow e^{-4 \frac{\sigma^2}{c^2} \sin^2 \left( \frac{Q_z c}{2} \right)}$$

- Binomial distribution (limits to a Gaussian for large roughness)
- Preserves translational symmetry in the roughness

Physica B 221, 65 (1996)
• Sharper interface (real space) gives broader scattering
• Gaussian roughness does not give translational symmetry
Transversely-integrated scattering shows no effect of roughness:

\[
S^{\text{Bragg}}(\mathbf{Q}) \propto \frac{|b|^2}{\left|1 - e^{iQ_zc}\right|^2} e^{-4\frac{\sigma^2}{c^2}\sin^2 \left(\frac{Q_zc}{2}\right)}
\]

Bragg is narrow: it samples laterally uncorrelated roughness at long distances

Transversely-integrated scattering shows no effect of roughness:

\[
\int \int d^2Q_p \ S(\mathbf{Q}) \propto \frac{|b|^2}{\left|1 - e^{iQ_zc}\right|^2}
\]

(for 1 interface)
In practice, at every $Q_z$ the diffuse must be subtracted from the total intensity to get the Bragg rod intensity:
What do we expect from a Thin Film?

1st let’s recall Young’s slit interference…
Recall...

**N-Slit Interference and Diffraction Gratings**

**Principle maxima**

\[ d \sin \theta = m\lambda \]
Principle maxima always in the same place for N slits:
But they narrow: width $\sim 1/N$

Double Slit
(no subsidiary maxima)

$Principle\ maxima$  
$d\ \sin\ \theta = m\lambda$
(N-2 subsidiary maxima)

N large:
• Weak subsidiary maxima
• Sharp principle maxima
“5-slit” interference of x-rays from 5 layers of atoms

5 AL ErAs

Counts/min

\[ \log_{10} \text{Counts/min} \]

\[ \log_{10} 2\Theta \text{ (deg.)} \]

Thin Films

Reciprocal Space

Specular rods overlap

Non-specular rods: No overlap (incommensurate)

Real Space

substrate
Ag/Si(111)7x7

Specular Reflectivity: 0.3ML Ag/Si(111)7x7

Sensitive to Ag-Si distance

0.3 ML Ag in 7x7 wetting layer

Yiyao Chen et al.
Ag/Si(111)\(7\times 7\)

**Specular Reflectivity**: \(0.9\text{ML} \text{Ag/Si}(111)7\times 7\)

\[\Theta = 0.9\text{ML}\]

\(3\)-layer islands
2ML above wetting layer

\(\Theta = 0.9\text{ML}\)

Mainly 3-layer islands

\(Q_z = 2\pi L/c\) \(L \text{ [rLU]}\)

Yiyao Chen et al.
Specular reflectivity cannot easily distinguish between these two cases:

FCC Ag islands on a Ag 7x7 wetting layer?

FCC Ag islands all the way to the substrate?

Reflectivity = 3 layers
FCC CTR  = 2 layers

Reflectivity = 3 layers
FCC CTR  = 3 layers

Si
Specular reflectivity and rod give same thickness:
Island is FCC Ag all the way to the substrate
Islands *remove* the wetting layer!

Specular Reflectivity

**Yiyao Chen et al.**
Quantum-Size-Effects: Pb Nanocrystals on Si(111)7x7

Discoveries:
• anomalously (10^4) fast kinetics
• Non-classical coarsening
• Unusual behavior:
  fast growth => most stable structures

Height Selection: “Magic” crystal heights

Quantum Mechanics Influences Nanocrystal Growth

C. A. Jeffrey et al., PRL 96, 106105 (2006)
Electrons in a “box”

Electrons will be confined to the metal

Electrons will exhibit discrete quantum mechanical energies

Coarsening

Rain Drops On Your Winshield

laist.com
greeneurope.org
Kinetics: In Situ Surface X-ray Scattering

Surface Chamber
Advanced Photon Source

Mean island separation, $<L>$:

\[ \Delta n = \frac{2\pi}{\langle L \rangle} \]

Experiment:
- Deposit Pb (1.2 to 2 ml) at 208K
- Measure the island density vs time (flux off)

Island Density:

\[ n \propto \frac{\langle L \rangle^2}{\langle L \rangle} \]
Classical Coarsening: Ostwald Ripening

\[ n(t) = n_0 \left(1 + \frac{t}{\tau} \right)^{-\beta} \]

\[ \beta = \frac{2}{(m+2)}, m = 0, 1, 2 \]

**Long time**: independent of initial conditions

\[ n(t) \Rightarrow (n_0 \tau^{\beta}) t^{-\beta} \]

\[ \tau \propto n_0 \frac{1}{\beta} \]

Relaxation time depends only on the initial density.

**Graph**: Island density vs. time for high and low initial density.
Pb Nanocrystal Coarsening

...does not conform to the classical picture!

C. A. Jeffrey et al., PRL 96, 106105 (2006)

- Island densities do not approach each other at long times:
  \[ \text{QSE} \Rightarrow \text{Non-Oswald} \]
  Breakdown of Classical Coarsening

- Time constant \( \tau \sim 1/\text{Flux} \)
  Strong flux dependence!
  Unexpected!

- Anomalously fast relaxation
  \( \sim 1000\times \) faster than expected!
  \[ \Rightarrow \text{allows equilibrium!} \]

\[ n(t) = \frac{n_0}{\left(1 + \frac{t}{\tau}\right)} \]

1.2 ML of Pb at 208K
at various flux rates
Reciprocal Space is Superb for Obtaining Good Statistics of Distributions

Equivalent ML Time = t*F
Materials research problems require information on a broad range of length scales, from atomic to mesoscale.

Scattering from surfaces involves many different types of measurements:
- Reflectivity, Rods, Grazing Incidence Diffraction, Diffuse Scattering

Unique ability of x-rays: surface and subsurface structure simultaneously.