

X-ray and Neutron Scattering from Crystalline Surfaces and Interfaces

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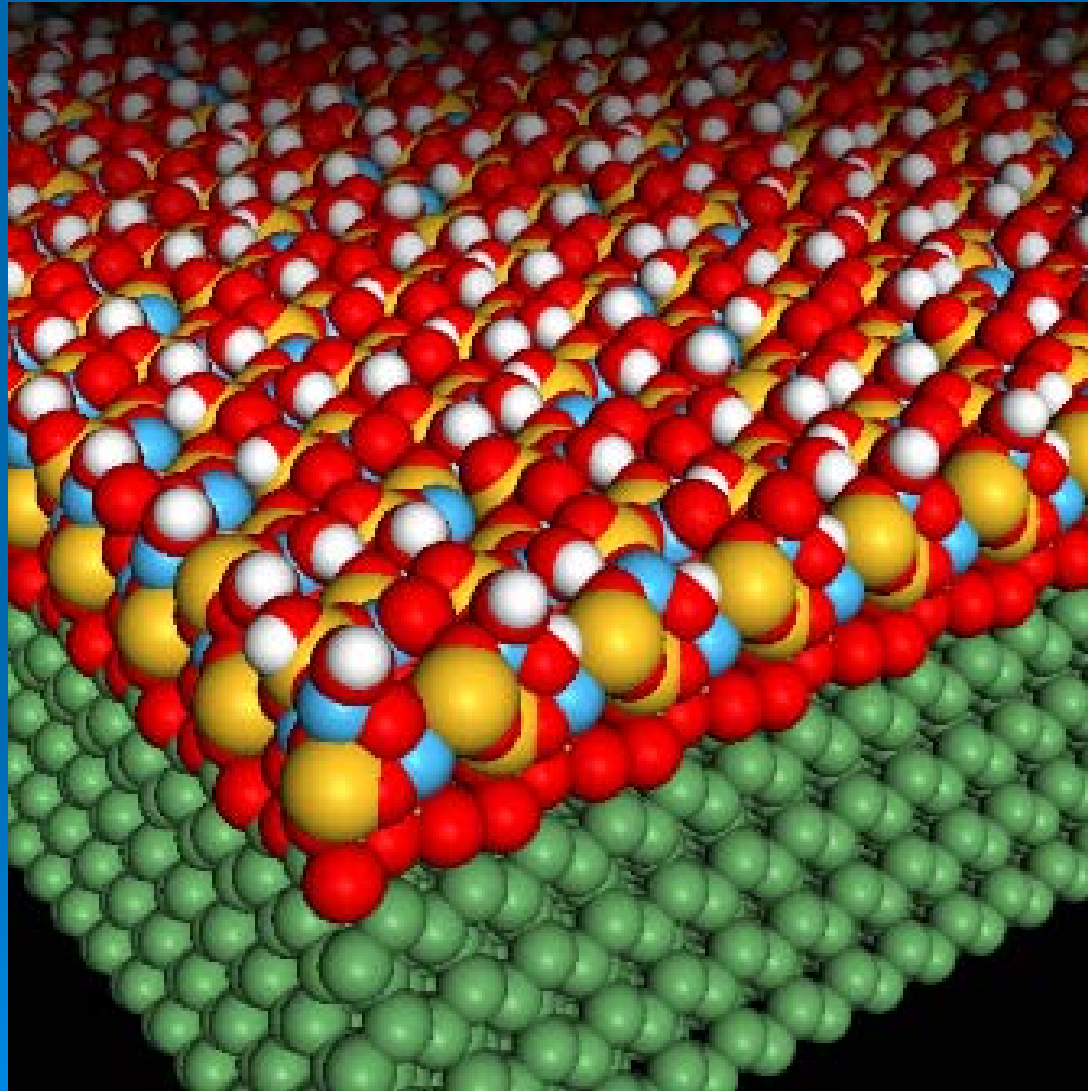
National School for X-ray and Neutron Scattering
Argonne and Oak Ridge National Laboratories

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Many thanks to students and collaborators:
W. Elliott, C. Botez, S.W. Han, M. Gramlich, S. Hayden, Y. Chen,
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M. Tringides; and to NSF and DOE for funding.

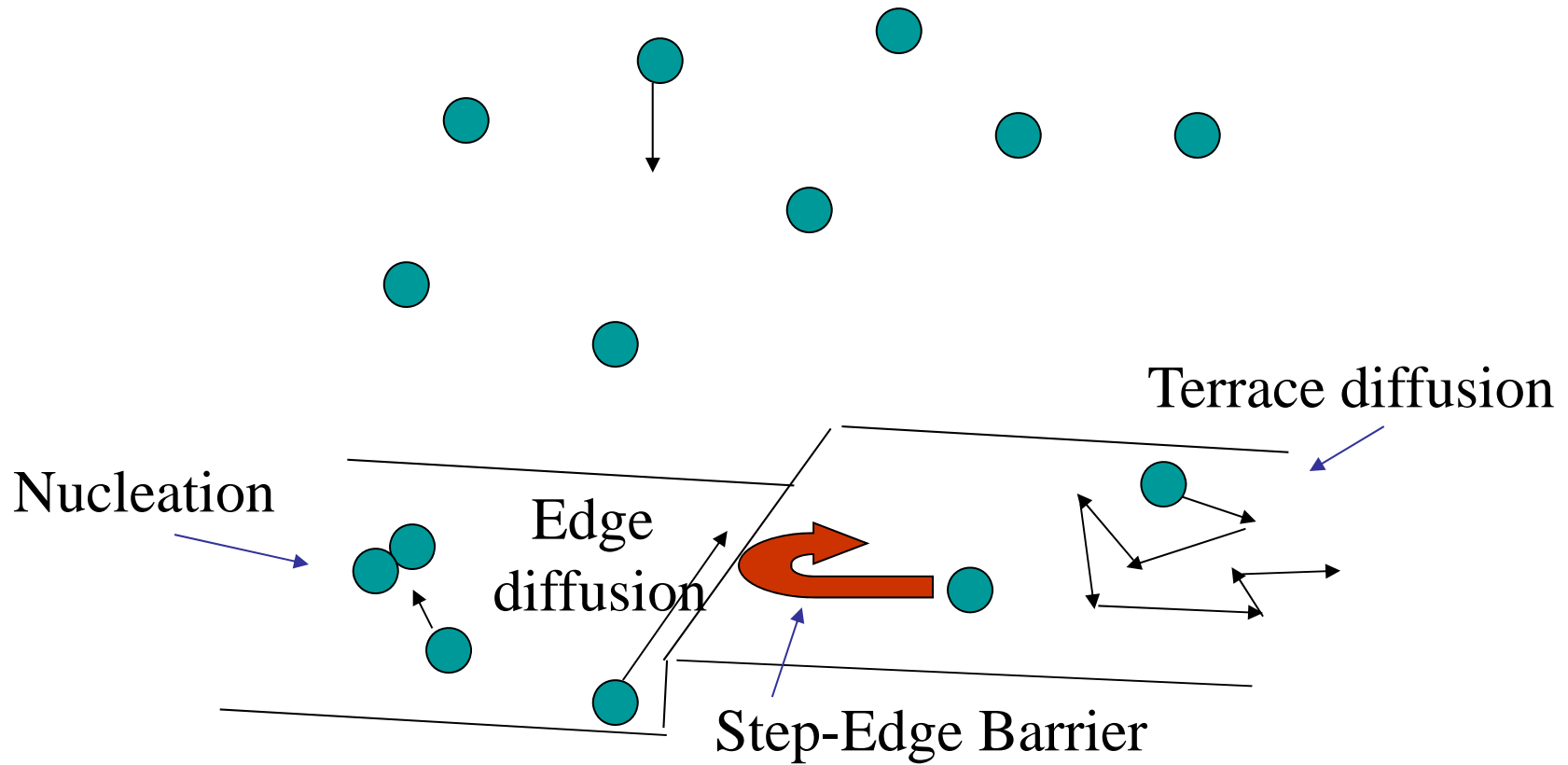
Buried Interface Structure

to understand the growth and function of materials

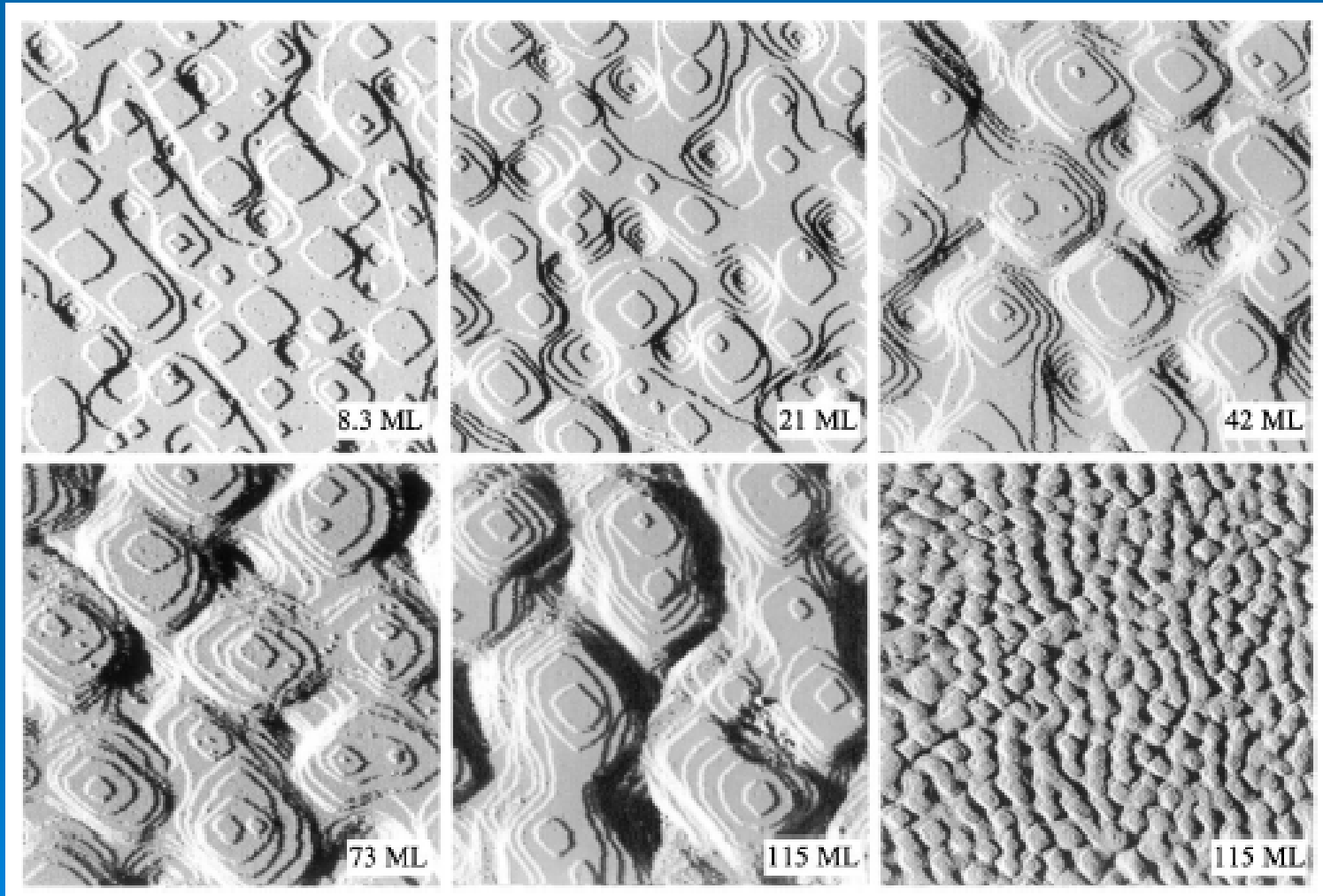


http://www.tyndall.ie/research/electronic-theory-group/thin_film_simulation.html

Crystal growth from a vapor



Morphology → 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:

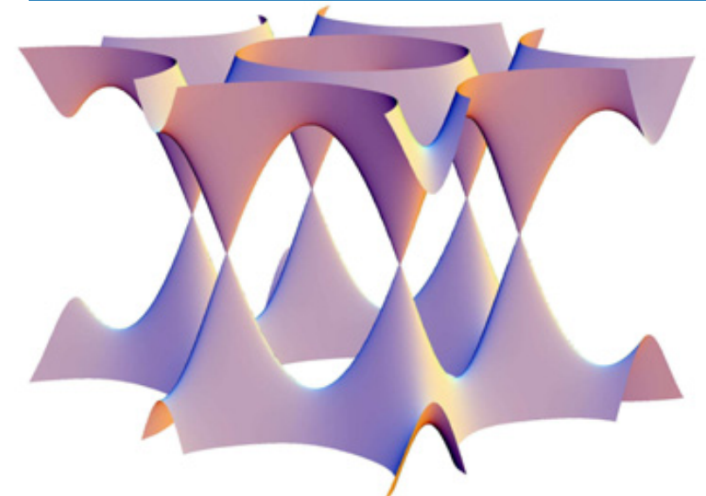
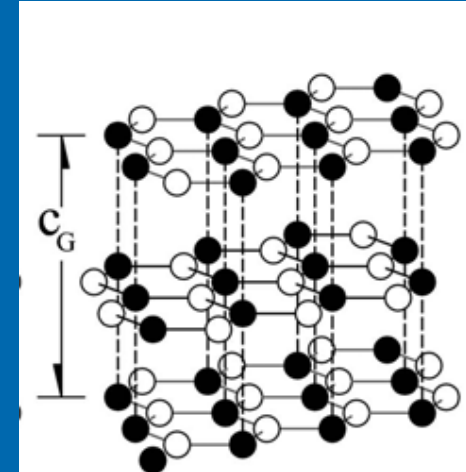
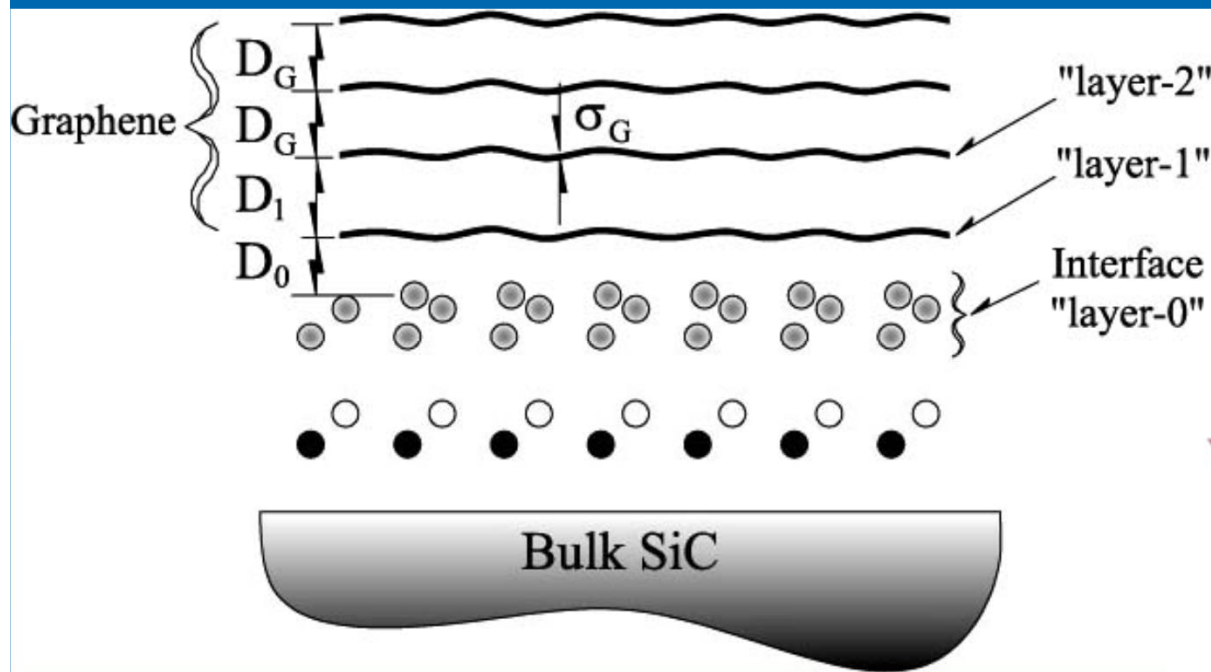
- Atomic-scale structure at a buried interface
- Morphological structure at buried interfaces
- Subsurface phenomena
 - Strains and defects near a surface
- Accurate statistics of distributions
(eg. Island size distributions)

Neutrons: low intensity- limited to reflectivity

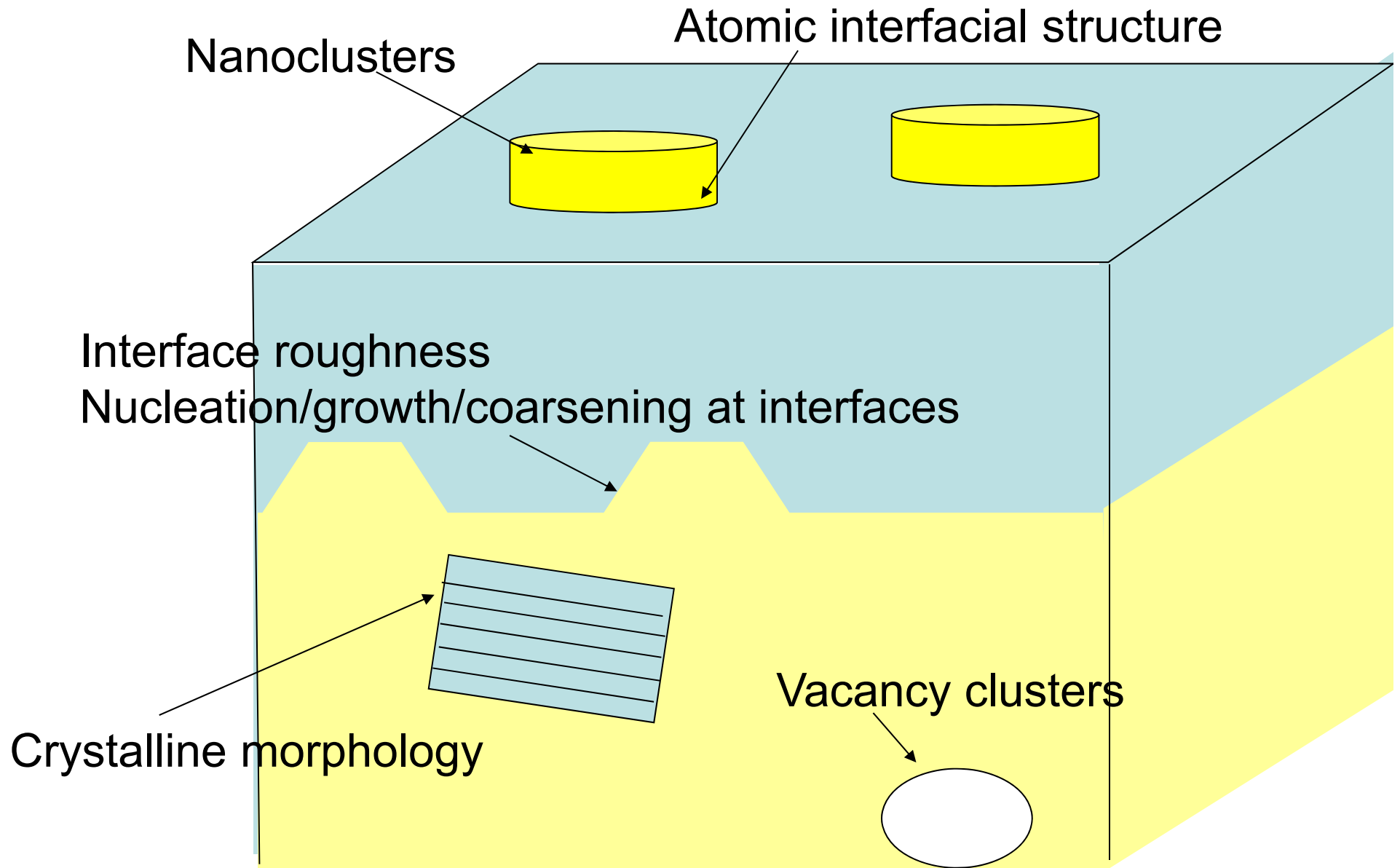
- Soft Matter and Bio materials; H_2O & D_2O
- Magnetic materials

Example: Rotation of graphene planes affect electronic properties

Graphene made from SiC



Morphology → atomic scale mechanisms



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

$$k = \frac{2\pi}{\lambda}$$

X-rays

Neutrons

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

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

$n(r)$ = inhomogeneous refractive index

Refractive Index for neutron:

$$n(\vec{r}) = \sqrt{1 - \frac{2m}{\hbar^2 k^2} V(\vec{r})} = \sqrt{1 - \lambda^2 \rho_b(\vec{r}) / \pi}$$

Scattering length density:

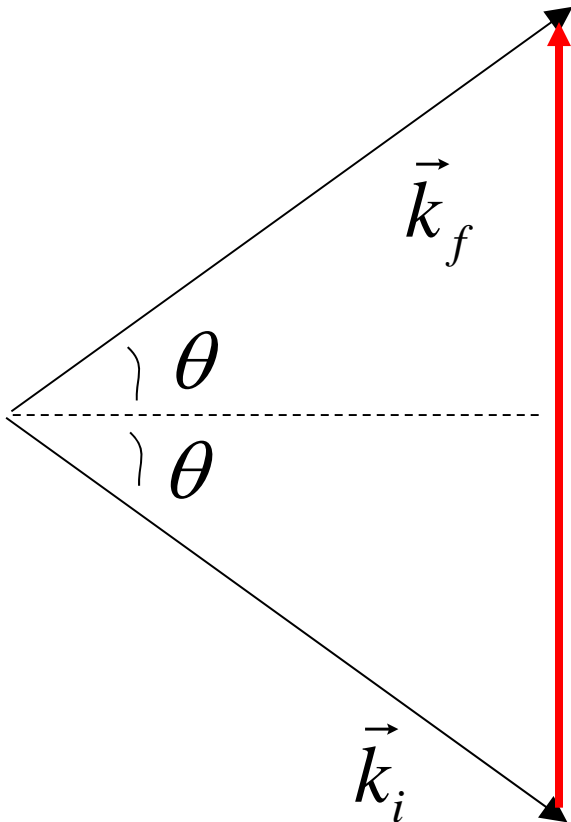
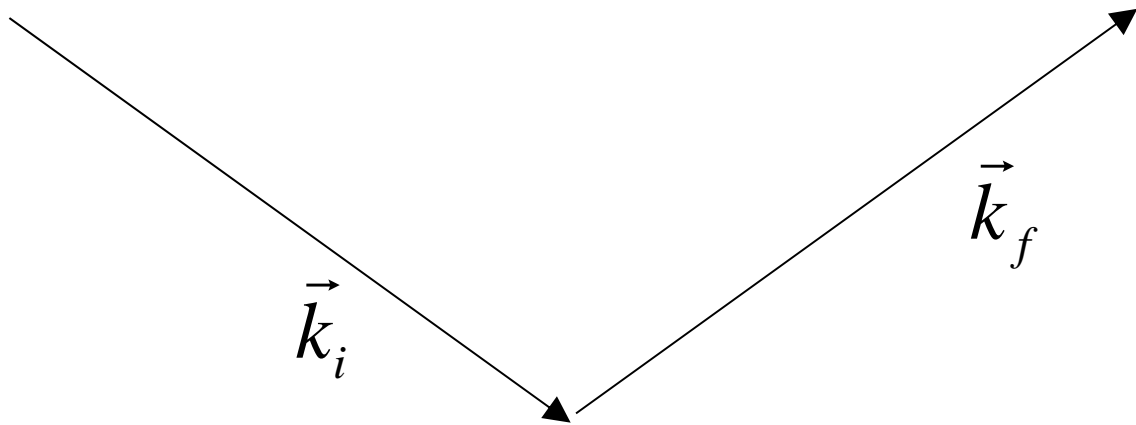
$$\rho_b(\vec{r}) \xrightarrow{\text{monoatomic}} \rho_N(\vec{r}) b$$

number density

scattering length:

$$b = \begin{cases} r_e f(Q) & \text{x-rays} \\ \text{tabulated} & \text{neutrons} \end{cases}$$

One language for both x-rays and neutrons



Wavevector Transfer:

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

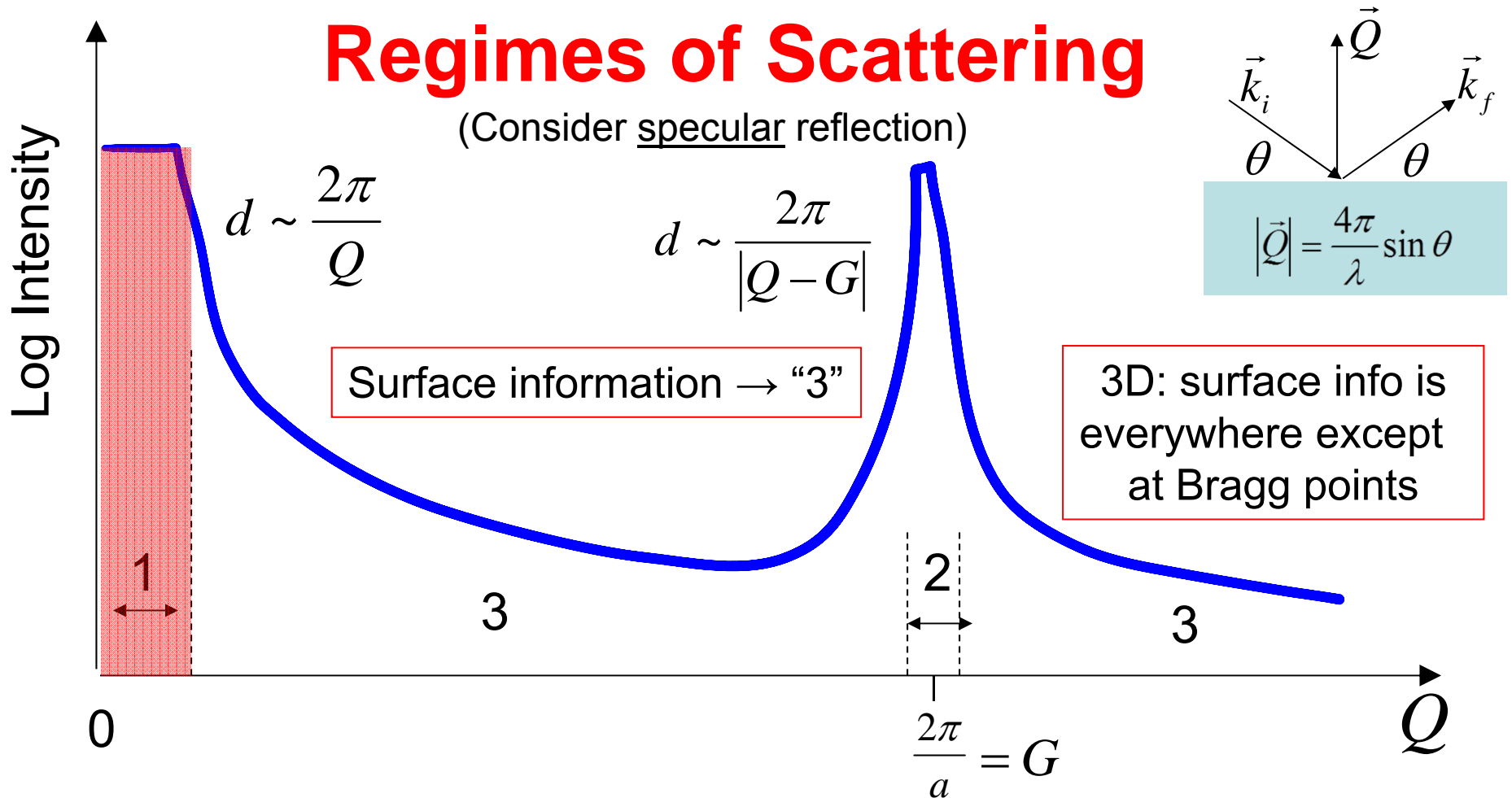
$$|\vec{Q}| = \frac{4\pi}{\lambda} \sin \theta \sim \frac{2\pi}{d}$$

Probing Length Scale

d

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.

Grazing Angles: Refraction and Total Reflection

$d \gg a$: consider homogenous medium

Use average refractive index:

$$n = \sqrt{1 - \lambda^2 \rho_b / \pi} \equiv 1 - \delta$$

$$\delta = \frac{\lambda^2 \rho_b}{2\pi} \ll 1 \quad (\sim 10^{-5})$$

With absorption: $n = 1 - \delta - i\beta$

Snell's Law:

$$\sin^2 \theta' = \sin^2 \theta - 2\delta$$

Critical Angle for
Total Reflection:

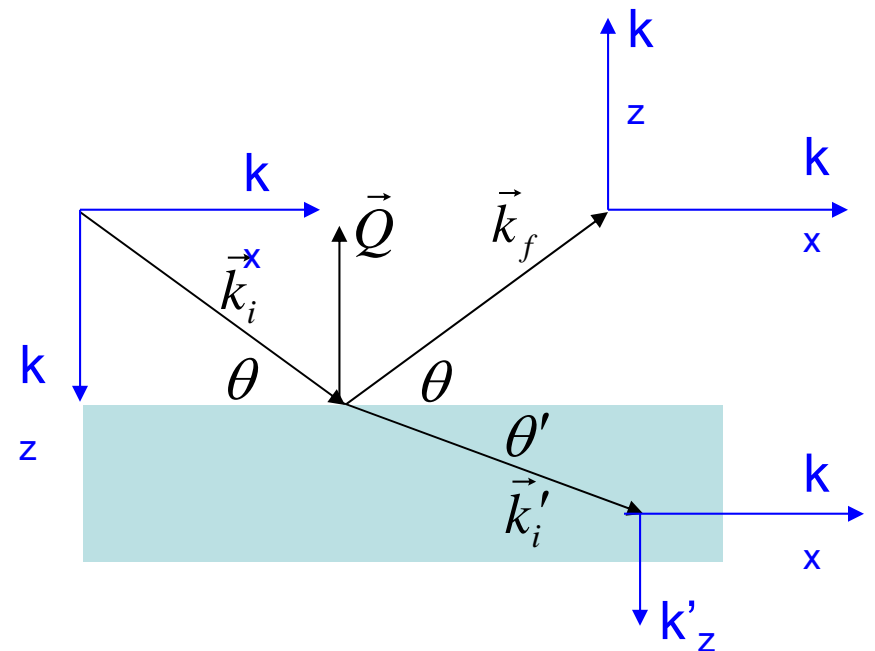
$$\theta_c = \sqrt{2\delta}$$

Wavevector transfer:

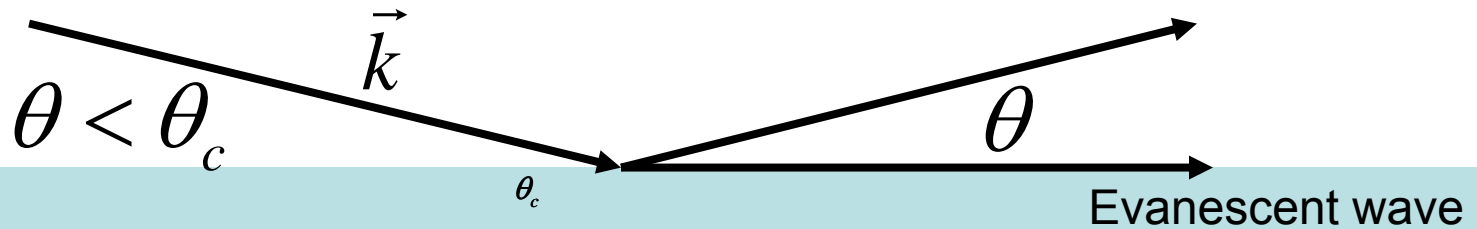
$$Q'^2 = Q^2 - Q_c^2$$

$$Q_c^2 = 16\pi\rho_b$$

Only k_z component is affected by the surface.
 k_x is unchanged.



Total Reflection



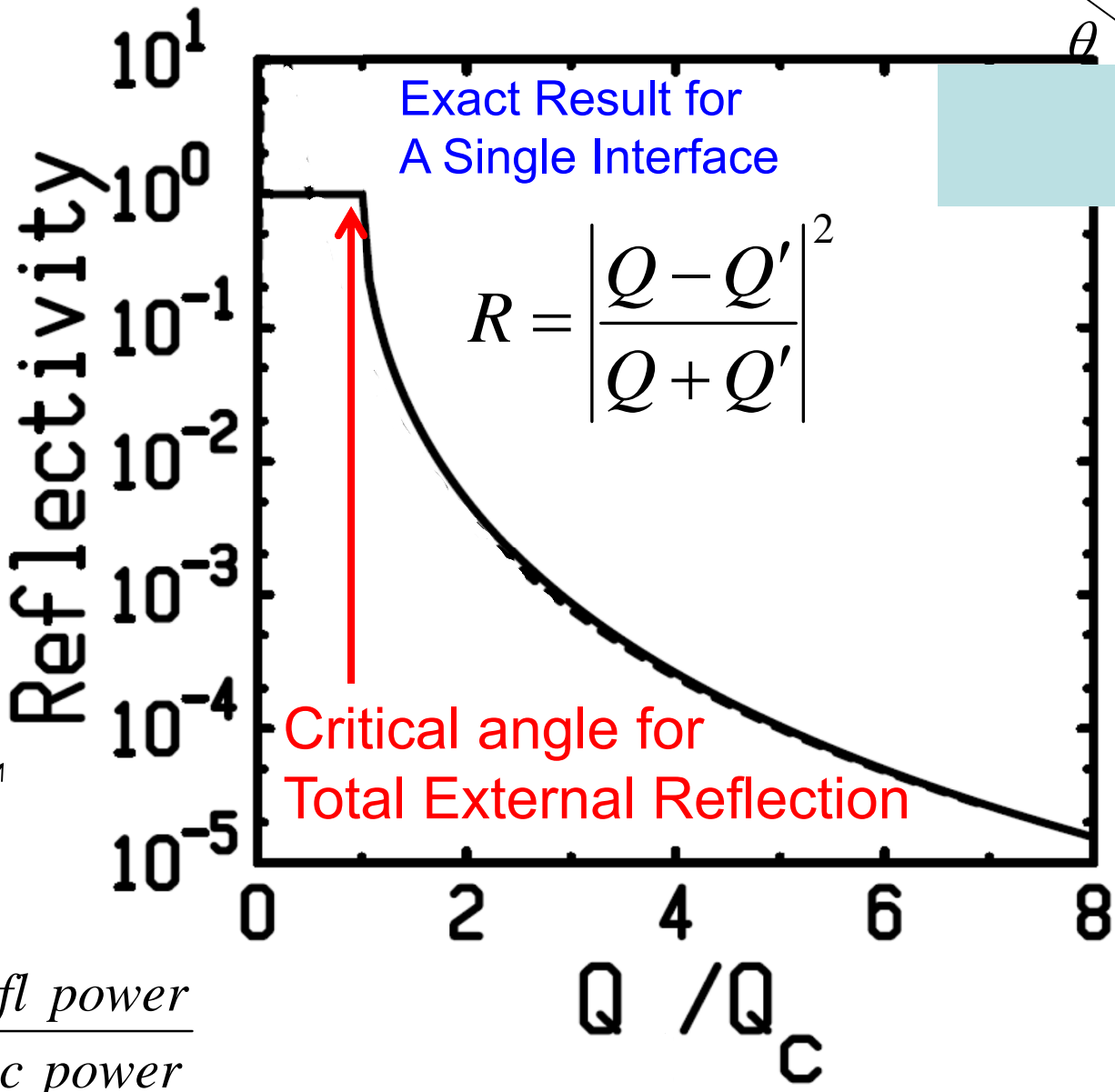
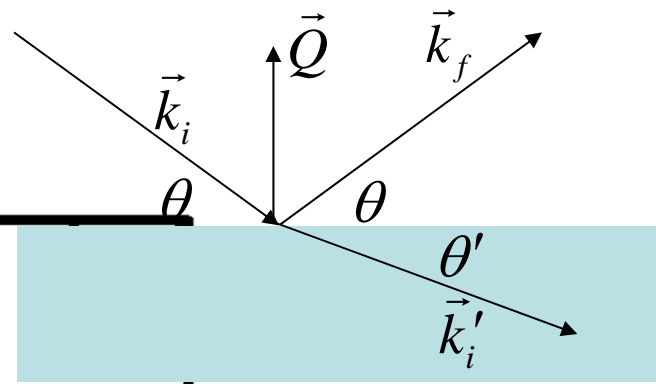
$$\sin^2(\theta') = 0 = \sin^2(\theta_c) - 2\delta$$

Critical Angle for Total External Reflection:

$$\theta_c = \sqrt{2\delta} \quad Q_c = \frac{4\pi}{\lambda} \theta_c$$

Beam does not transmit below θ_c

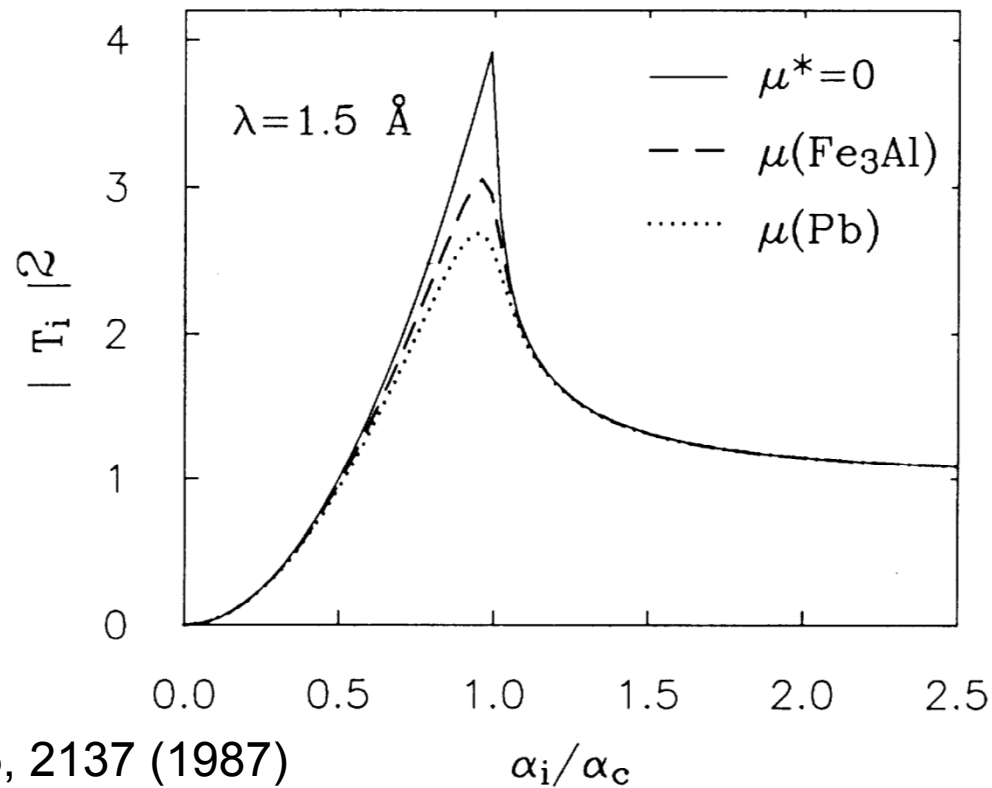
Frenel Reflectivity for a Single Interface



$$R = \frac{\text{refl power}}{\text{inc power}}$$

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)

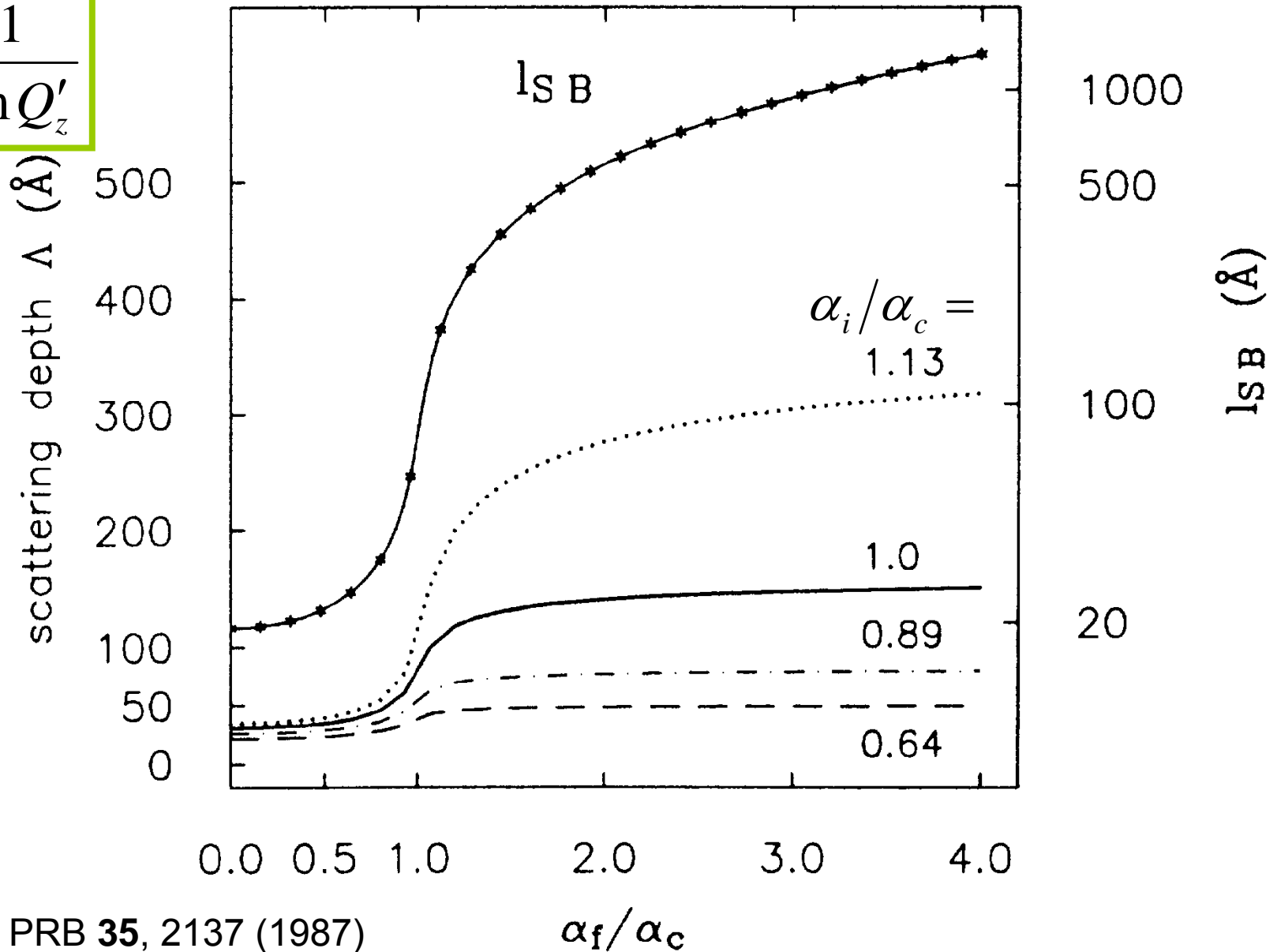
FIG. 1. Fresnel transmissivity $|T_i|^2$ as a function of α_i/α_c for a transparent medium and the real systems Fe_3Al and Pb .

$$\Lambda = \lambda / [2\pi(l_i + l_f)]$$

Penetration Length

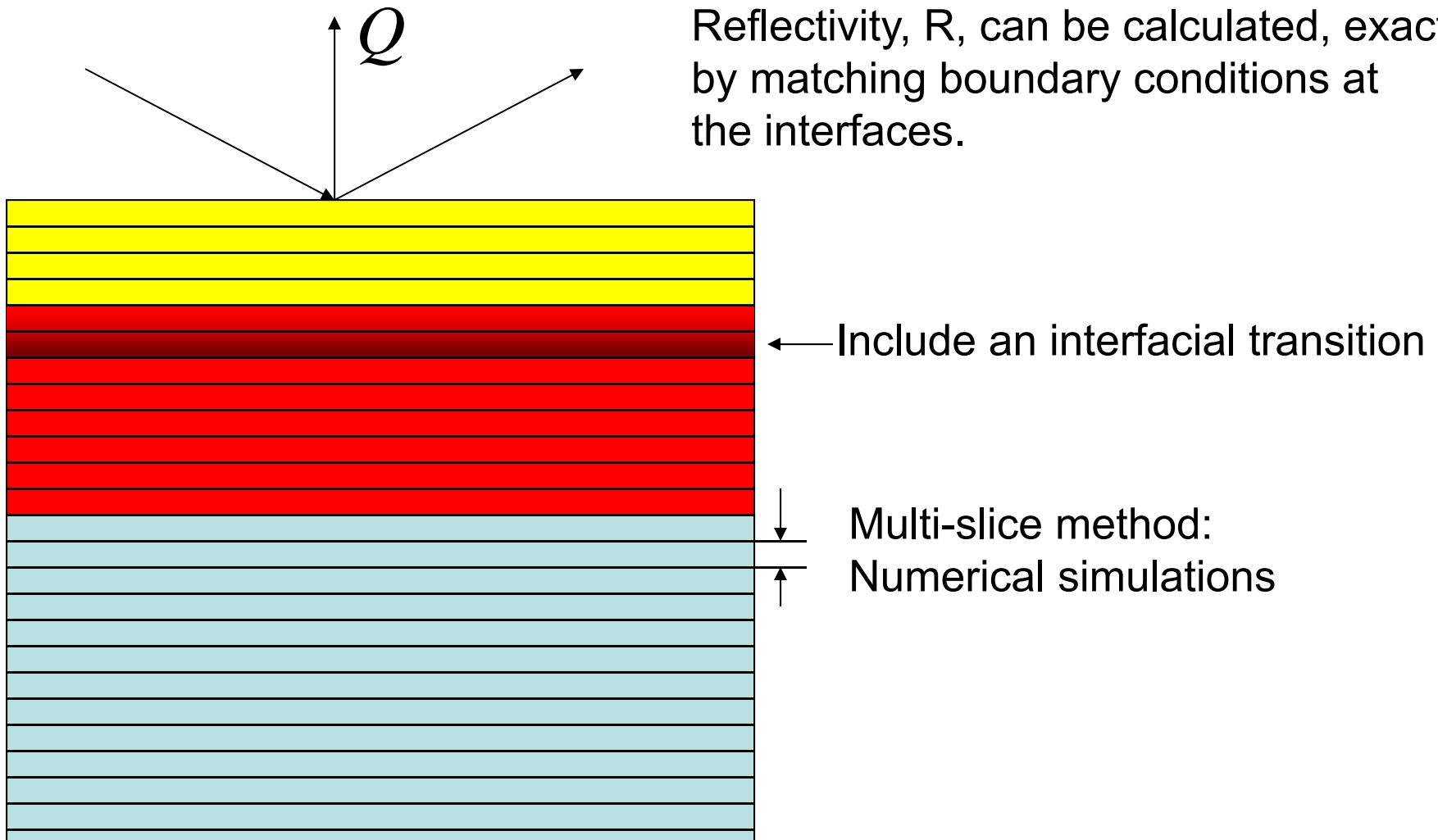
$$l_{i,f} = \frac{1}{2}\sqrt{2} \left\{ (2\delta - \sin^2\alpha_{i,f}) + [(\sin^2\alpha_{i,f} - 2\delta)^2 + (2\beta)^2]^{1/2} \right\}^{1/2}$$

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



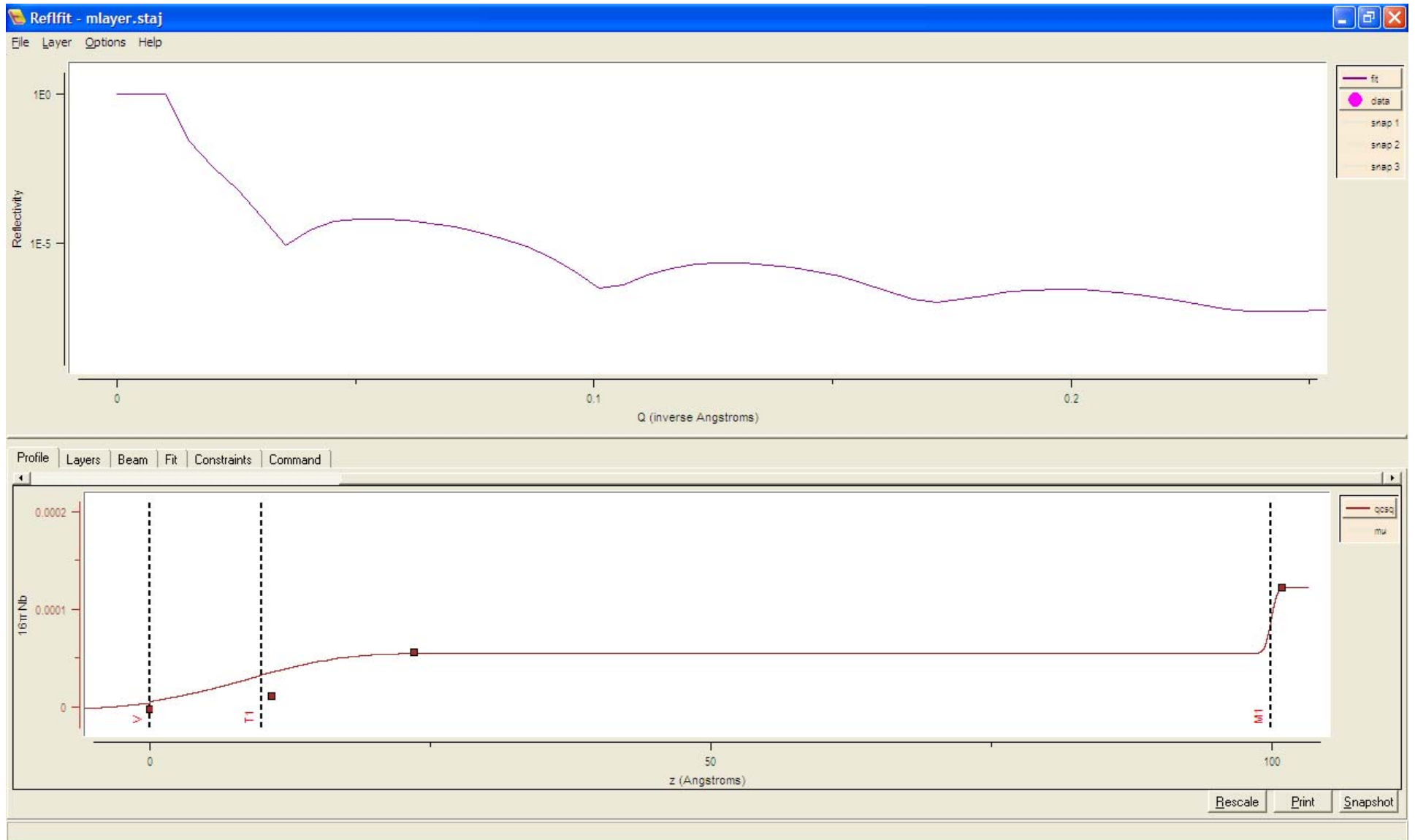
Calculation of reflectivity

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



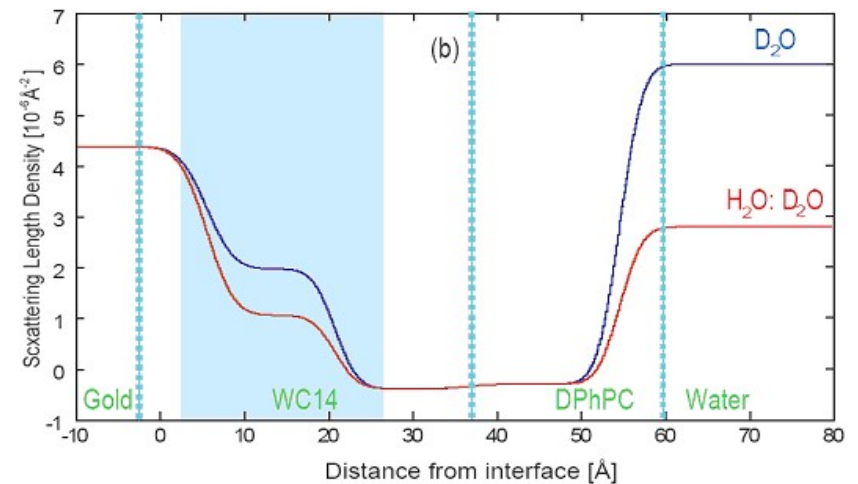
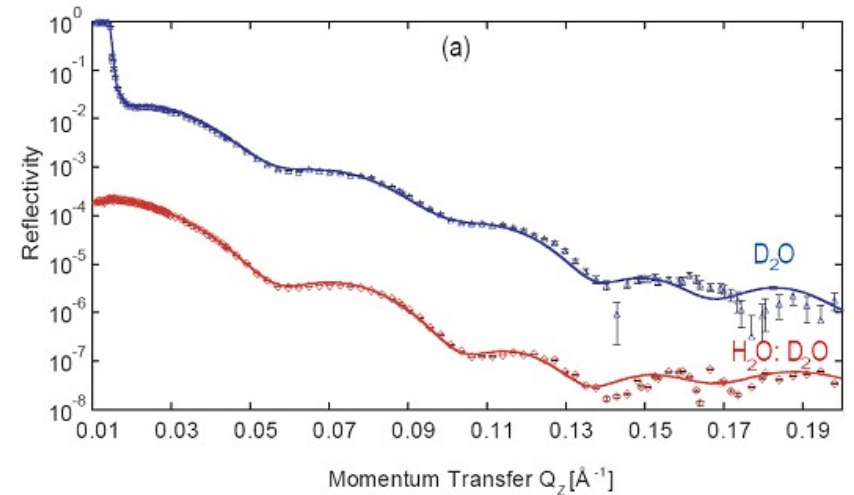
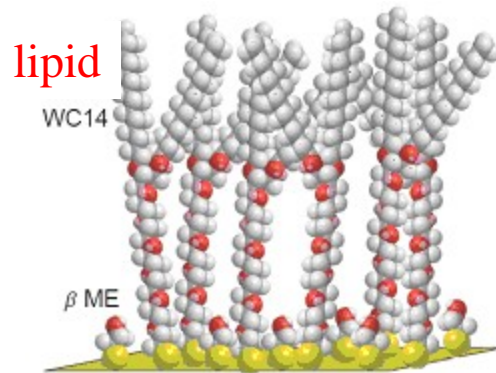
M-layer

<http://www.ncnr.nist.gov/reflpak/>



Soft Matter: Neutron Reflectivity

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

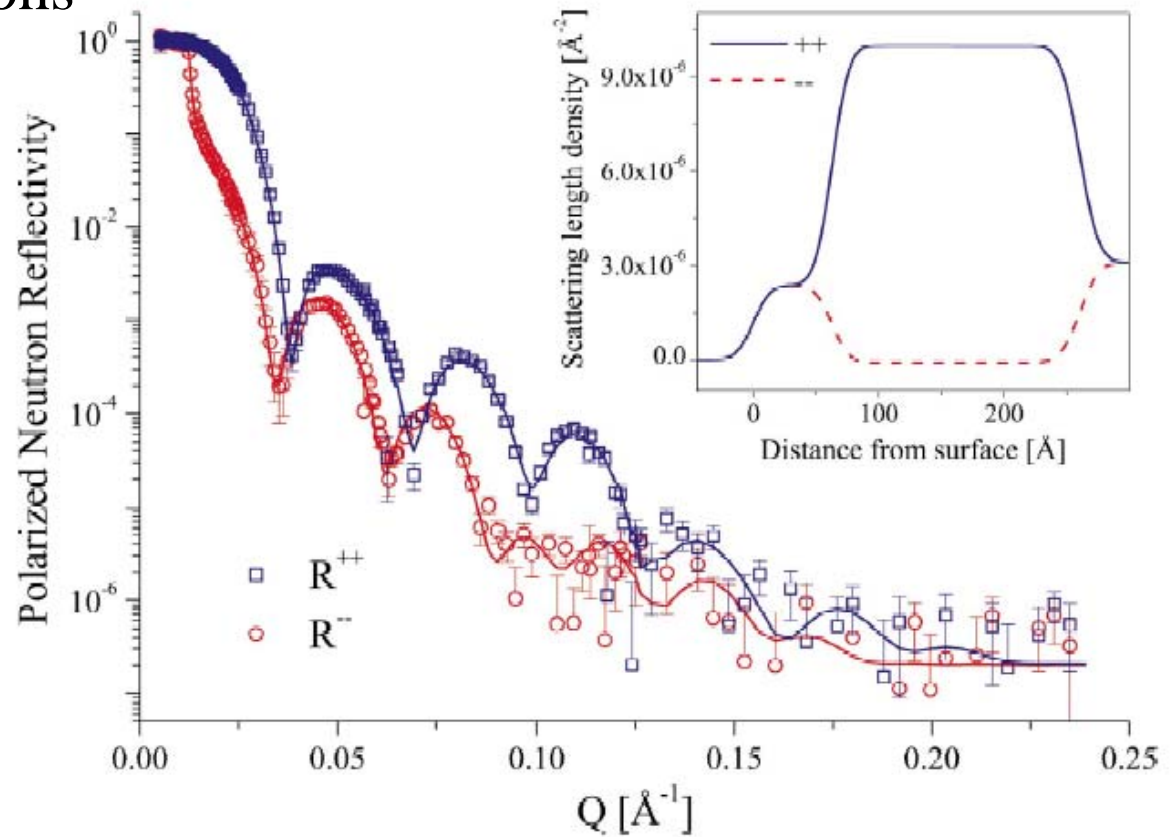


D. J. McGillivray and M. Lösche
D. J. Vanderah and J. J. Kasianowicz
G. Valincius

Magnetic Films: Neutron Reflectivity

- Magnetic thin films
Spin-polarized neutrons

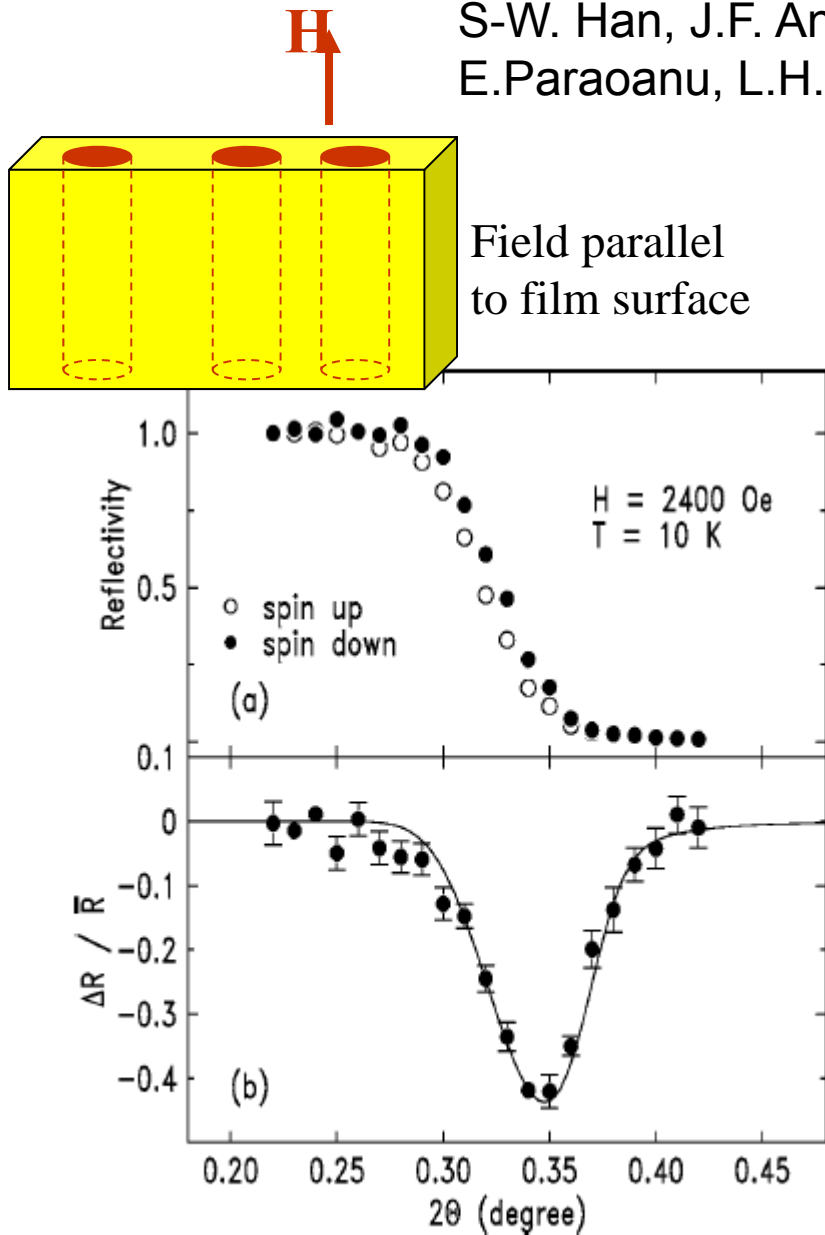
FeCo/GaAs



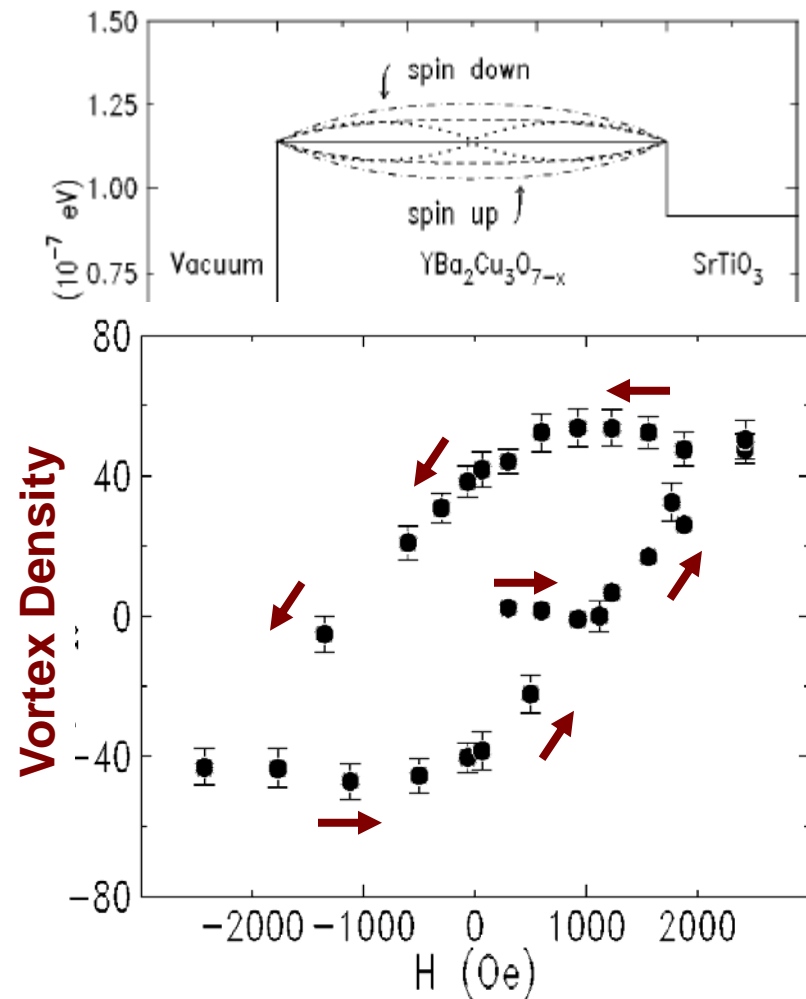
S. Park, M. R. Fitzsimmons, X. Y. Dong,
B. D. Schultz, and C. J. Palmstrøm, Phys Rev B 70 104406 (2004)

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)

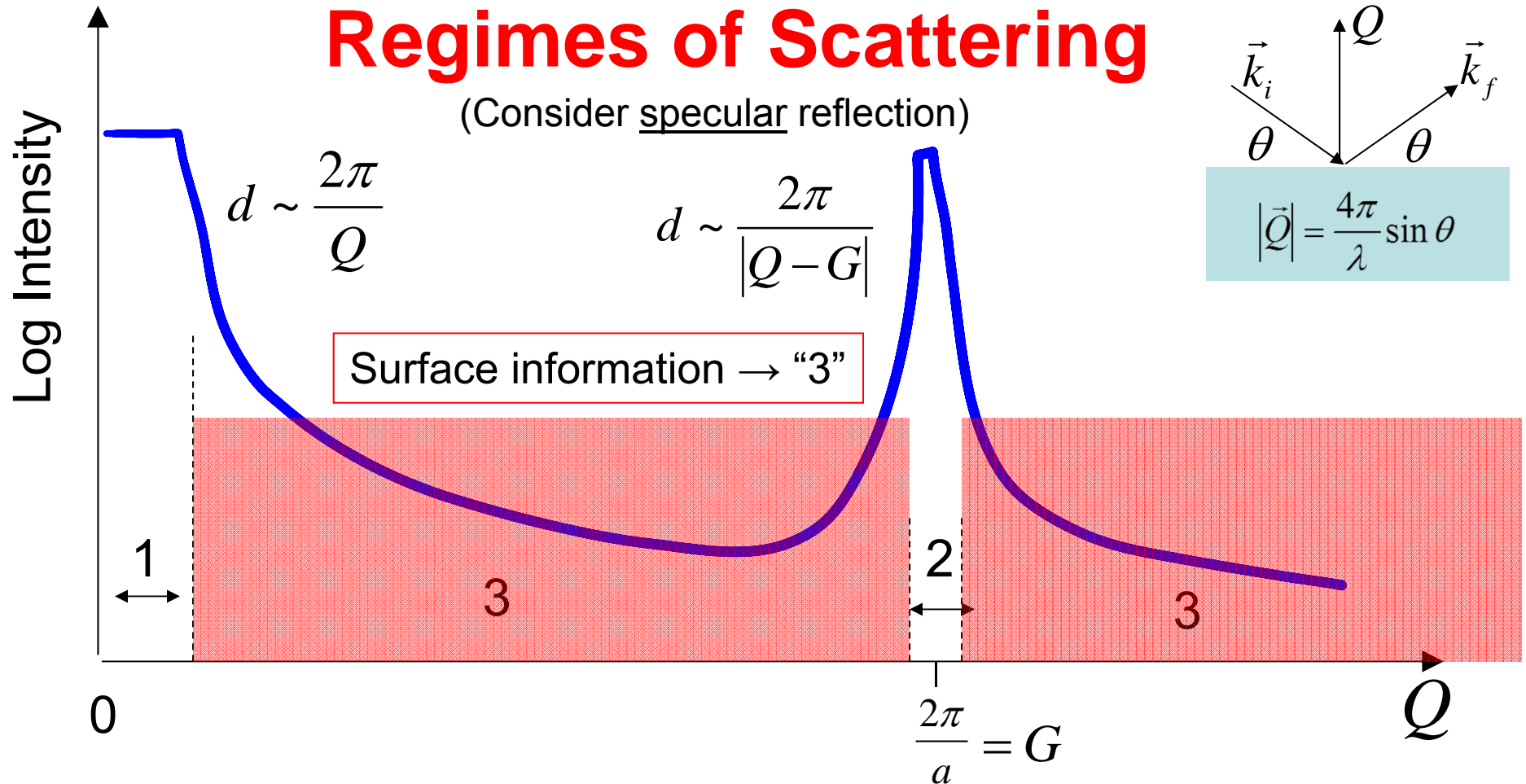
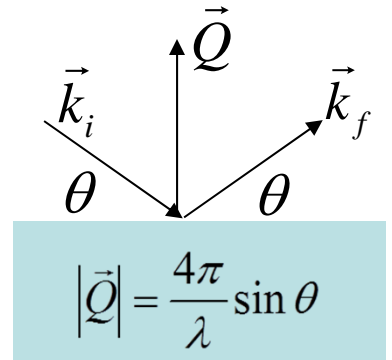


YBCO 600 nm Superconducting Film



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.

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

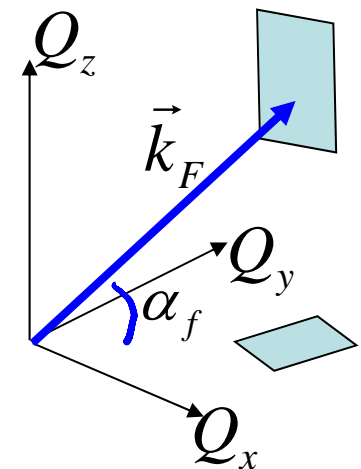
f(Q) is the atomic form factor

ρ_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

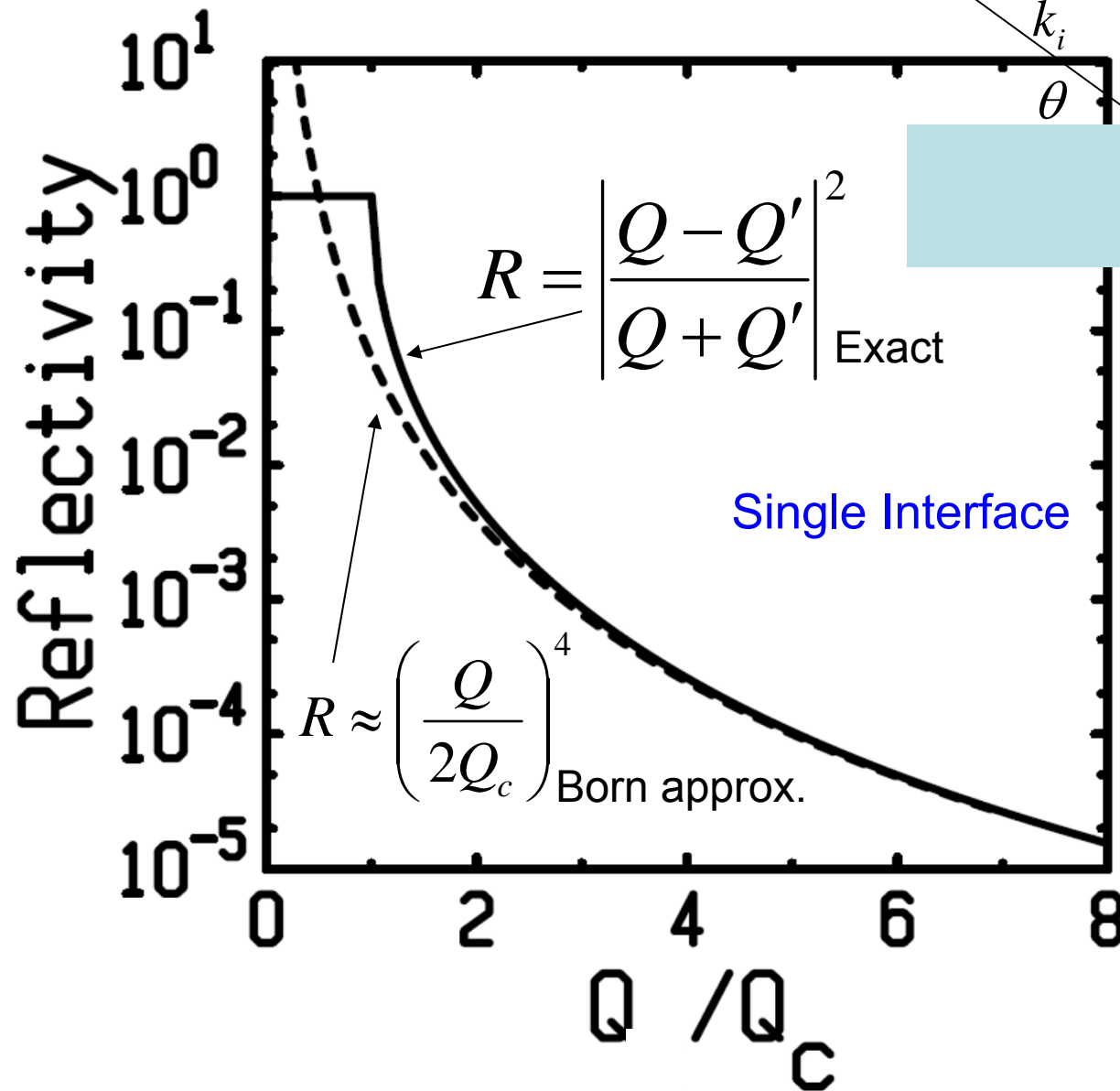
Sum over all atomic positions

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

$b = r_e f(Q)$ for x-rays or tabulated for neutrons

Born Approximation works if the reflectivity is not too large.

Specular Reflection



General Case: non-specular scattering

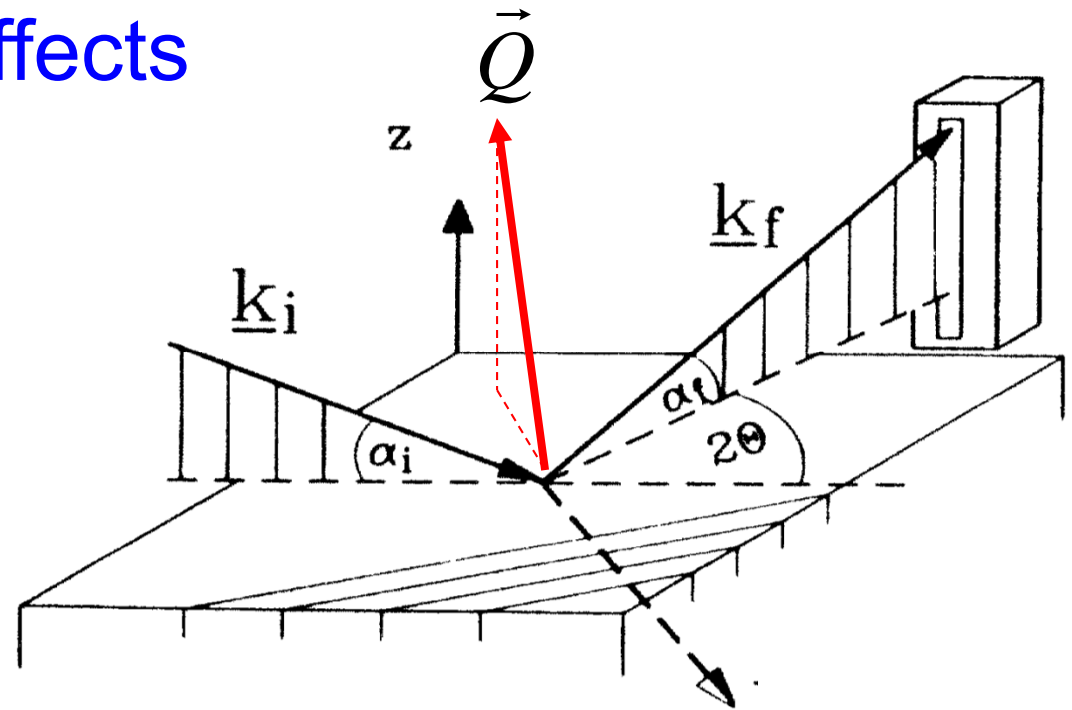
Grazing Incidence Effects

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 \mathbf{Q}' and external \mathbf{Q} are different

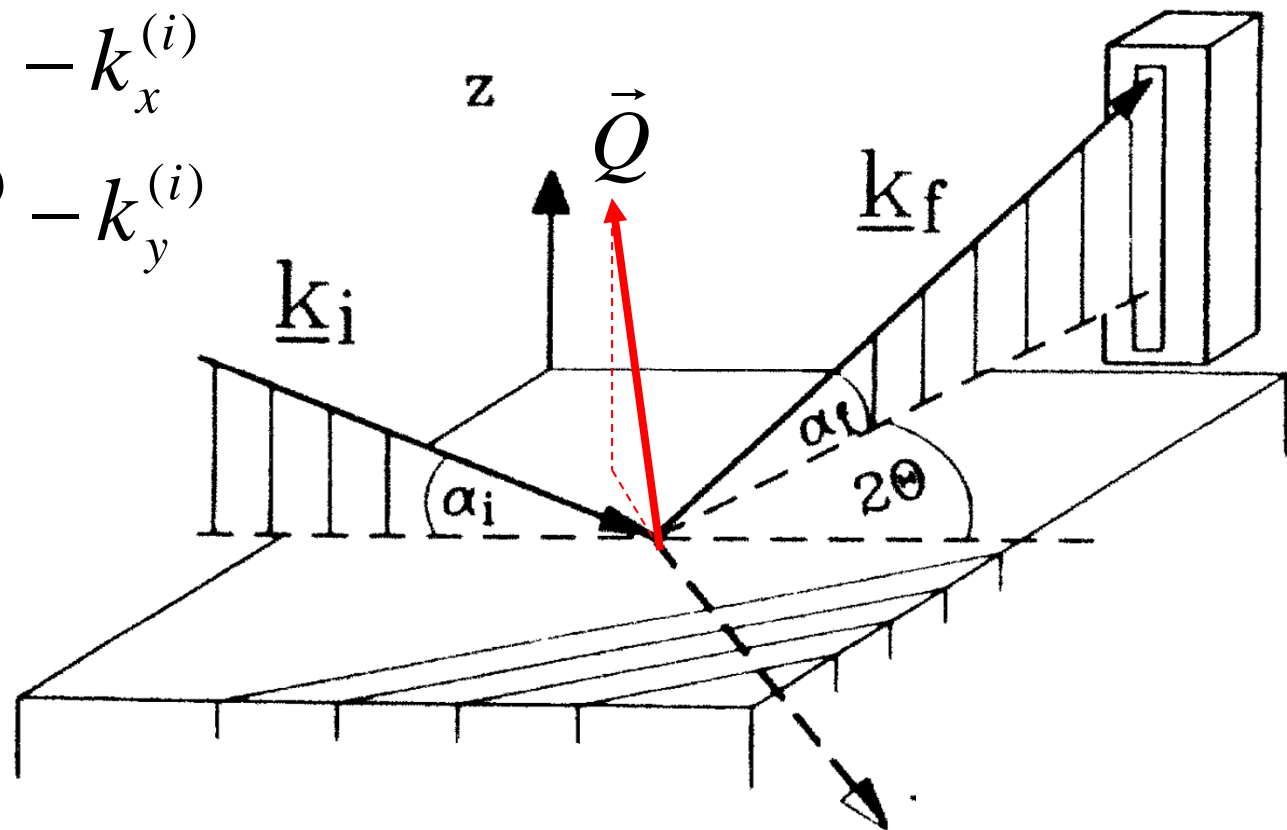
$$Q_z = k_z^{(f)} - k_z^{(i)} = (2\pi/\lambda) [\sin\alpha_f + \sin\alpha_i].$$

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

Parallel to Surface: internal \mathbf{Q}' and external \mathbf{Q} are same

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

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

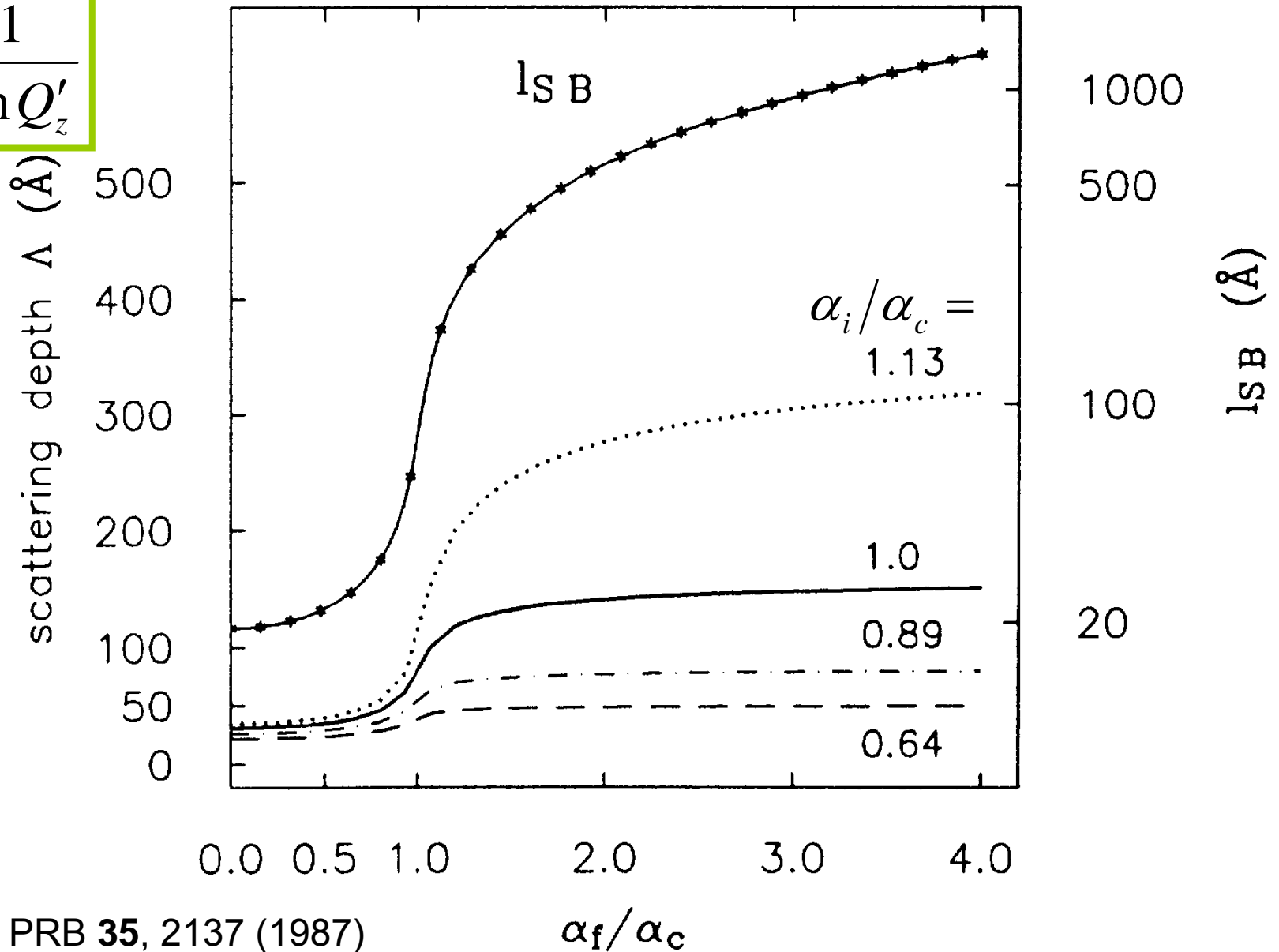


$$\Lambda = \lambda / [2\pi(l_i + l_f)]$$

Penetration Length

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

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



Fe₃Al

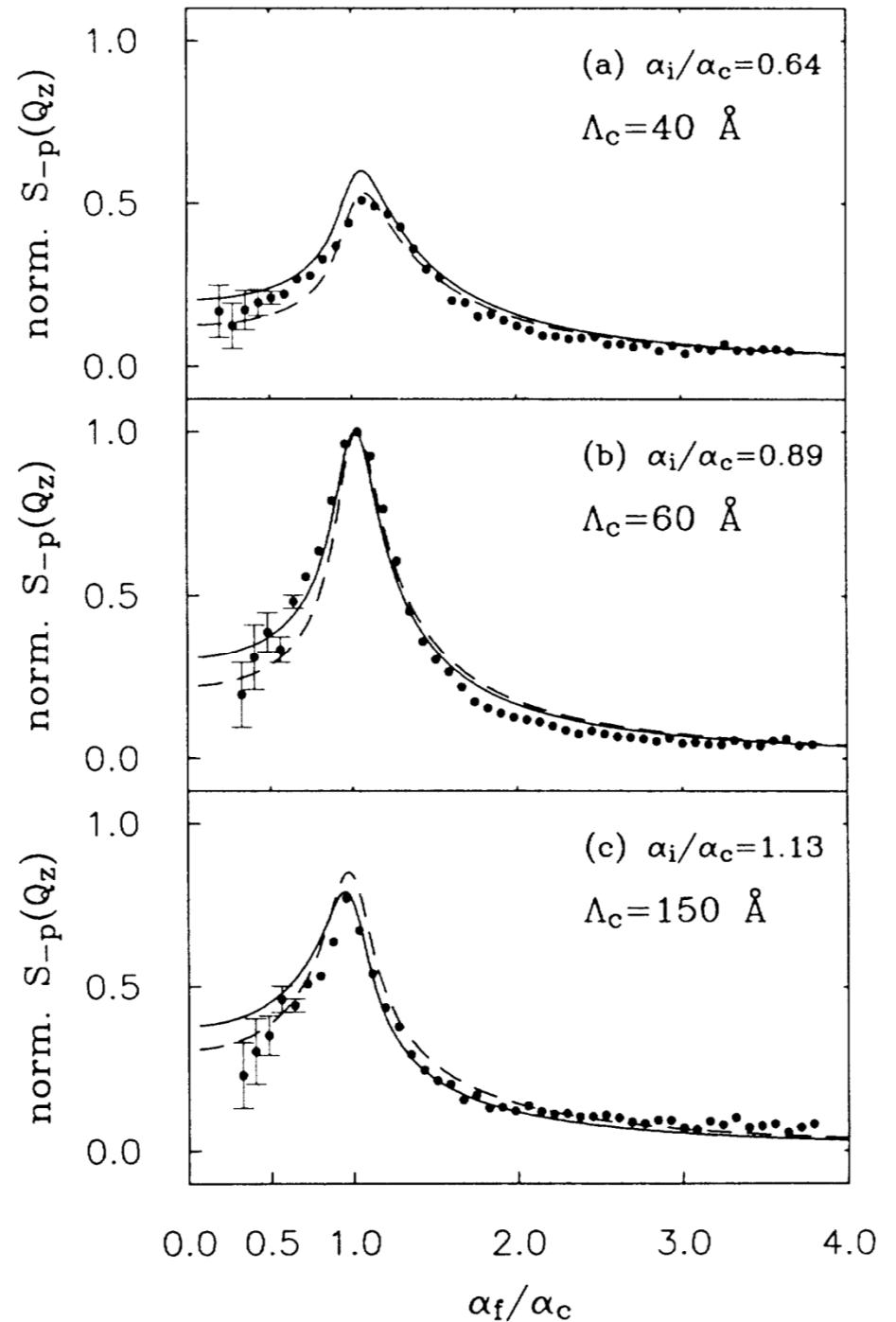
H. Dosch, PRB **35**, 2137 (1987)

Distorted Wave Born Approximation

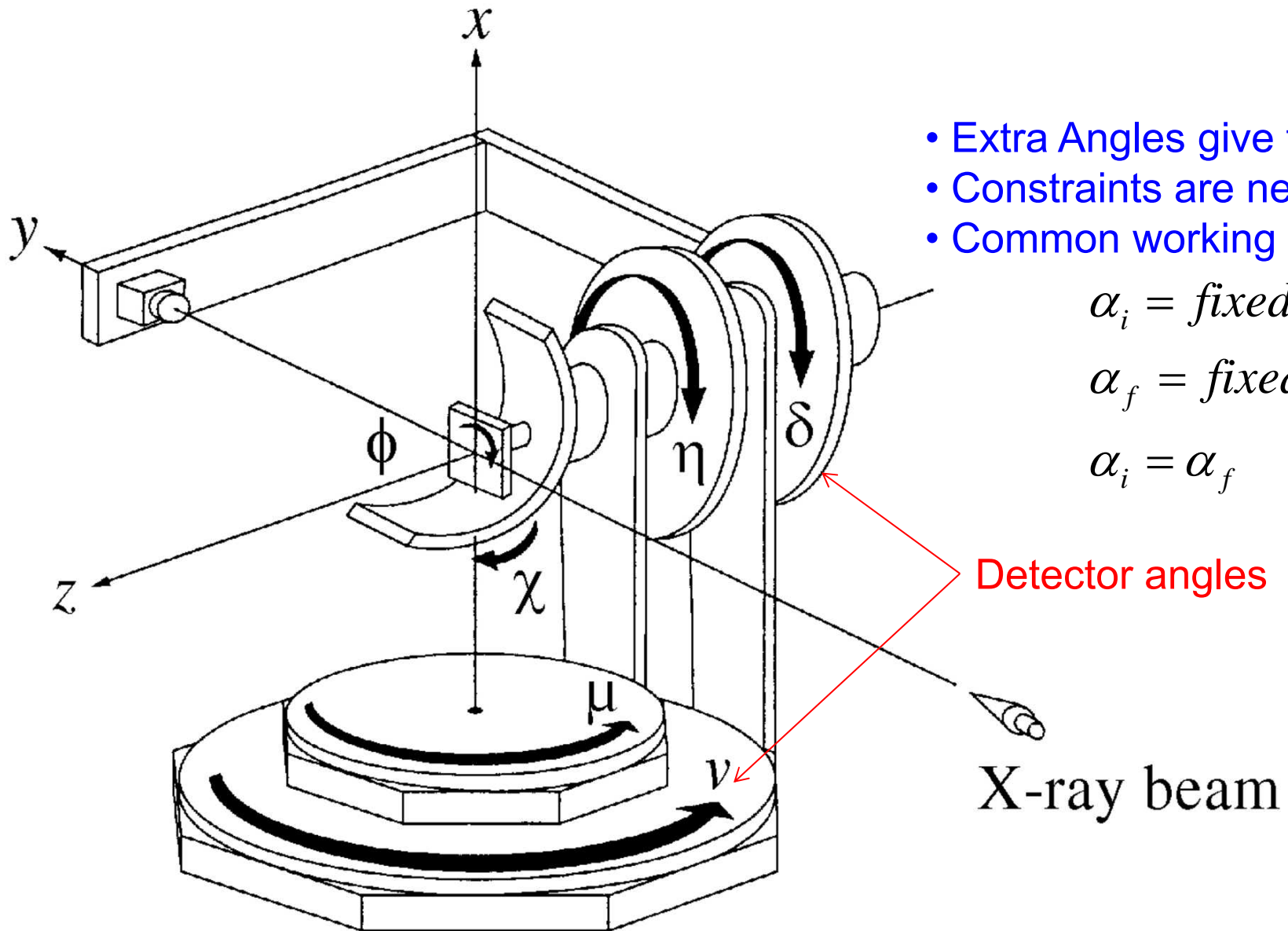
$$I_{\text{GID}}(\vec{Q}') \propto |T_i|^2 S(\vec{Q}') |T_f|^2$$

- refraction
- transmission

$S(\vec{Q}')$ is the structure factor using
the internal wavevector transfer

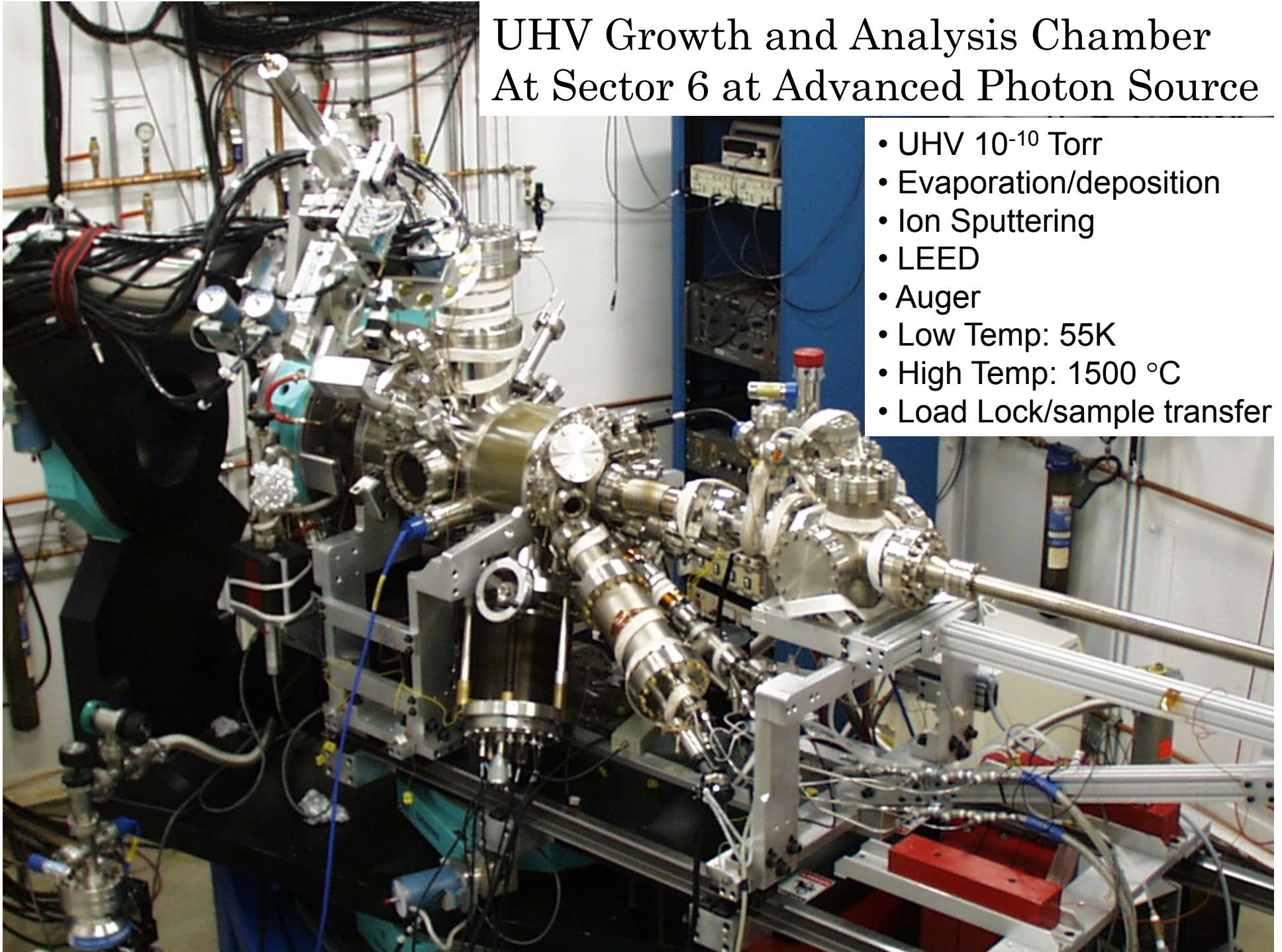


A Six-Circle Diffractometer

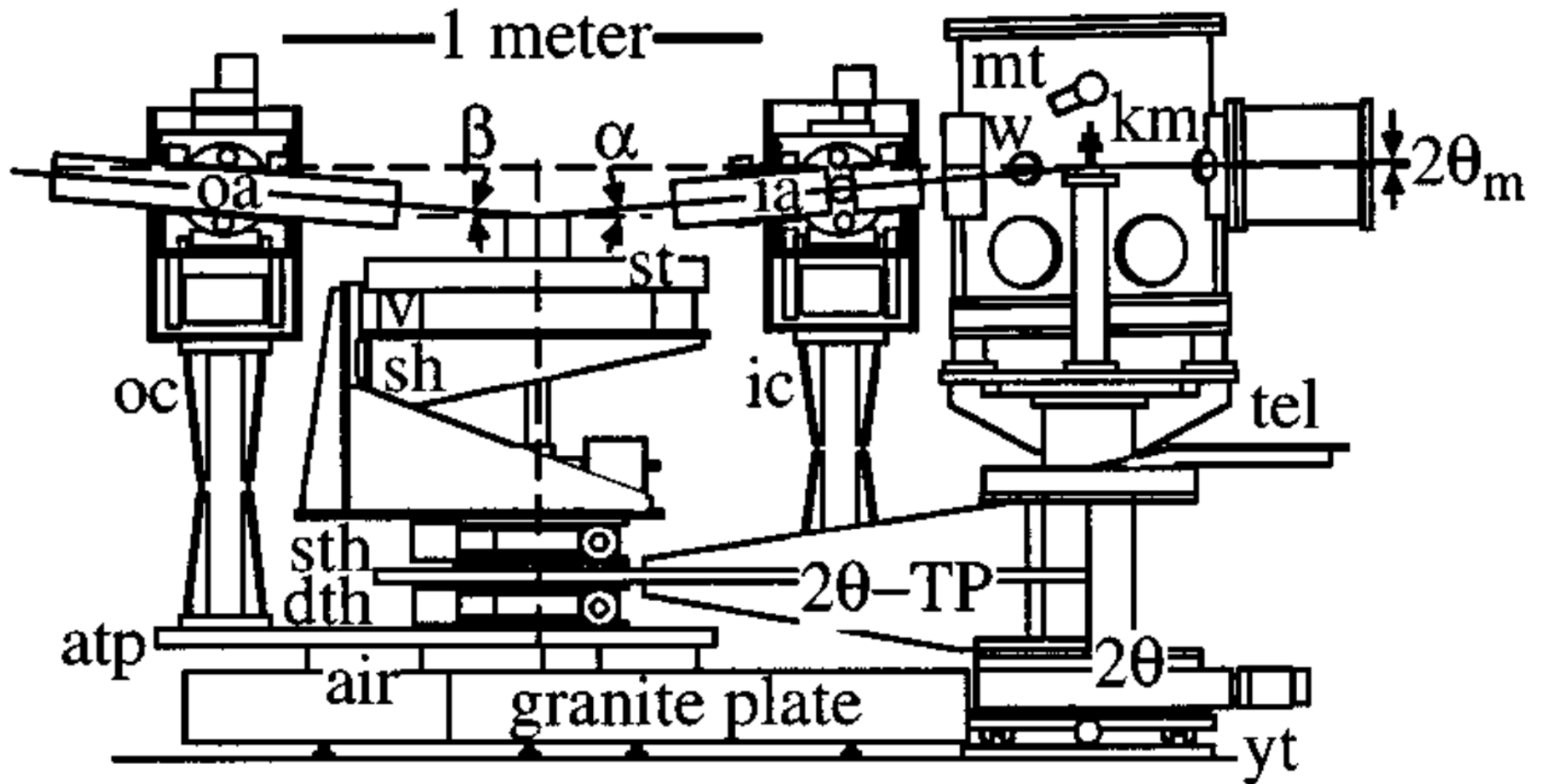


UHV Growth and Analysis Chamber At Sector 6 at Advanced Photon Source

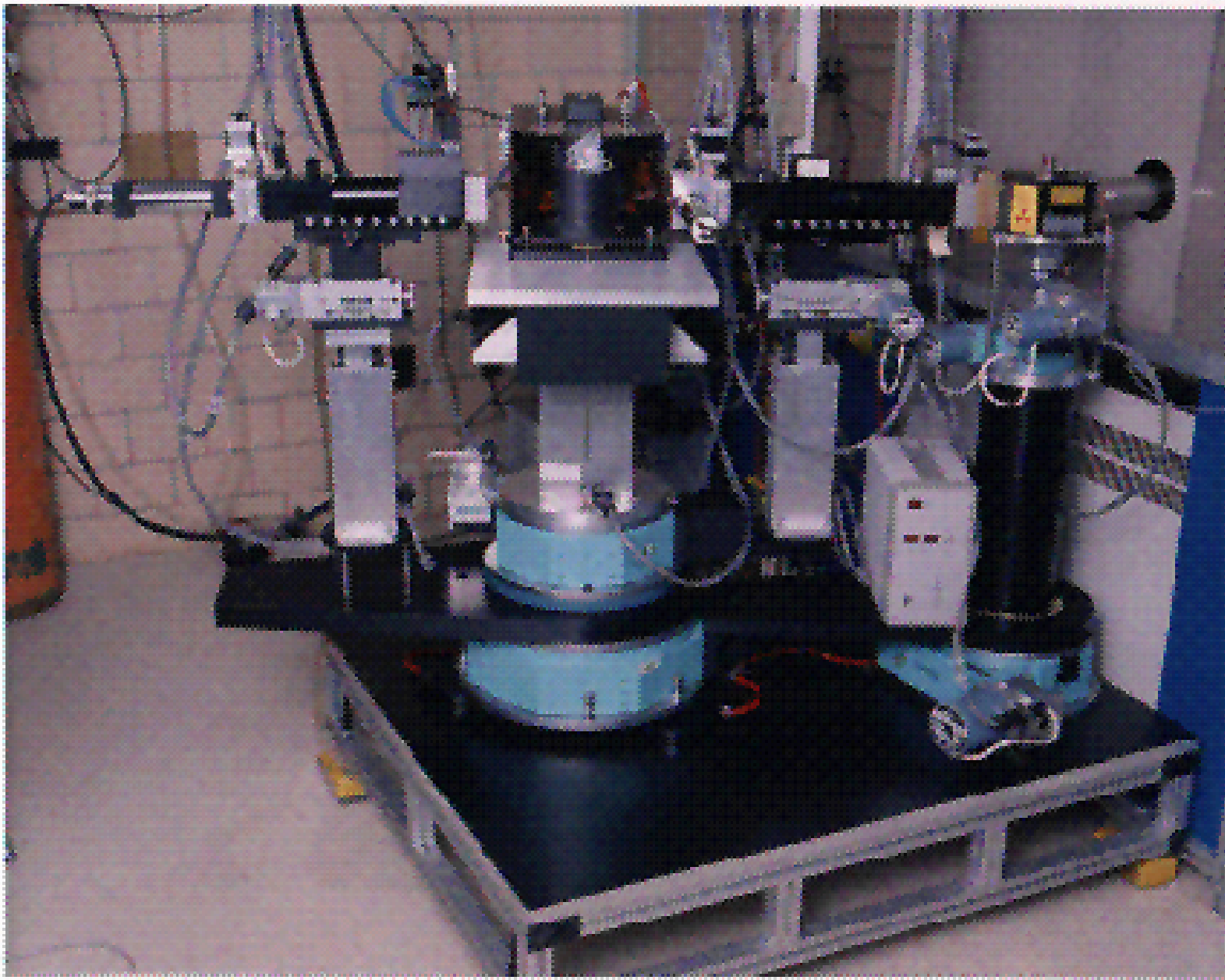
- UHV 10^{-10} Torr
- Evaporation/deposition
- Ion Sputtering
- LEED
- Auger
- Low Temp: 55K
- High Temp: 1500 °C
- Load Lock/sample transfer



Liquid Surface Diffractometer



M. Schlossman et. al., Rev. Sci. Inst. **68**, 4372 (1997)



David Vaknin, Ames Lab

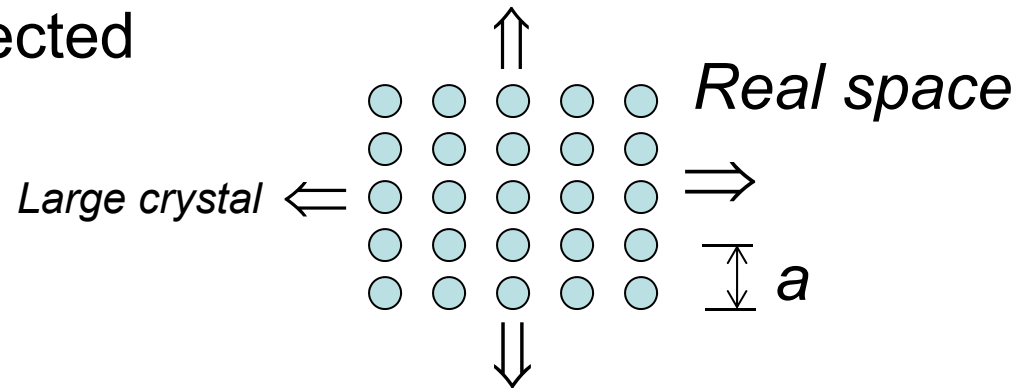
The Effect of a Crystalline Boundary



What is a crystal truncation rod?

First consider:

- Large crystals; rough and irregular boundaries
- Boundaries neglected



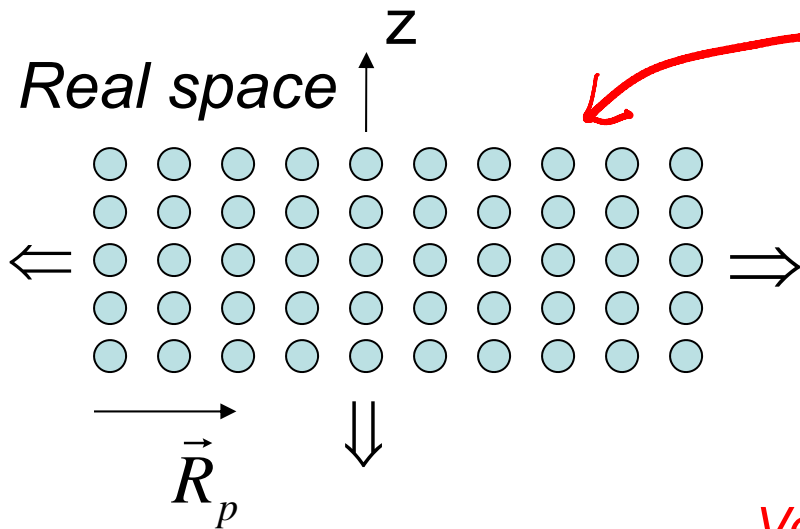
$$S(\vec{Q}) = \left| \sum_{n_x=0}^{N-1} e^{iQ_x a n_x} \sum_{n_y=0}^{N-1} e^{iQ_y b n_y} \sum_{n_z=0}^{N-1} e^{iQ_z c n_z} \right|^2 = \frac{\sin^2\left(\frac{NQ_x a}{2}\right) \sin^2\left(\frac{NQ_y b}{2}\right) \sin^2\left(\frac{NQ_z c}{2}\right)}{\sin^2\left(\frac{Q_x a}{2}\right) \sin^2\left(\frac{Q_y b}{2}\right) \sin^2\left(\frac{Q_z c}{2}\right)}$$

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



\vec{G} is a reciprocal lattice vector

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



- Large crystal; flat boundary $z = 0$
- Neglect boundary at $z = -\infty$

Very small attenuation $\varepsilon < \sim 1$

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

Reflected wave vanishes

Crystal Truncation Rod Factor

$$\lim_{\varepsilon \rightarrow 1} \lim_{N \rightarrow \infty} \left| \frac{1 - \varepsilon^N e^{-iQ_z c N}}{1 - e^{-iQ_z c}} \right|^2 = \frac{1}{4 \sin^2 \left(\frac{Q_z c}{2} \right)} \approx \frac{1}{c^2 (Q_z - G_z)^2}$$

By neglecting the lateral boundaries:

$$\sum_{\vec{R}_p} \sum_{\vec{R}'_p} e^{i\vec{Q}_p \cdot (\vec{R}_p - \vec{R}'_p)} = N_{irr} \sum_{\vec{R}_p} e^{i\vec{Q}_p \cdot \vec{R}_p}$$

and
$$\sum_{\vec{R}_p} e^{i\vec{Q}_p \cdot \vec{R}_p} = \frac{(2\pi)^2}{s_c} \sum_{\vec{G}_p} \delta(\vec{Q}_p - \vec{G}_p)$$

N_{irr} = the number of irradiated atoms at the surface

s_c = area per surface atom

\vec{G}_p = an in-plane reciprocal lattice vector

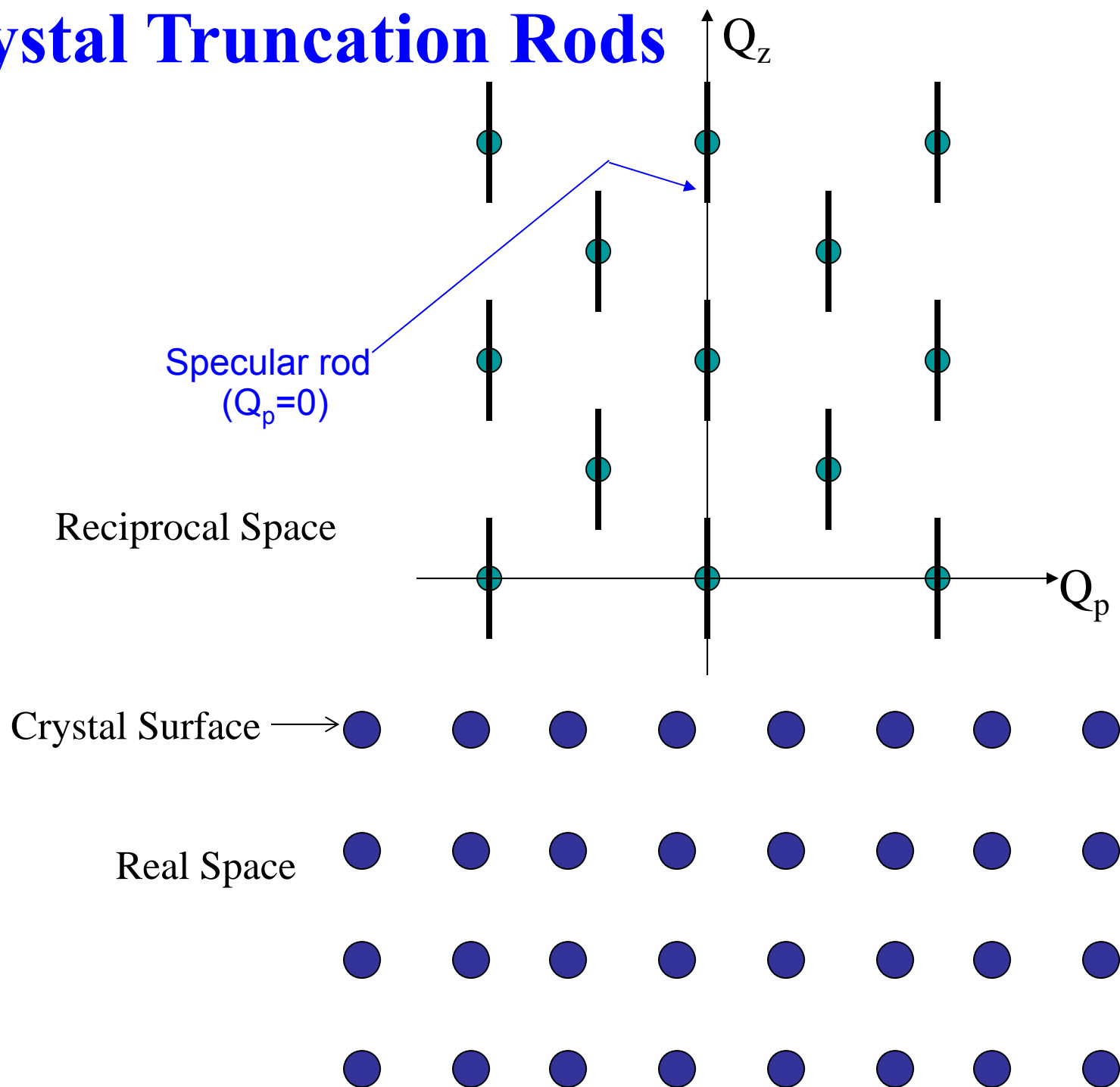
$$S(\vec{Q}) = \frac{(2\pi)^2 N_{irr} b^2}{s_c} \frac{1}{4 \sin^2\left(\frac{Q_z c}{2}\right)} \sum_{\vec{G}_p} \delta(\vec{Q}_p - \vec{G}_p)$$

CTR

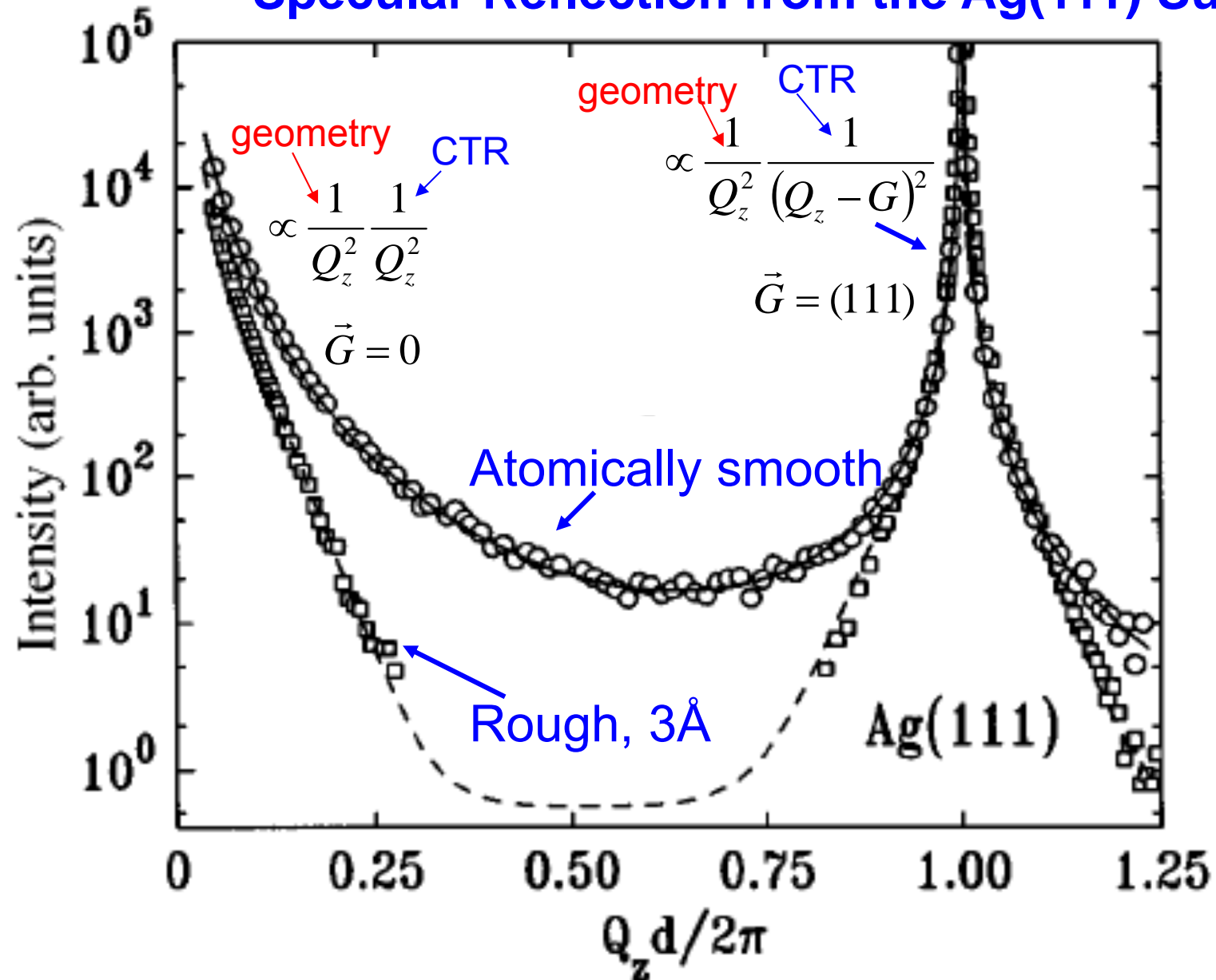
Narrow reflection in-plane

Intensity falls slowly

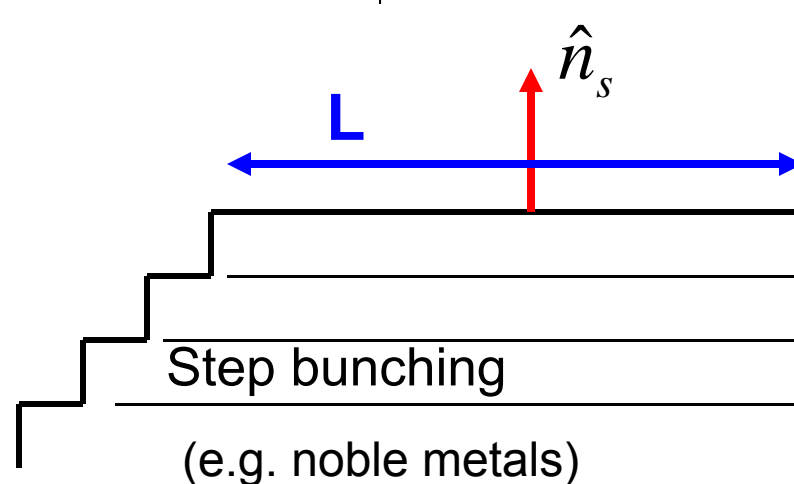
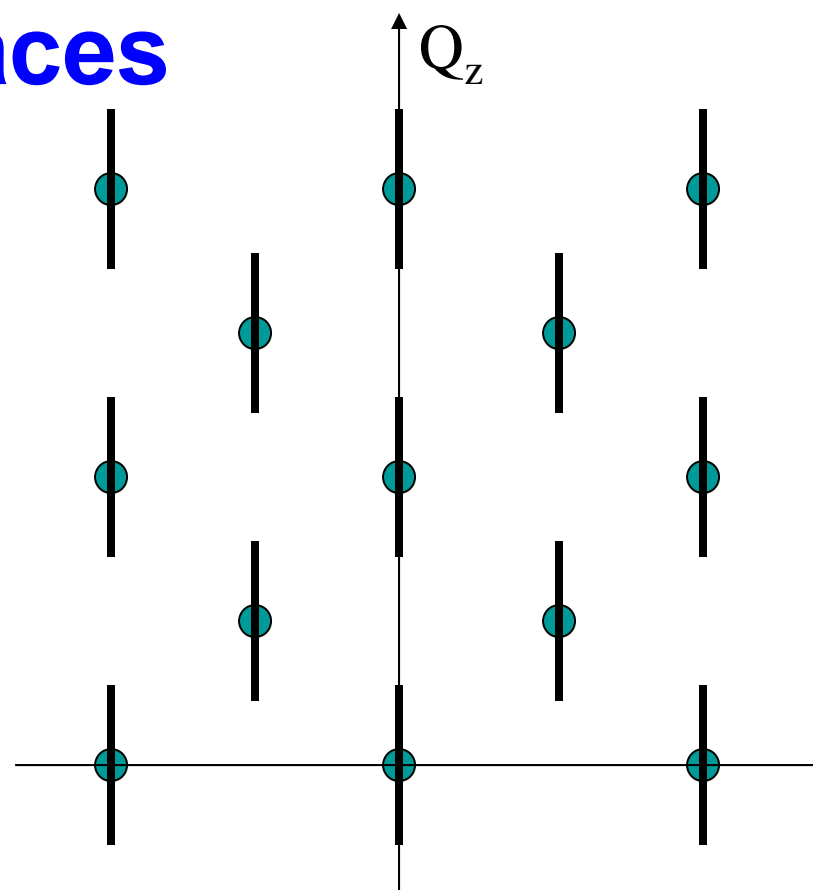
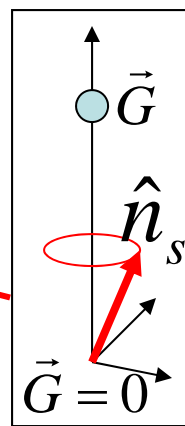
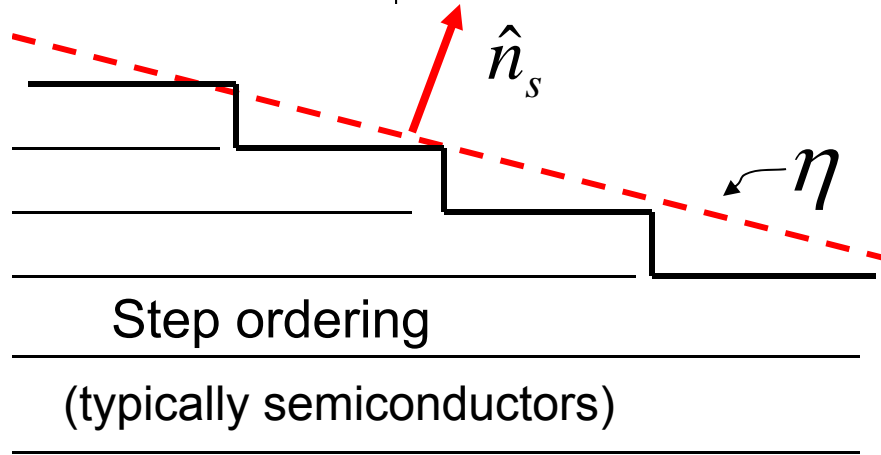
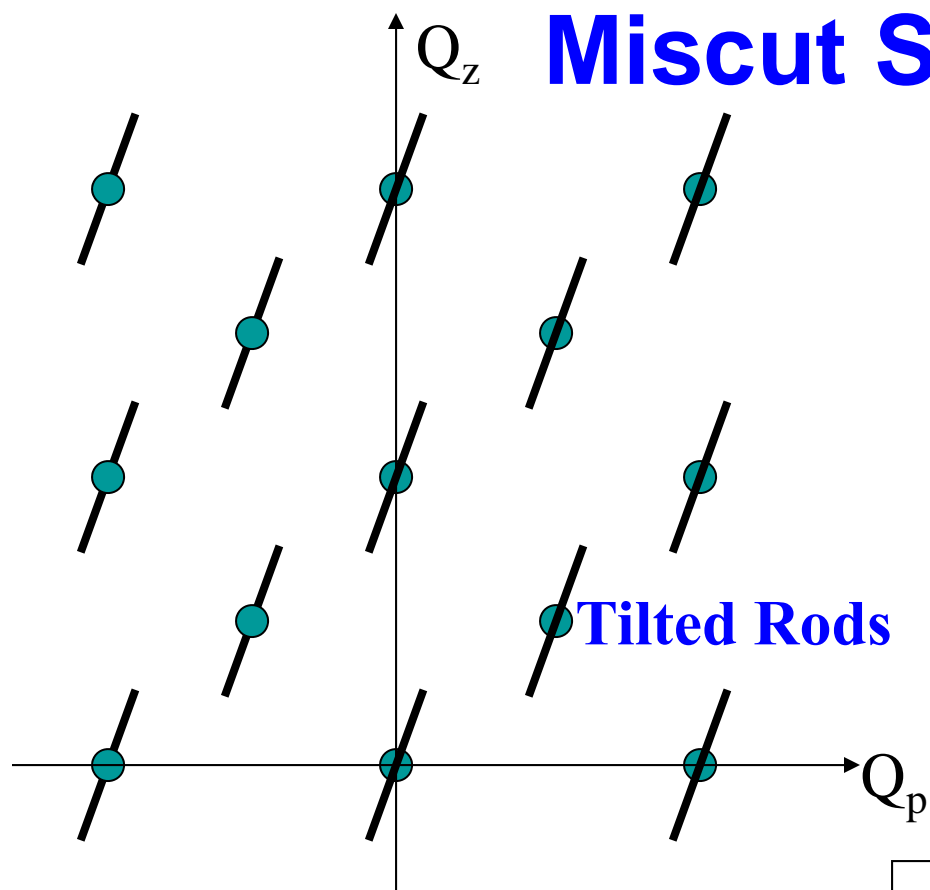
Crystal Truncation Rods



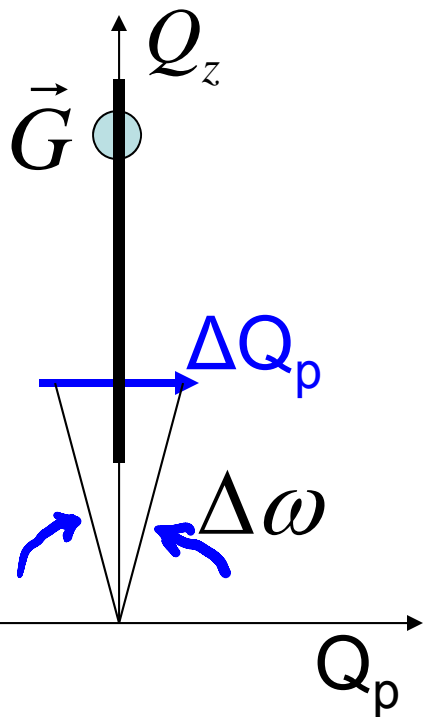
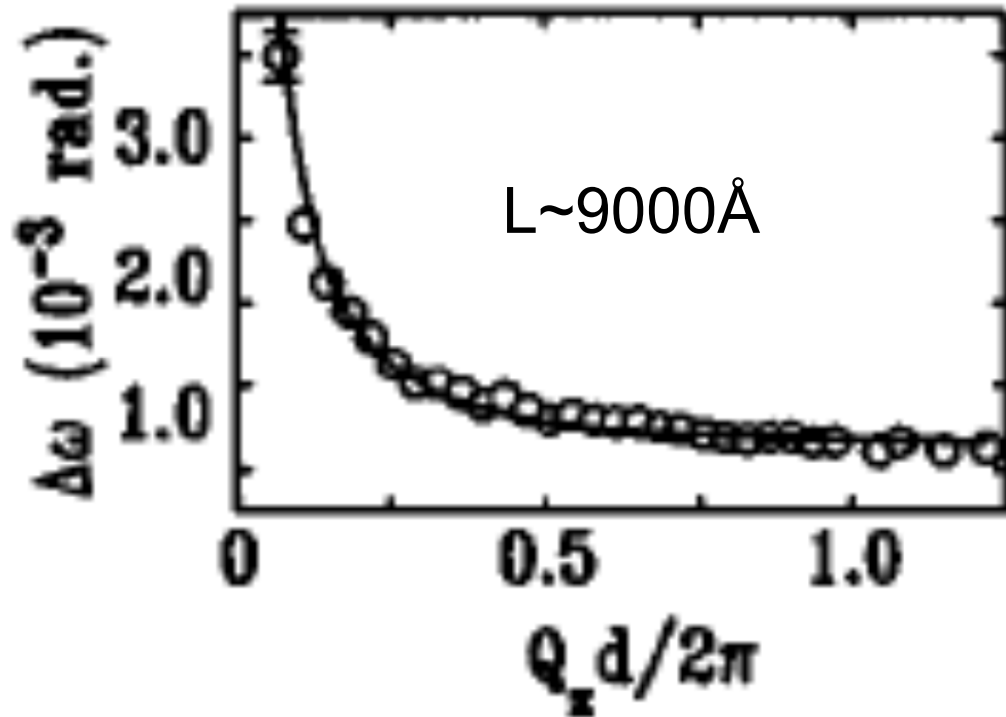
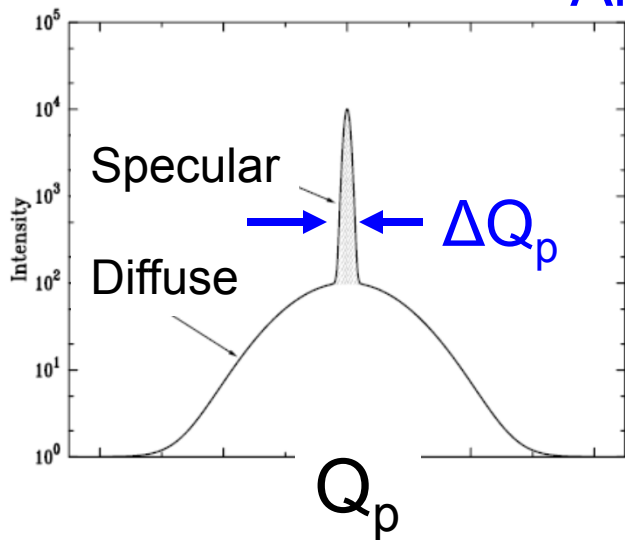
Crystal Truncation Rod Scattering for Specular Reflection from the Ag(111) Surface



Miscut Surfaces



Angular Width of Specular Decreases with Q_z



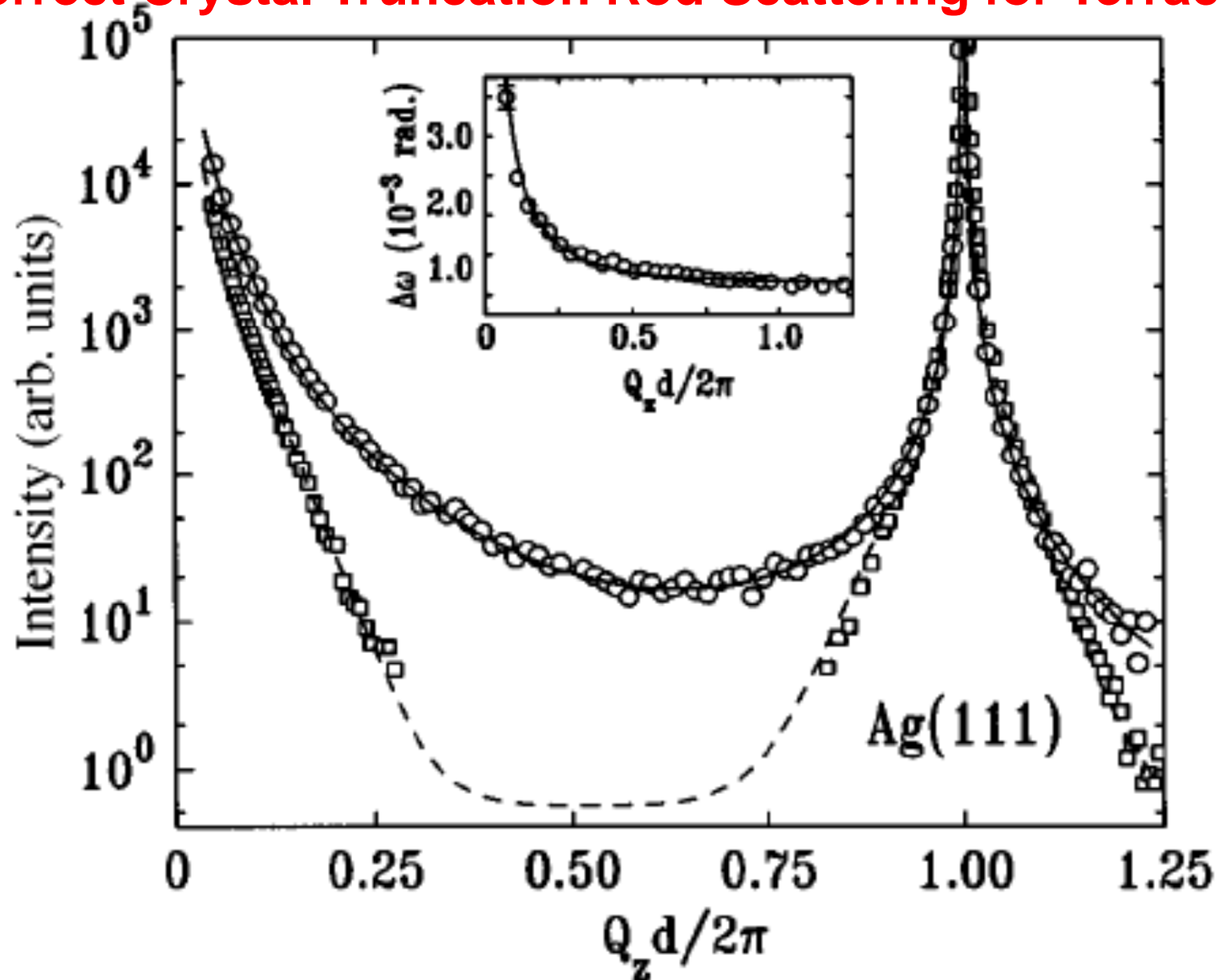
$$\Delta\omega = \frac{\Delta Q_p}{Q_z}$$

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

Can determine terrace size, L

Specular Reflection from the Ag(111) Surface

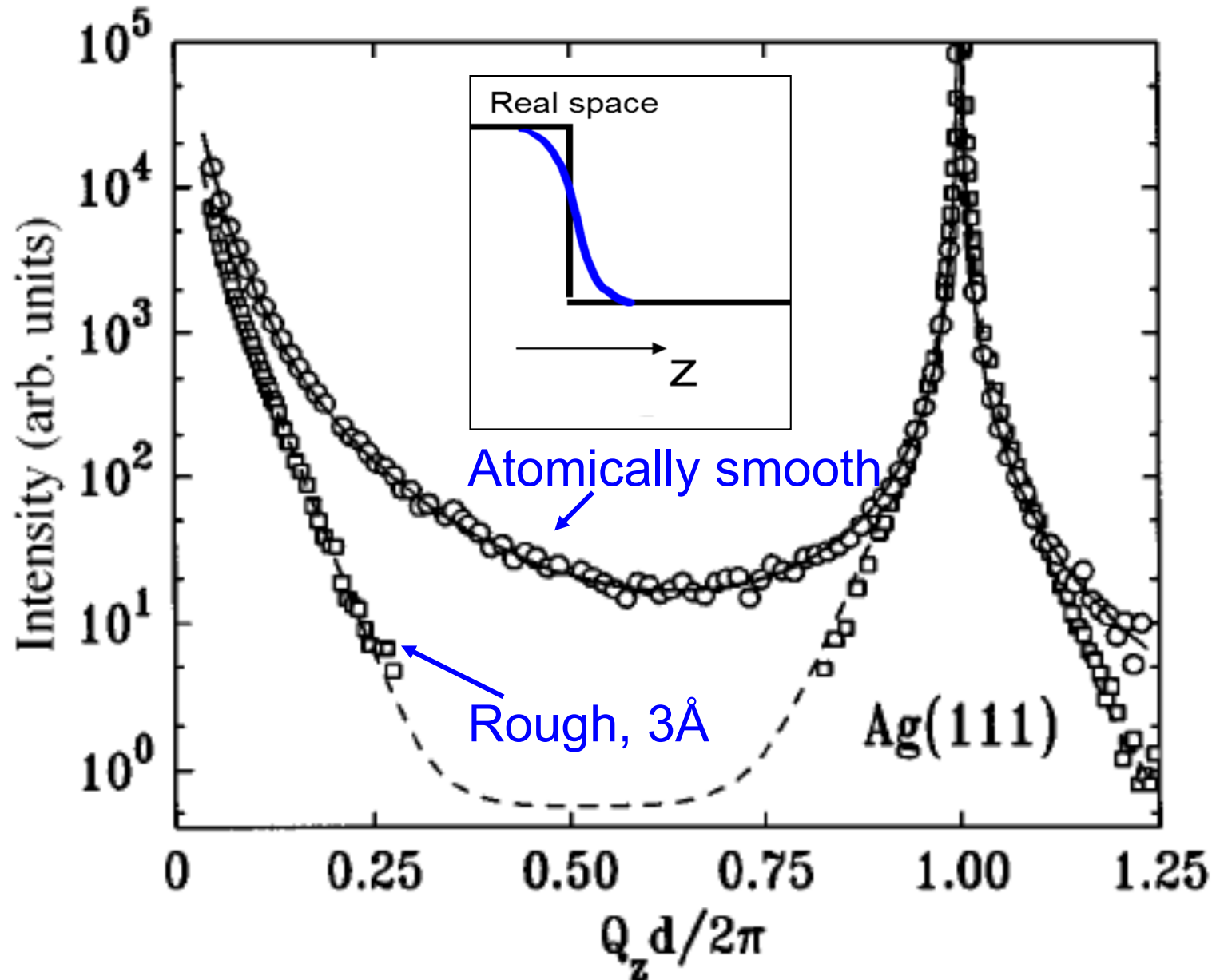
Correct Crystal Truncation Rod Scattering for Terrace Size



The Effect of a Rough Surface



Sharper interface (real space) gives “broader” scattering



Special location along CTR: anti-Bragg

Bragg Position:

$$Q_z c = 2\pi m$$

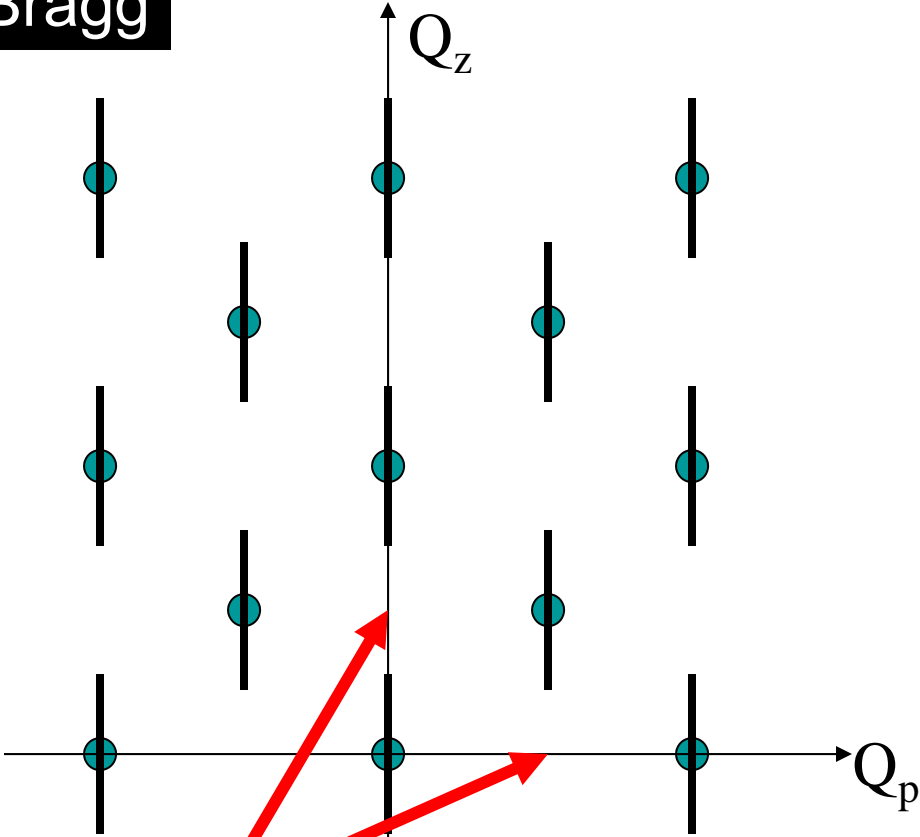
$$I = \left| \sum_{n_z=0}^{N-1} e^{-i2\pi n_z} \right|^2 \rightarrow N^2$$

Anti-Bragg Position:

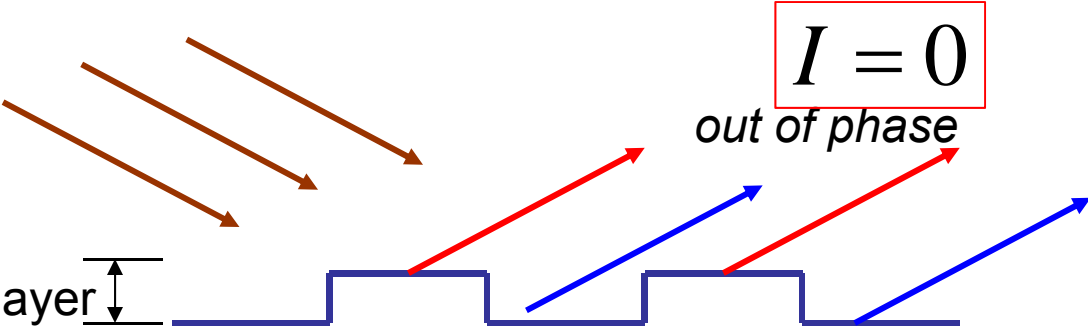
$$Q_z c = \pi m \quad (m \text{ odd})$$

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

For a smooth surface



Anti-Bragg Positions

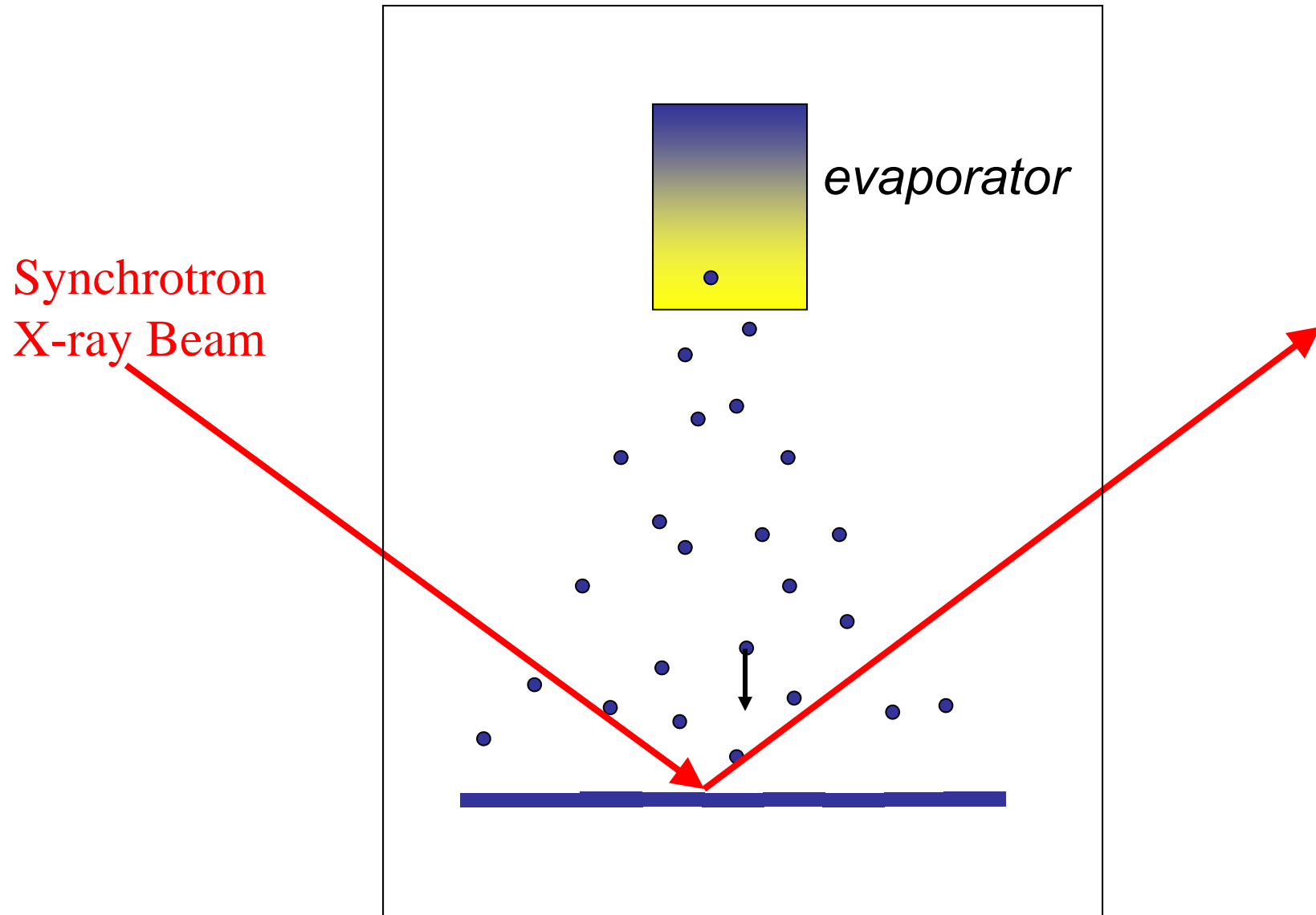


$I = 0$

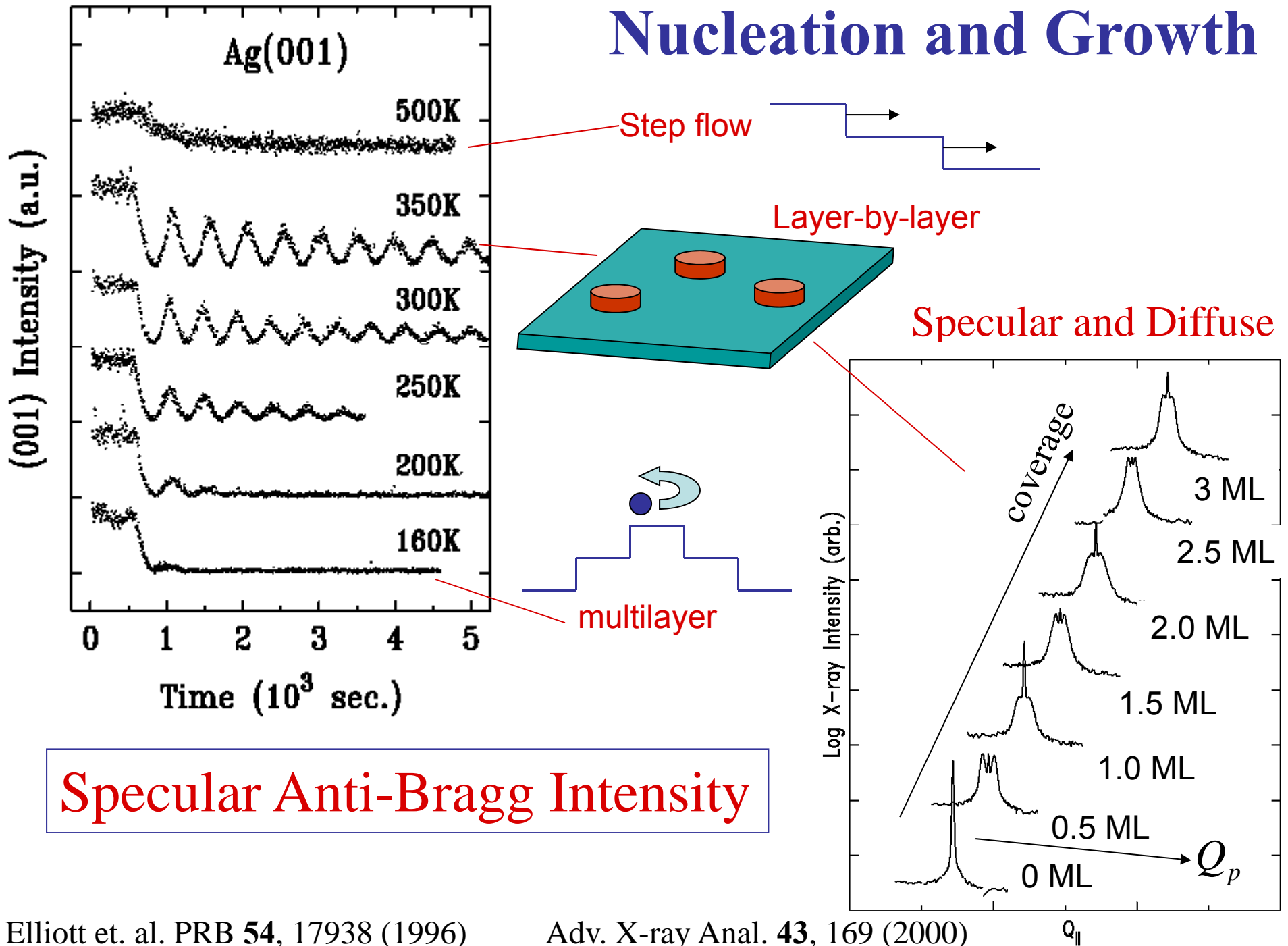
out of phase

1 atomic layer

In situ vapor deposition in UHV



Nucleation and Growth



Specular Anti-Bragg Intensity

Diffuse Scattering

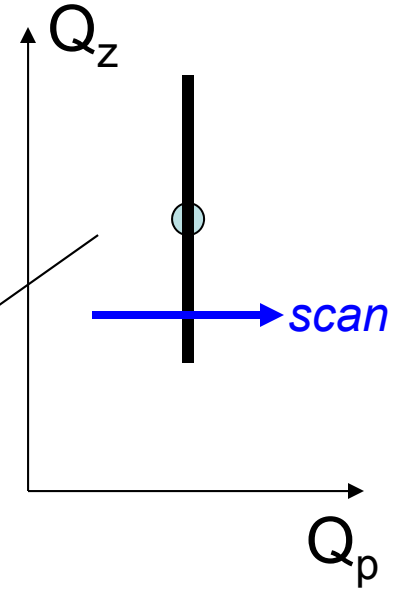
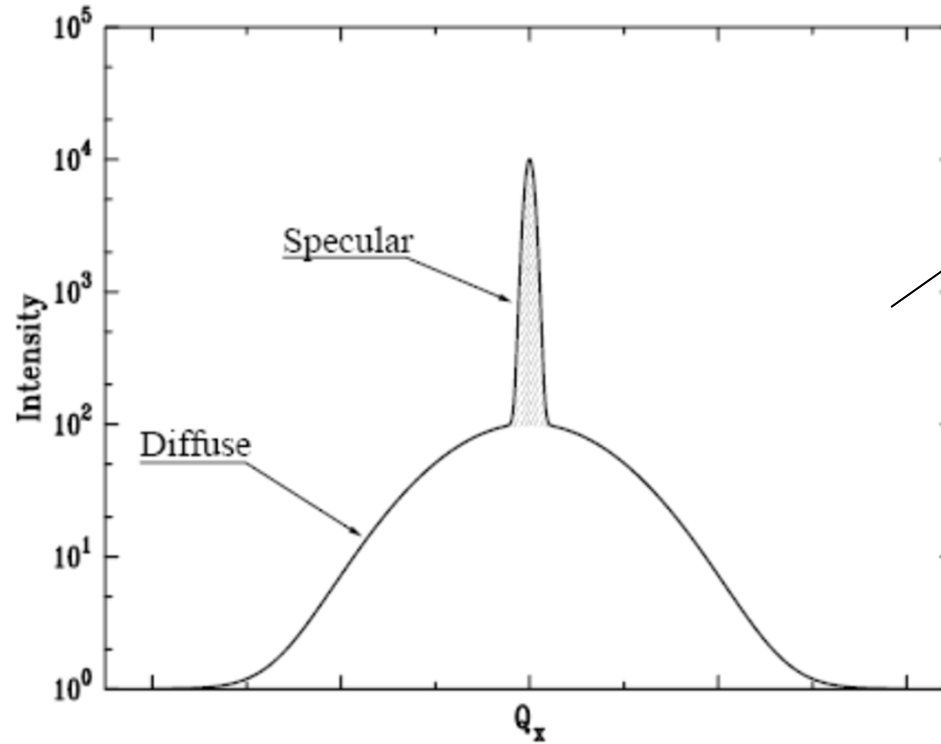
Caused by lateral structure

$$\begin{aligned}
 |A(\vec{Q})|^2 &= \\
 &= |b|^2 \sum_{\vec{R}_p} \sum_{\vec{R}'_j} \\
 &= \frac{N_{irr} |b|^2}{|1 - e^{iQ_z c}|}
 \end{aligned}$$

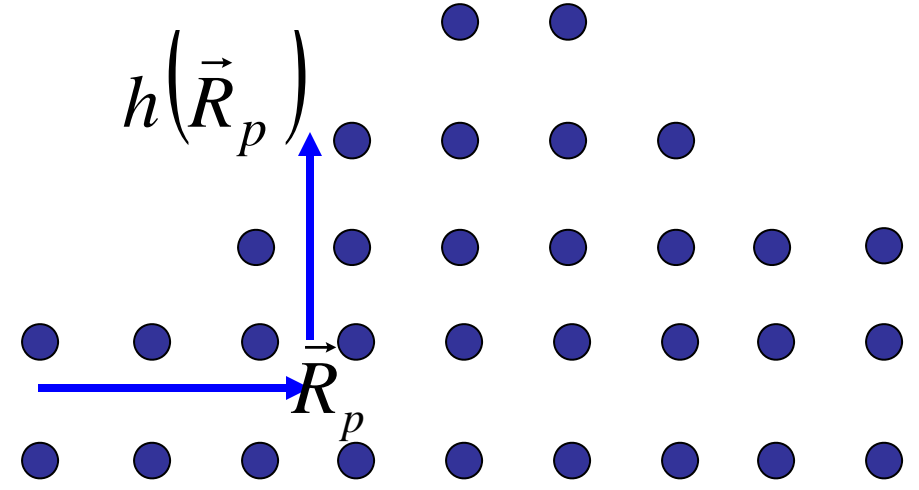
CTR factor

FT of average phase difference due to lateral height-differences

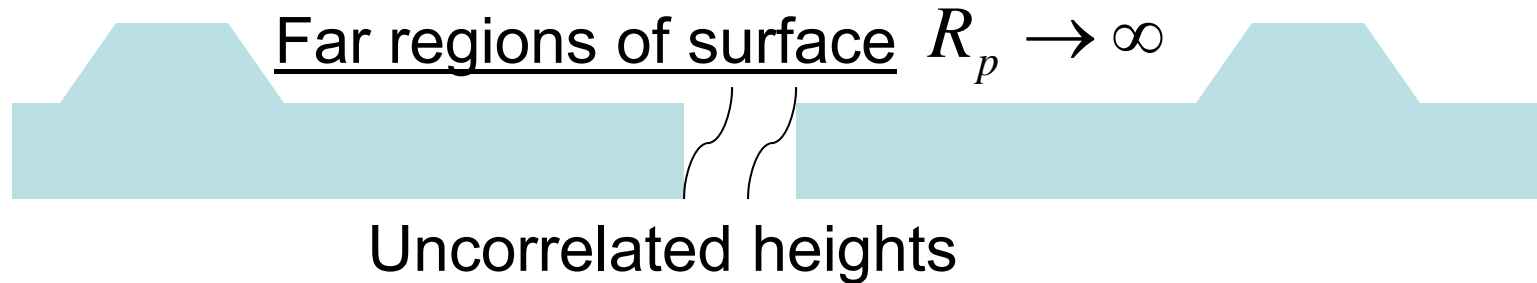
- Neglect lateral boundaries



Q_p dependence
 $\vec{R}'_p = S_T(Q_p)$



Transverse Lineshape



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

Uncorrelated Roughness @ Large Distance Gives Bragg:

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

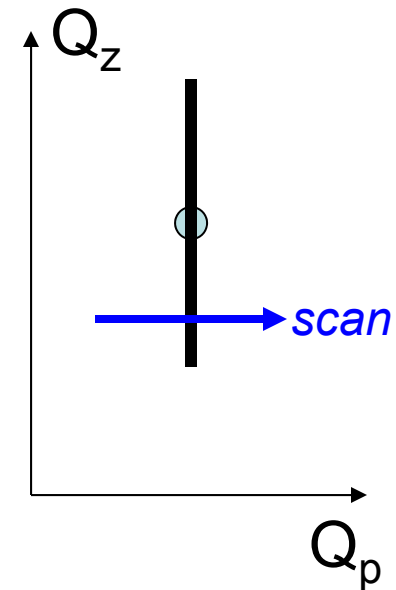
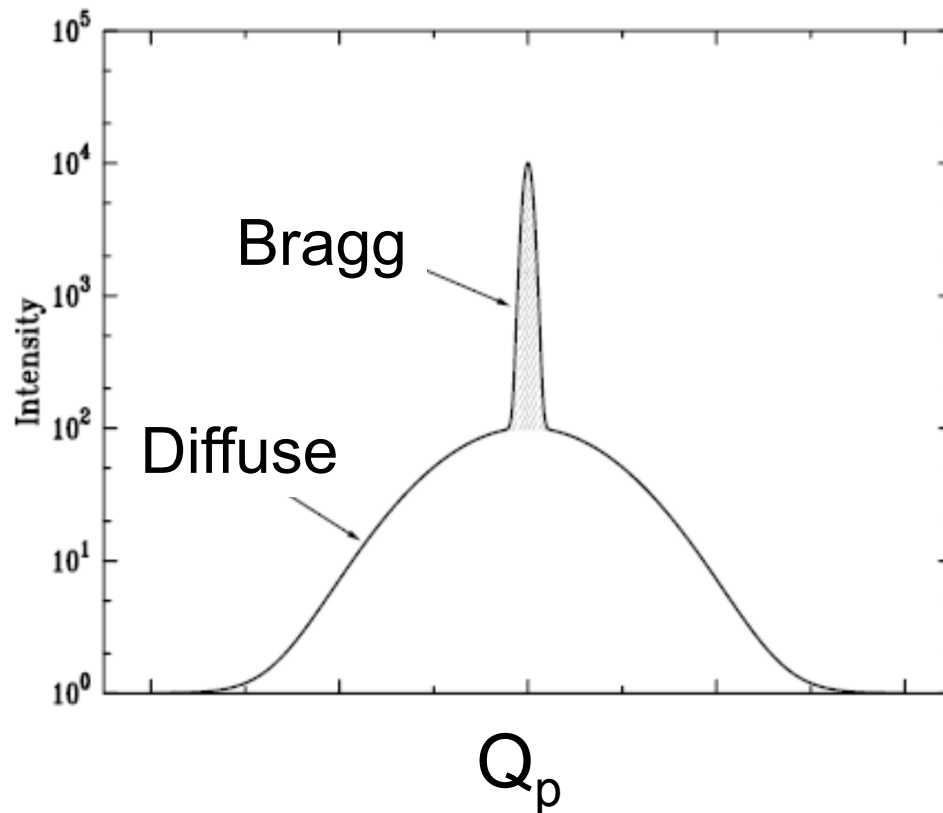
Short-Range Correlations Give Diffuse Scattering:

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

Two Component Line Shape: Bragg + Diffuse

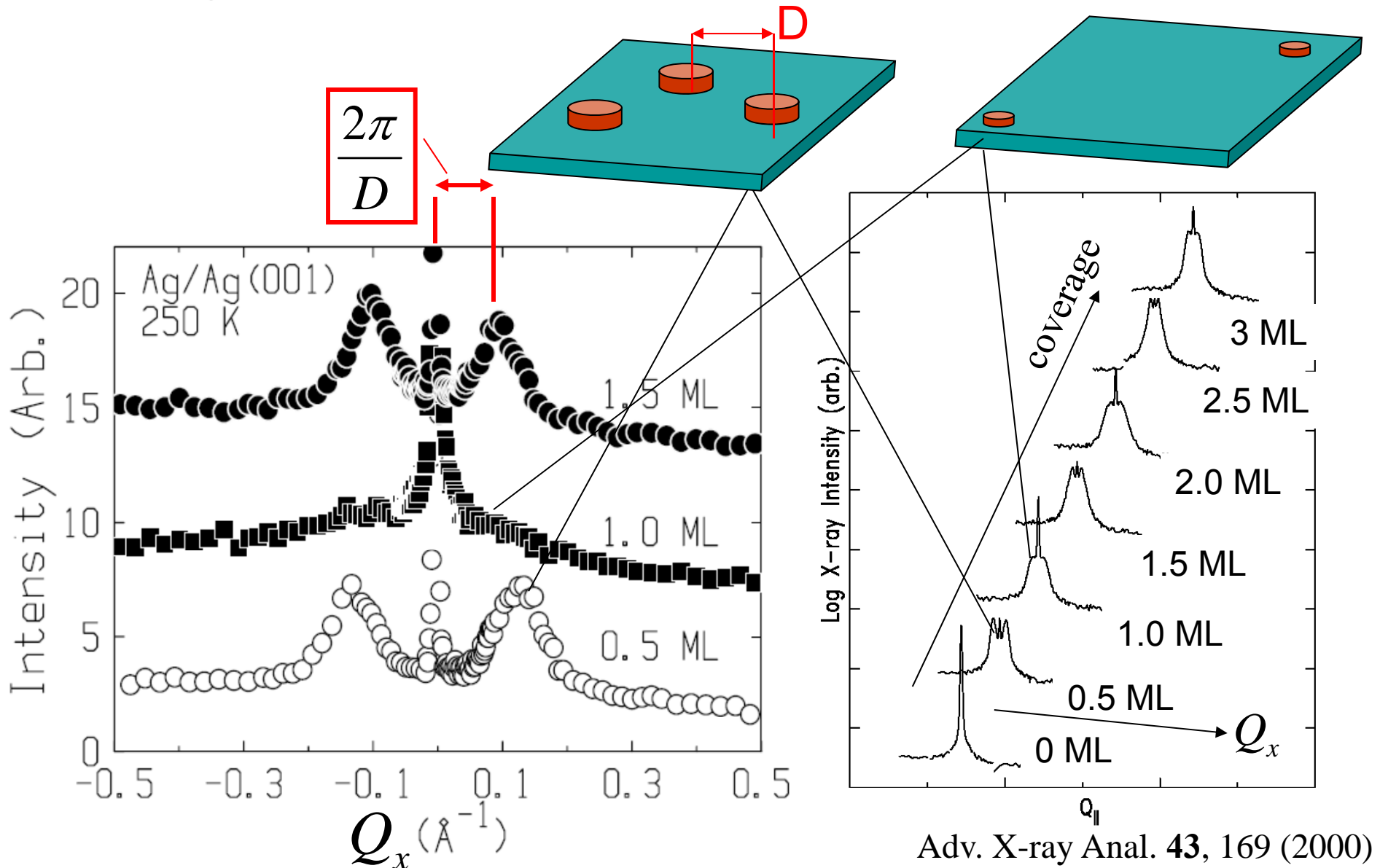
$$S_T(\vec{Q}_p) = S_T^{Bragg}(\vec{Q}_p) + S_T^{Diffuse}(\vec{Q}_p)$$

- Bragg due to laterally uncorrelated disorder at long distances
- Diffuse due to short-range correlations



Layer-by-layer growth

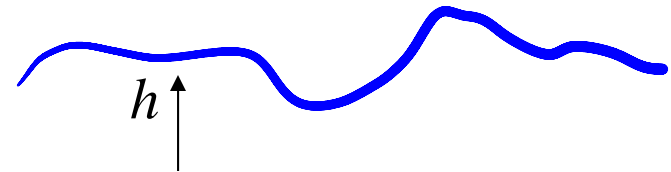
- Specular Bragg Rod: intensity changes with roughness
- Strong inter-island correlations seen in the diffuse



Attenuation of the Bragg Rod and Surface Roughness

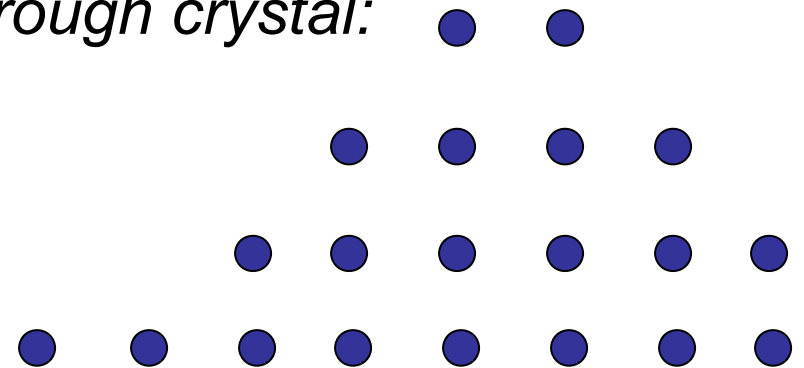
If height fluctuations are Gaussian: σ is rms roughness

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



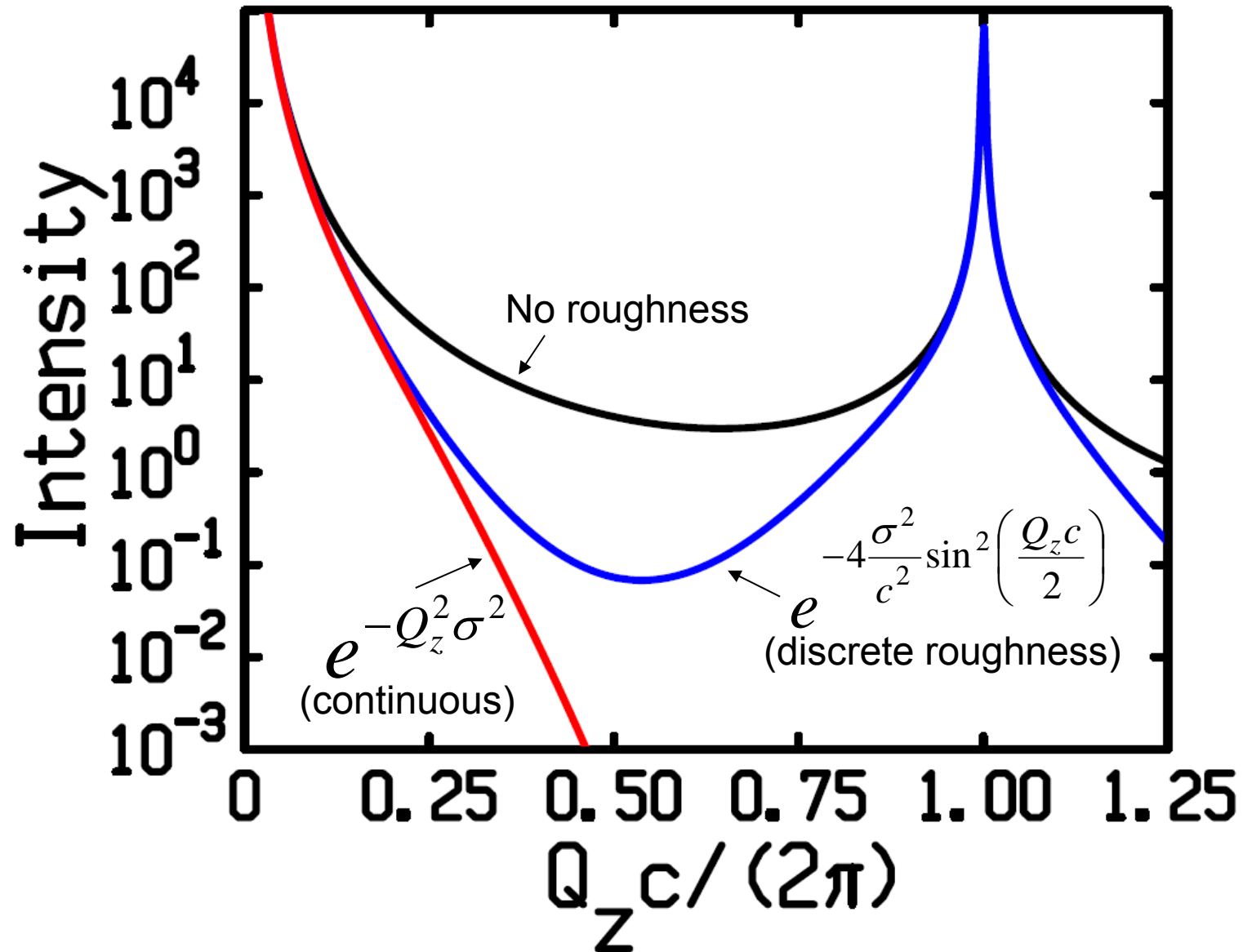
But crystal heights are discrete for a rough crystal:

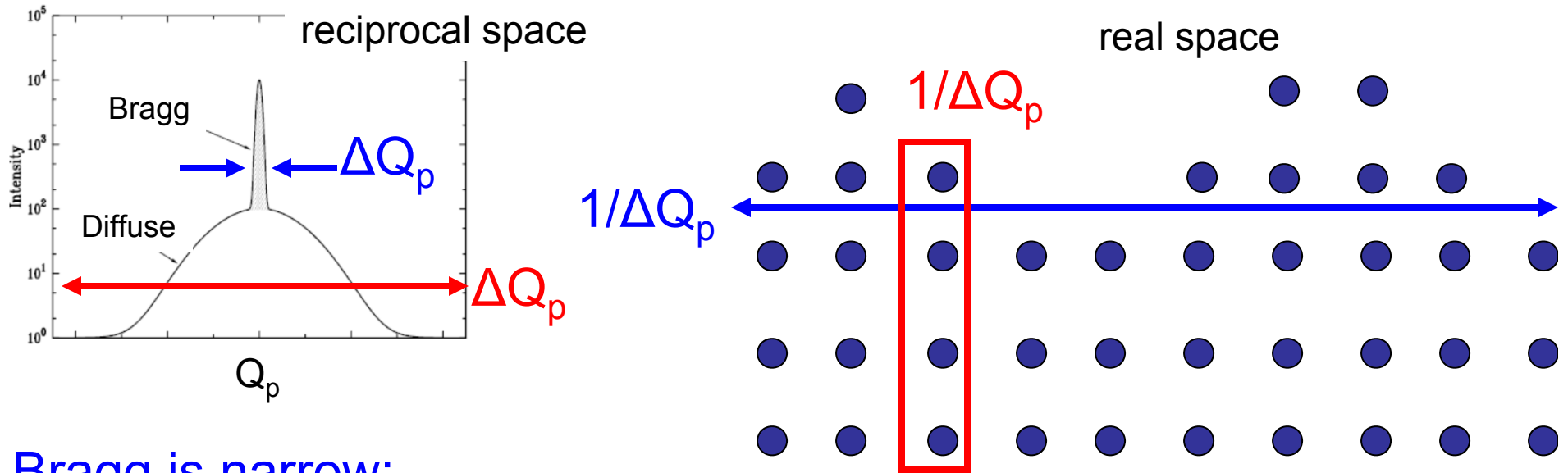
$$\left| \left\langle e^{iQ_z h} \right\rangle \right|^2 \rightarrow e^{-4 \frac{\sigma^2}{c^2} \sin^2 \left(\frac{Q_z c}{2} \right)}$$



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

- Sharper interface (real space) gives broader scattering
- Gaussian roughness does not give translational symmetry





Bragg is narrow:

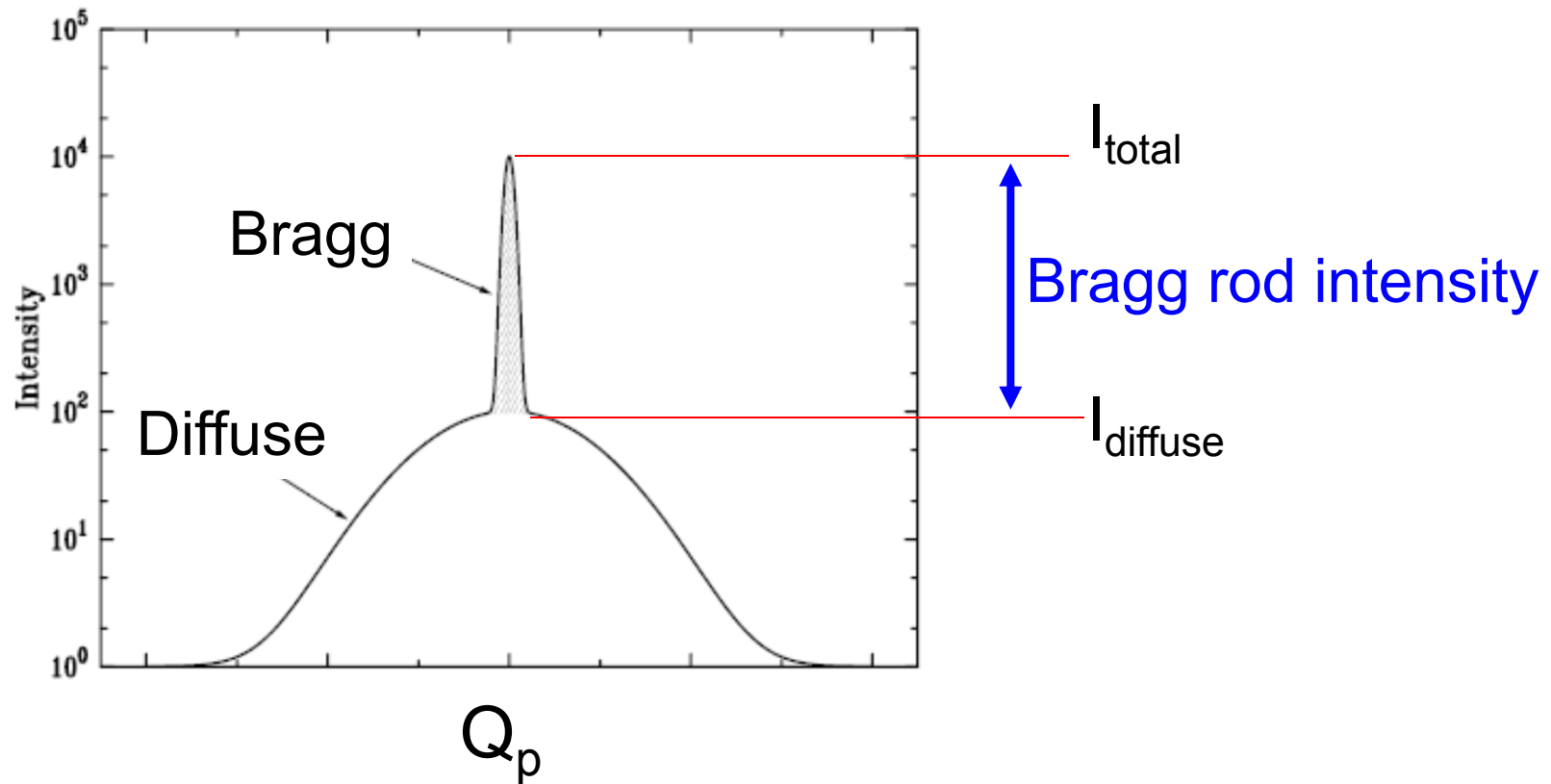
it samples laterally uncorrelated roughness at long distances

$$S^{Bragg}(\vec{Q}) \propto \frac{|b|^2}{|1 - e^{iQ_z c}|^2} e^{-4 \frac{\sigma^2}{c^2} \sin^2\left(\frac{Q_z c}{2}\right)}$$

Transversely-integrated scattering shows no effect of roughness:

$$\iint d^2 Q_p S(\vec{Q}) \propto \frac{|b|^2}{|1 - e^{iQ_z c}|^2} \quad (\text{for 1 interface})$$

In practice, at every Q_z the diffuse must be subtracted from the total intensity to get the Bragg rod intensity:

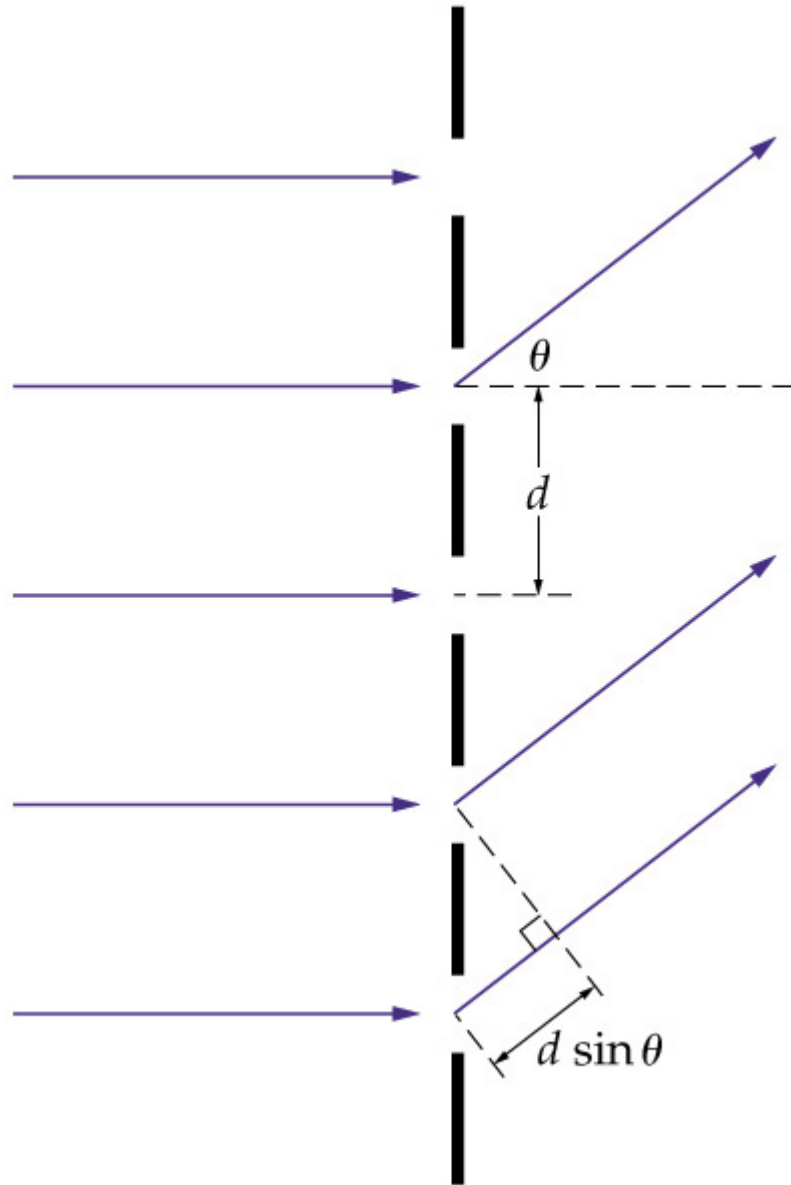


What do we expect from a Thin Film?

1st let's recall Young's slit interference... 

Recall...

N-Slit Interference and Diffraction Gratings



Principle maxima

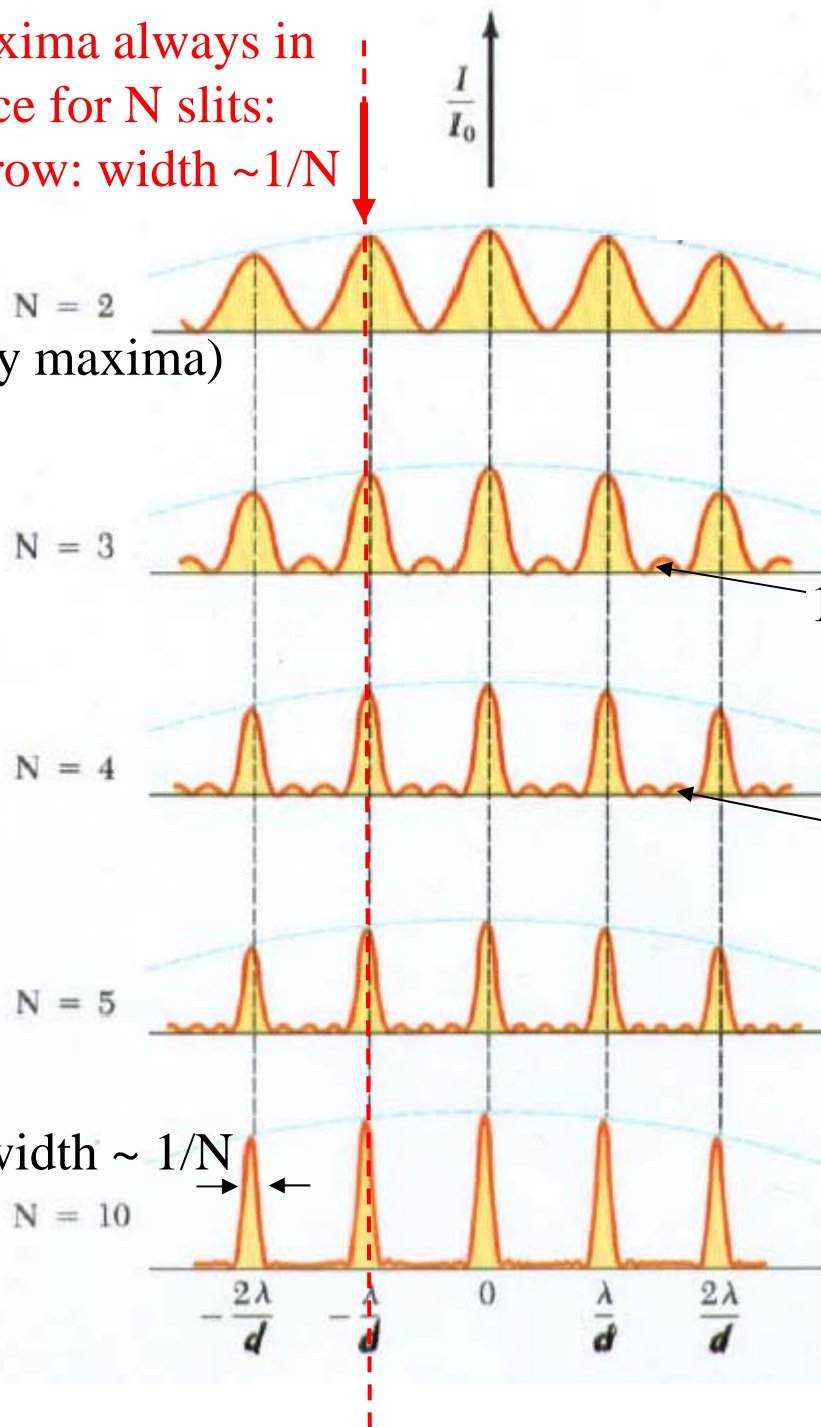
$$d \sin \theta = m\lambda$$

Principle maxima always in the same place for N slits:
But they narrow: width $\sim 1/N$

Principle maxima
 $d \sin \theta = m\lambda$

(N-2 subsidiary maxima)

Double Slit $N = 2$
(no subsidiary maxima)



1 subsidiary maximum

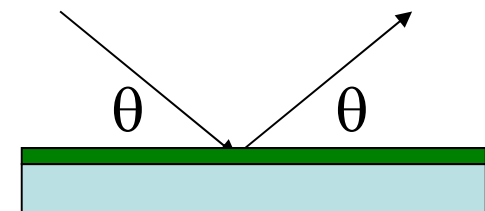
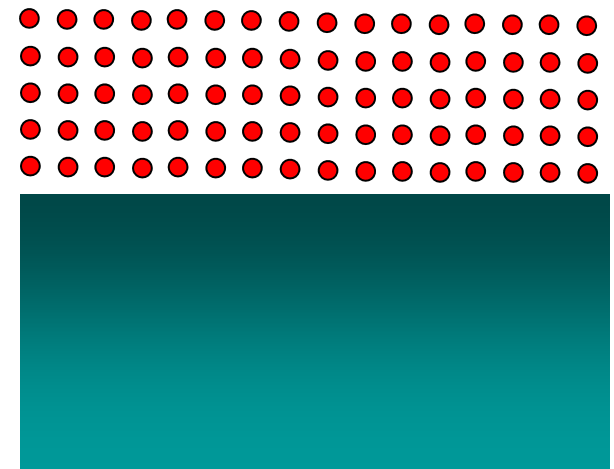
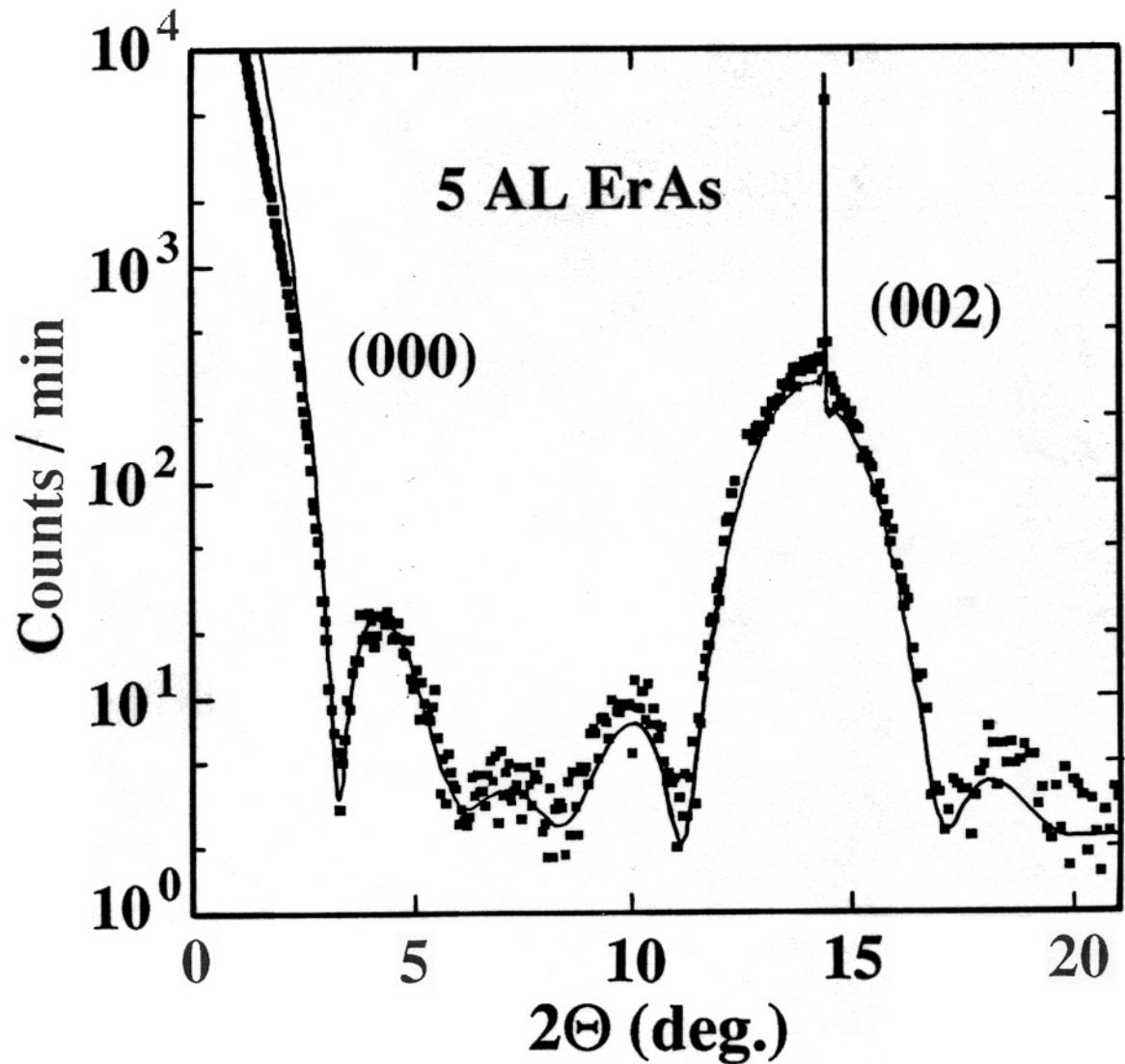
2 subsidiary maximum

width $\sim 1/N$

N large:

- Weak subsidiary maxima
- Sharp principle maxima

“5-slit” interference of x-rays from 5 layers of atoms

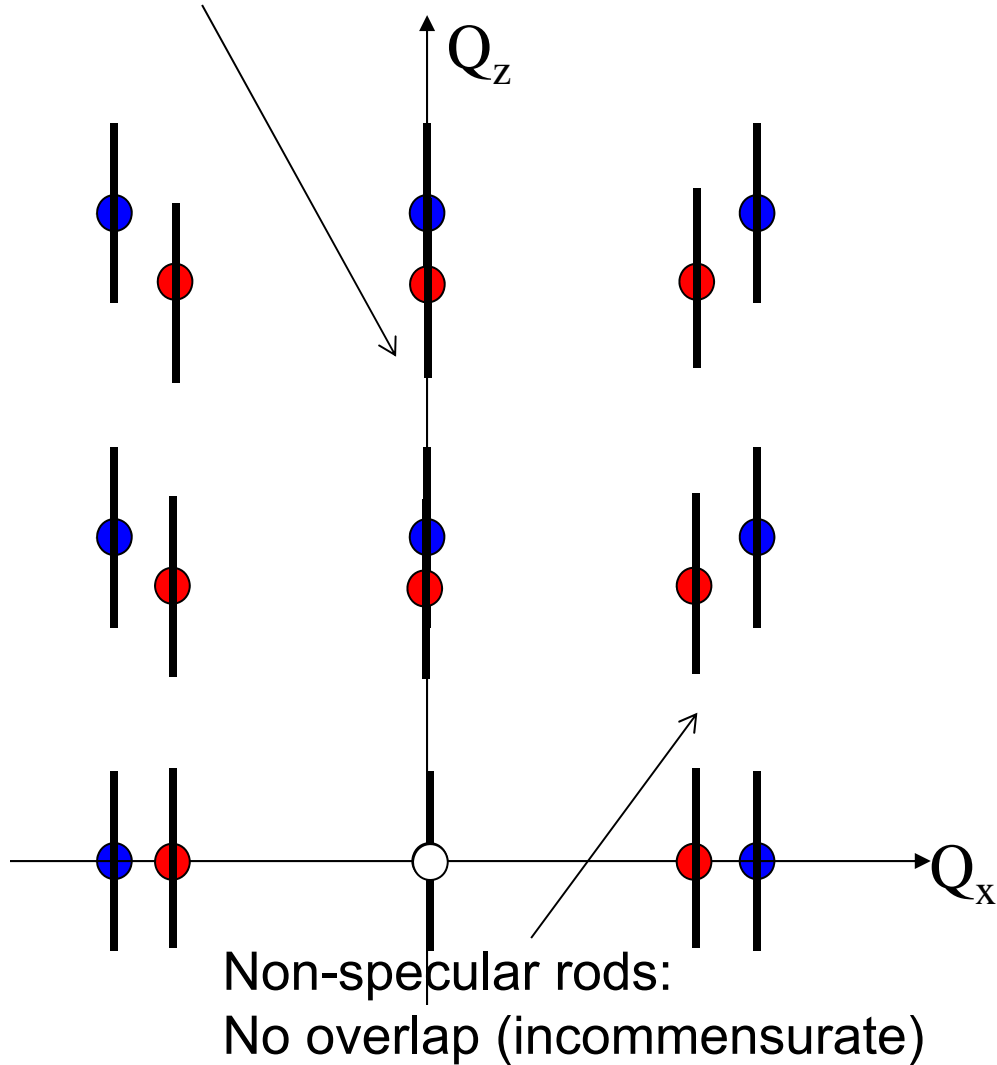


Miceli et al., Appl. Phys. Lett. 62, 2060 (1992)

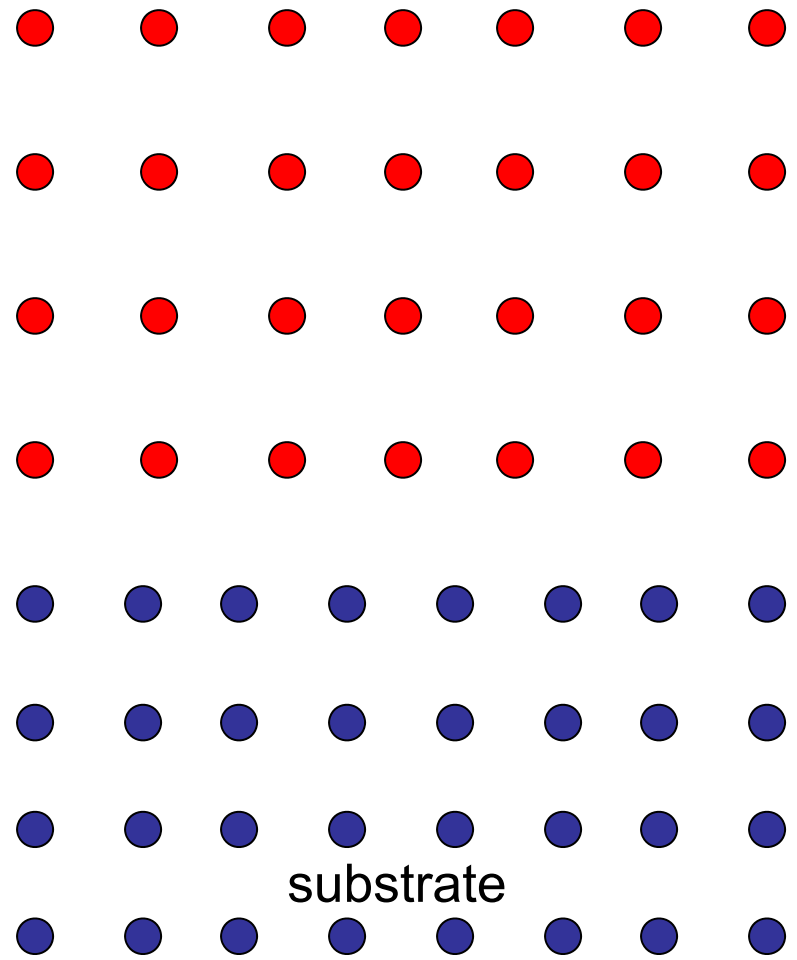
Thin Films

Reciprocal Space

Specular rods overlap

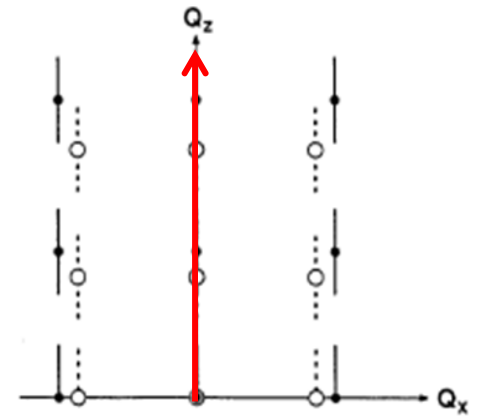
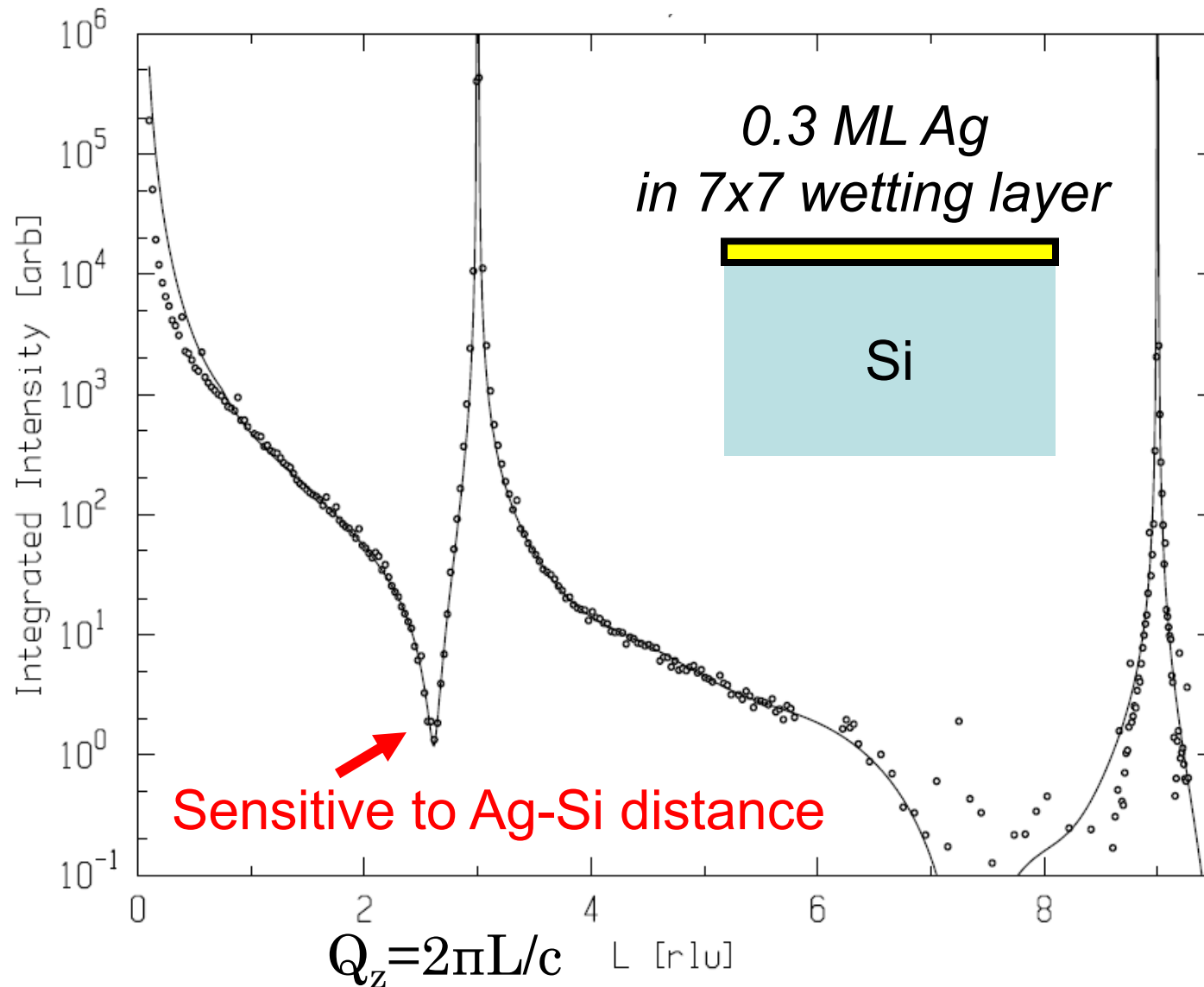


Real Space



Ag/Si(111)7x7

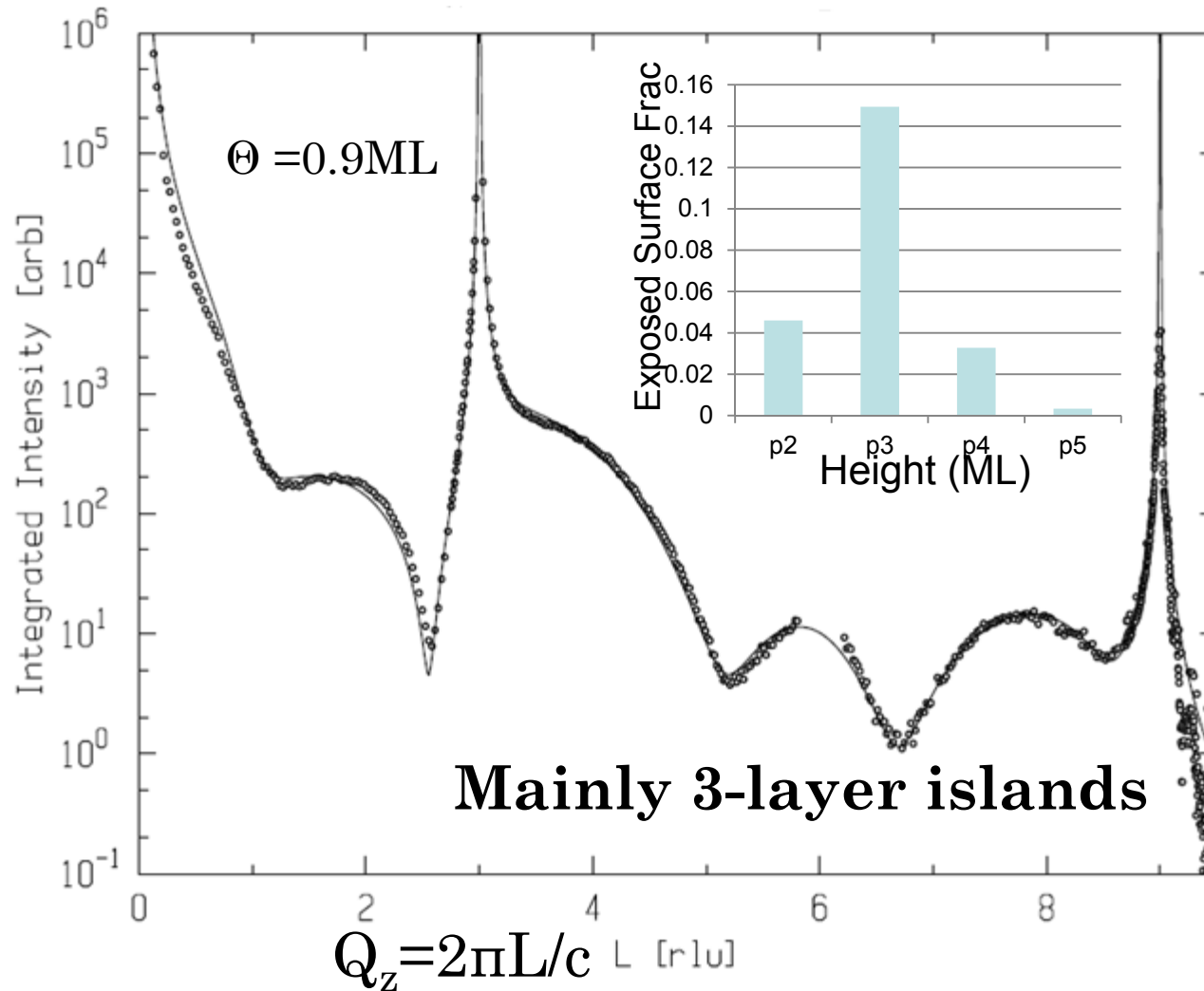
Specular Reflectivity: 0.3ML Ag/Si(111)7x7



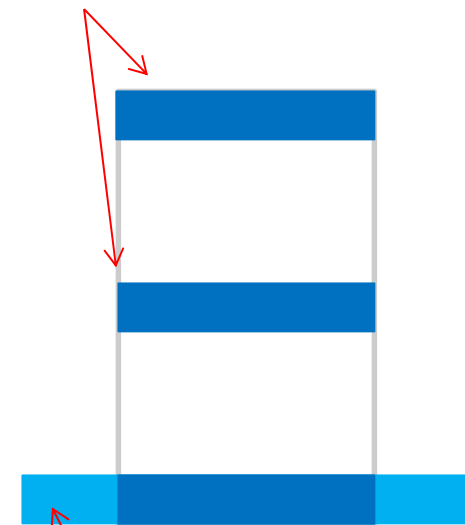
Yiyao Chen et al.

Ag/Si(111)7x7

Specular Reflectivity: 0.9ML Ag/Si(111)7x7



3-layer islands
2ML above wetting layer



Wetting layer

Yiyao Chen et al.

Specular reflectivity cannot easily distinguish between these two cases:

FCC Ag islands on
a Ag 7x7 wetting layer?



Reflectivity = 3 layers
FCC CTR = 2 layers

Si

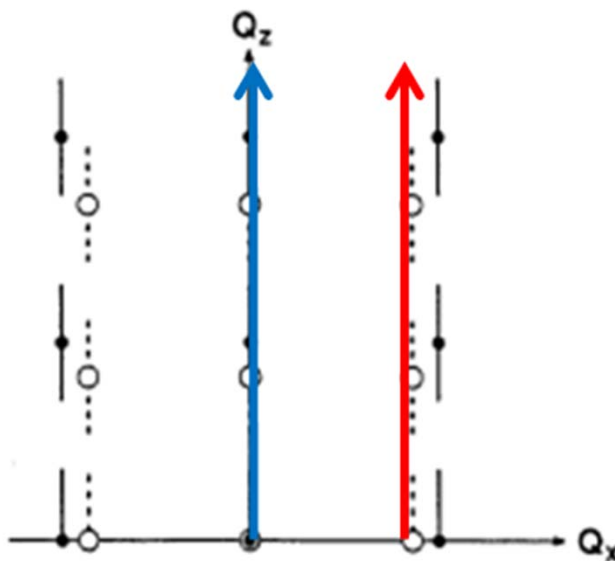
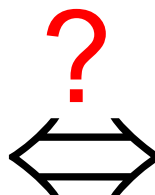
Ag7x7 wetting layer

FCC Ag islands all the way
to the substrate?

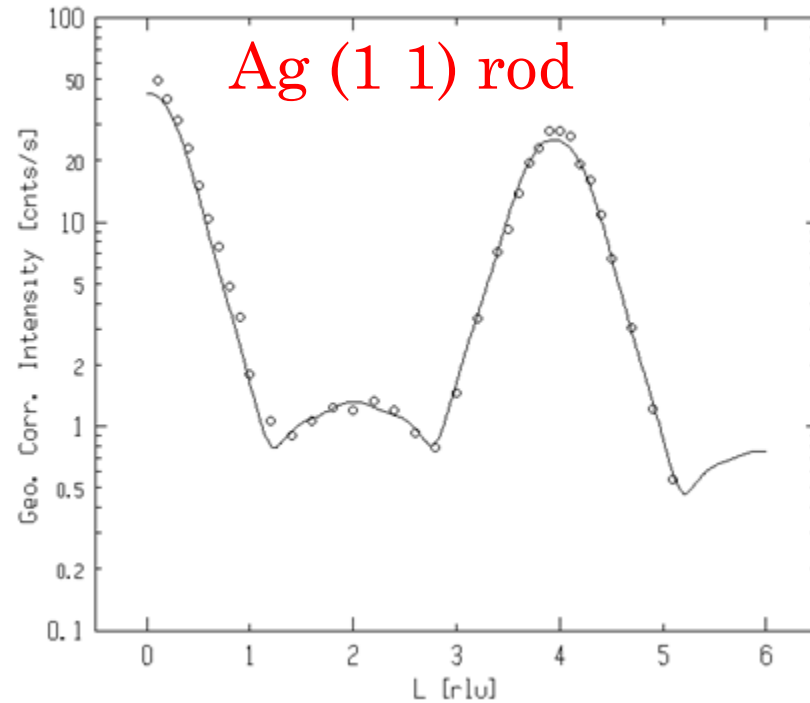
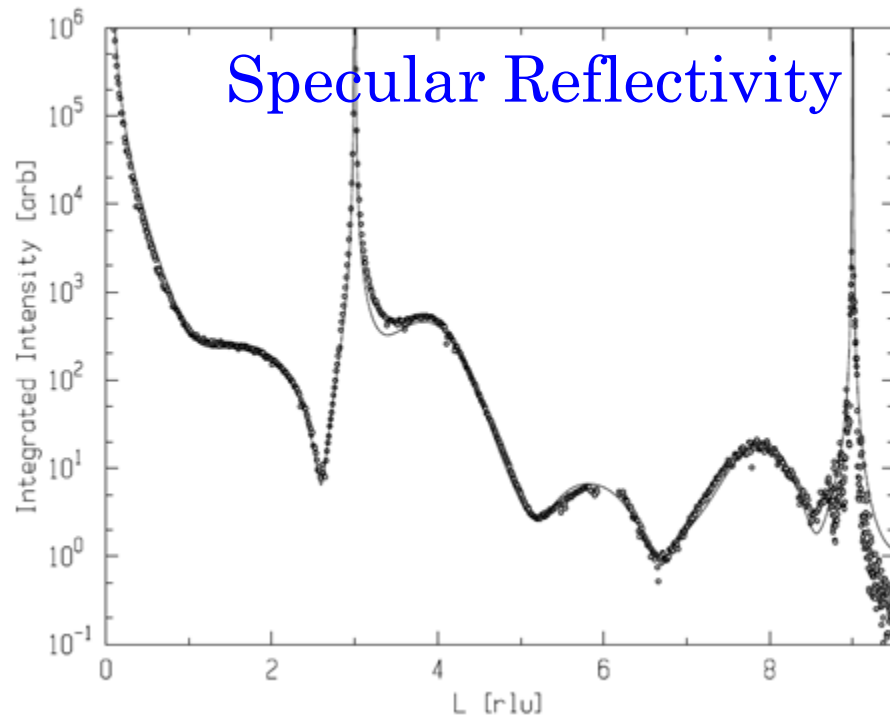


Reflectivity = 3 layers
FCC CTR = 3 layers

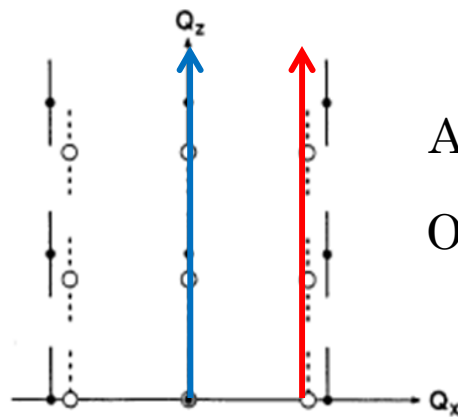
Si



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



↑
 Specular Reflectivity
 Probes Si substrate, Ag
 wetting layer and Ag island



↑
 Ag truncation rod
 Only probes FCC Ag

Yiyao Chen et al.

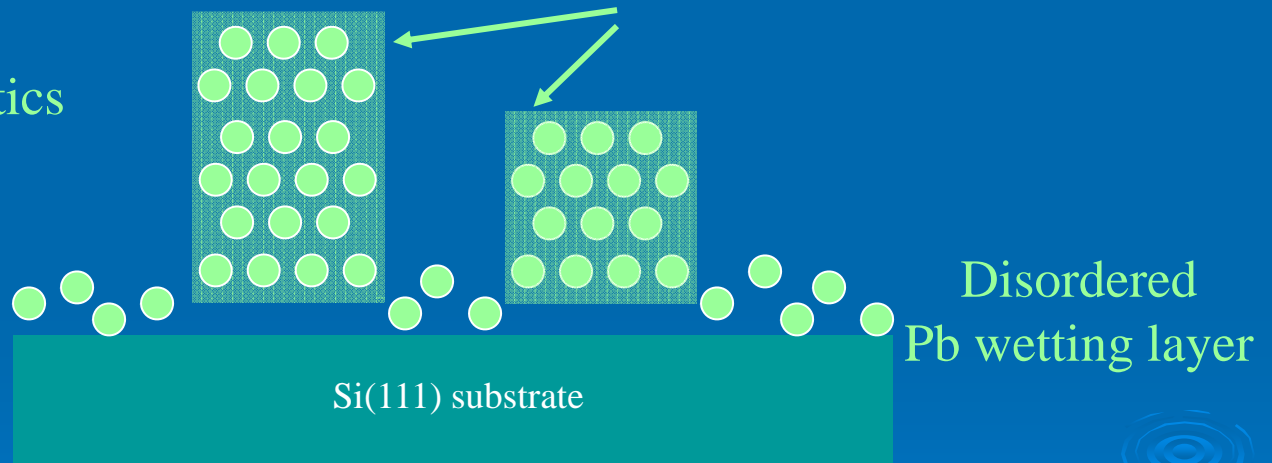
Quantum-Size-Effects: Pb Nanocrystals on Si(111)7x7

Height Selection: “Magic” crystal heights

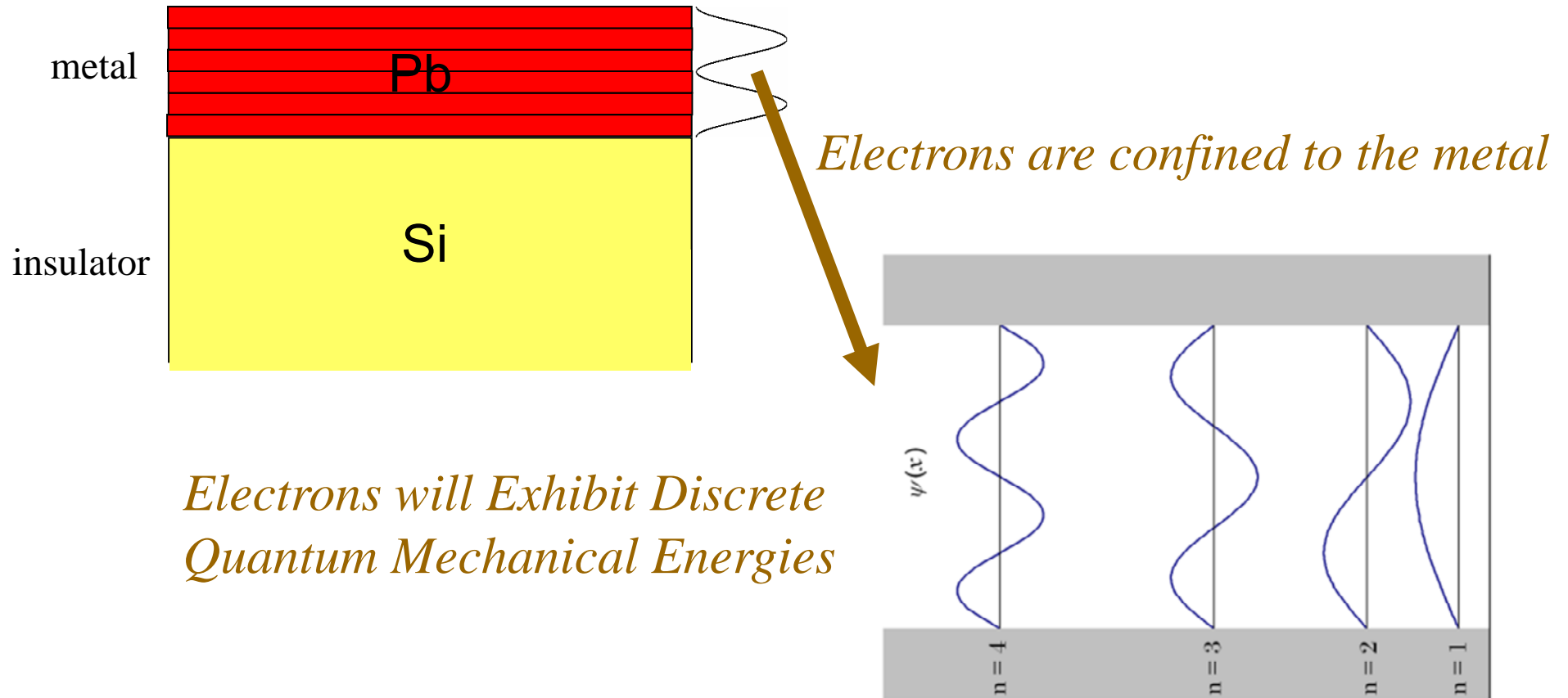
Quantum Mechanics Influences Nanocrystal Growth

Discoveries:

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



Electrons in a “box”



F. K. Schulte, Surf. Sci. **55**, 427 (1976)
P. J. Feibelman, PRB **27**, 1991 (1983)

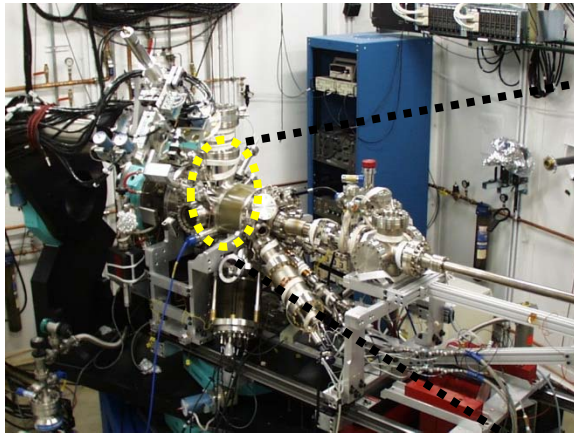
Rain Drops On Your Winshield



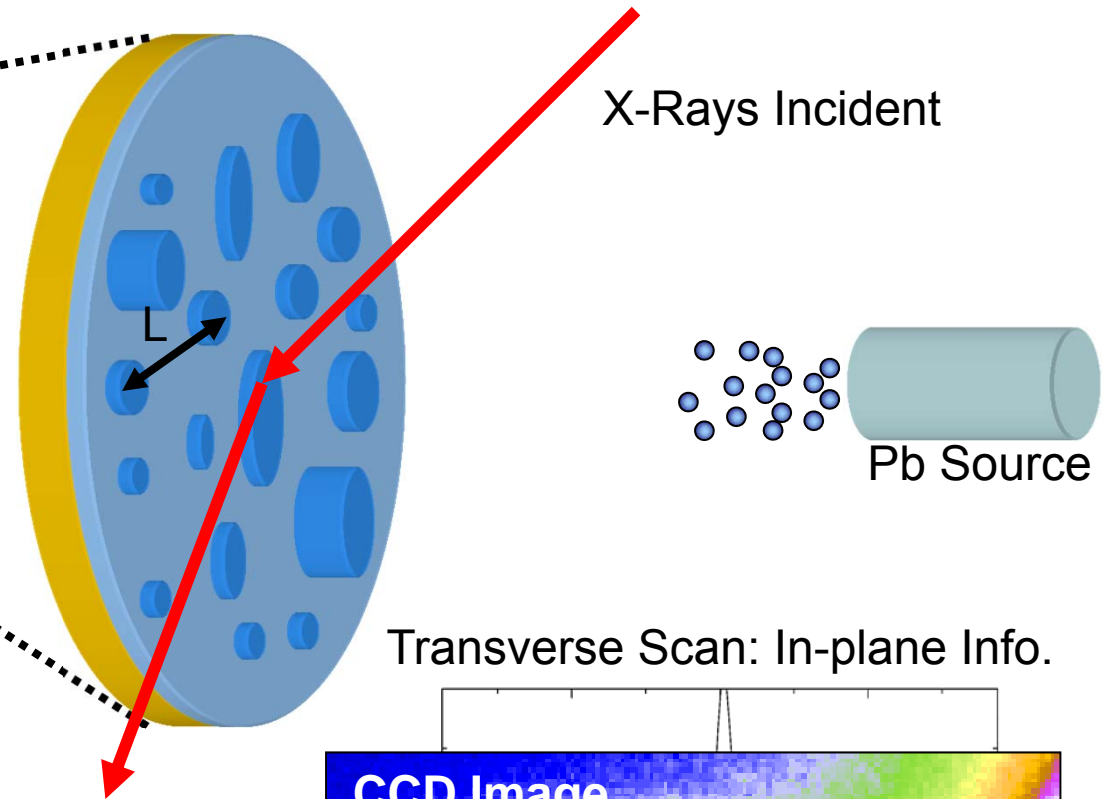
Coarsening



Kinetics: In Situ Surface X-ray Scattering



Surface Chamber
Advanced Photon Source

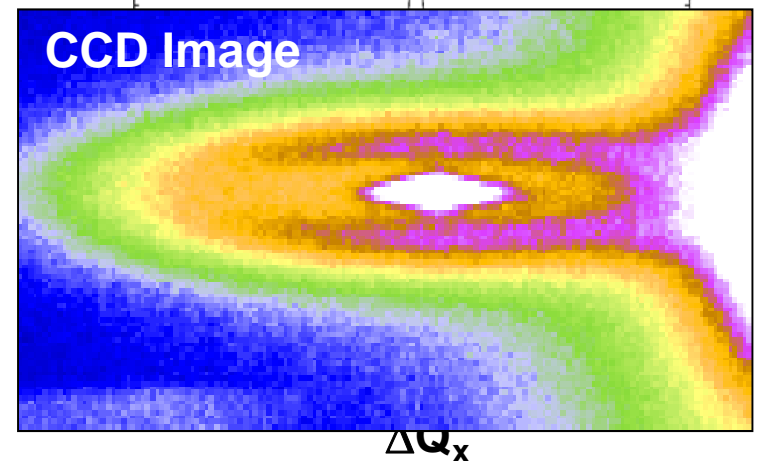


Mean island separation, $\langle L \rangle$:

$$\text{Experiment: } \Delta n = \frac{2\pi}{\langle L \rangle}$$

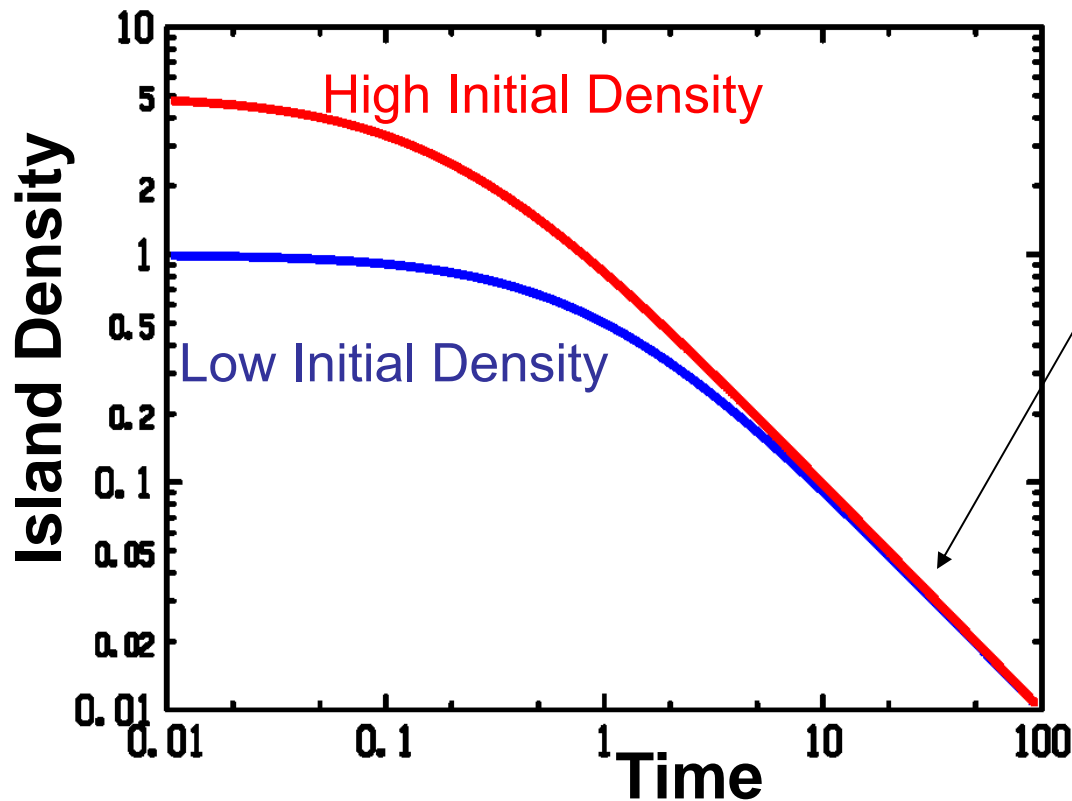
- Deposit Pb (1.2 to 2 ml) at 208K
- Island Density: Measure the island density vs time

$$(\text{flux off}) \propto \overline{\langle L \rangle^2}$$



Classical Coarsening: Ostwald Ripening

$$n(t) = n_0 \left(1 + \frac{t}{\tau} \right)^{-\beta} \quad \beta = \frac{2}{(m+2)}, m = 0, 1, 2$$



Long time: independent of initial conditions

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

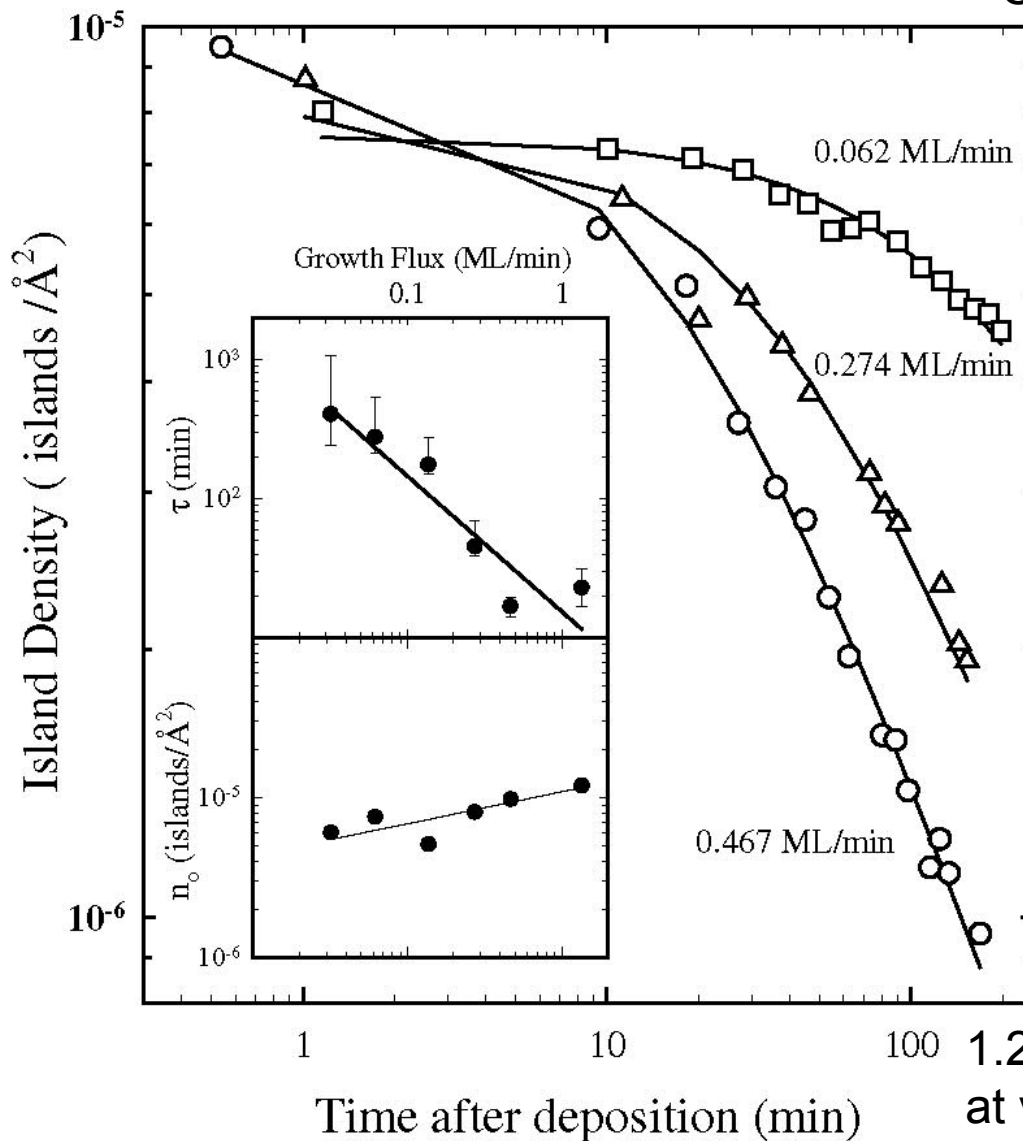
$$\tau \propto n_0^{-\frac{1}{\beta}}$$

Relaxation time depends only on the initial density

Pb Nanocrystal Coarsening

...does **not** conform to the classical picture!

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



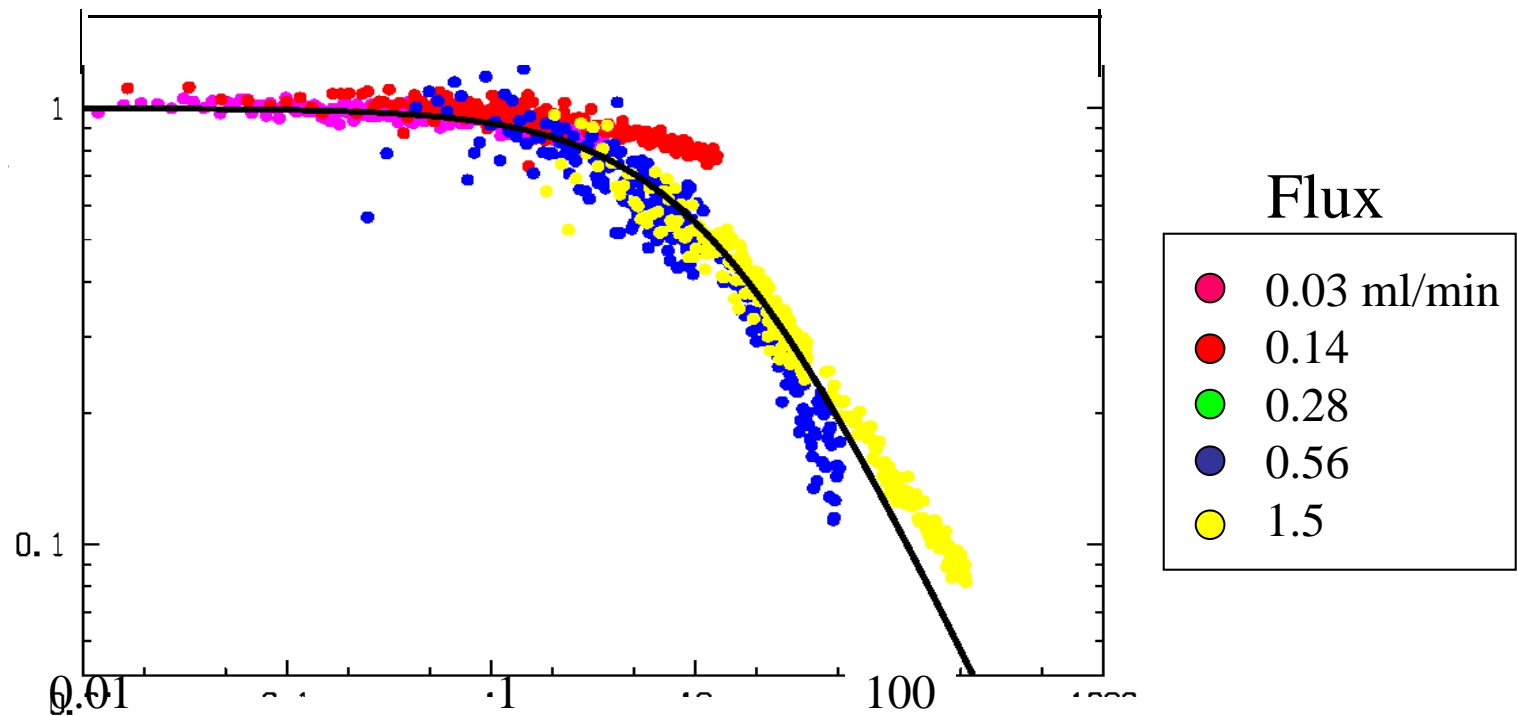
- Island densities do not approach each other at long times:
QSE ⇒ Non-Oswald
Breakdown of Classical Coarsening

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

- Anomalously fast relaxation
~1000x faster than expected!
⇒ allows equilibrium!

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

Reciprocal Space is Superb for Obtaining Good Statistics of Distributions



Equivalent ML Time = $t * F$

Summary

- 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