Surface Sensitive X-ray Scattering

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Introduction
- Concepts of surfaces
- Scattering (Born approximation)

Crystal Truncation Rods
- The basic idea
- How to calculate
- Examples

Reflectivity
- In Born approximation
- Exact formalism (Fresnel)
- Examples

Grazing Incidence Diffraction
- The basic idea
- Penetration depth
- Example

Grazing Incidence Diffraction (GID) **The basic idea**

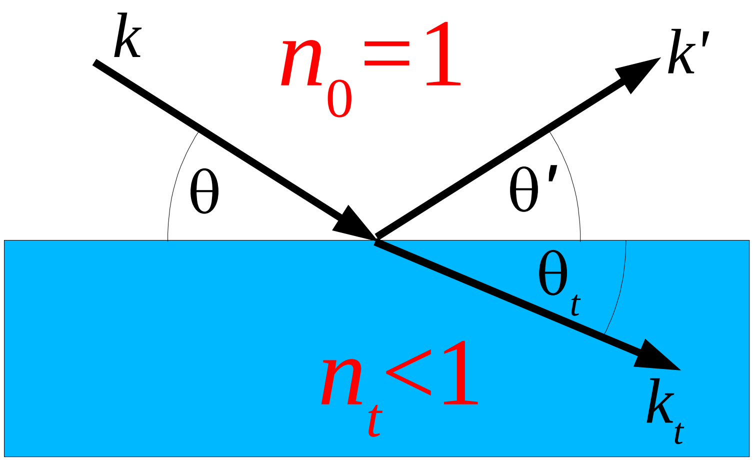
Mean value of the refractive index:

$$|n_t| = |1-\delta+i\beta| < 1$$

⇒ total external reflection

⇒ critical angle α_c

$$\alpha_c \approx \sqrt{2\delta}$$



$\theta > \alpha_c$

- some x-rays penetrate the sample
- some x-rays are reflected (Fresnel)

transmitted amplitude $t_f = \dfrac{2k_z}{k_z + k_{t,z}}$

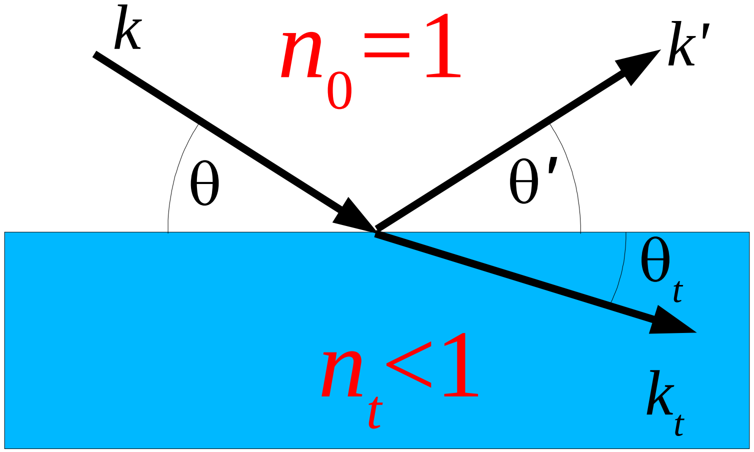
reflected amplitude $r_f = \dfrac{k_z - k_{t,z}}{k_z + k_{t,z}}$

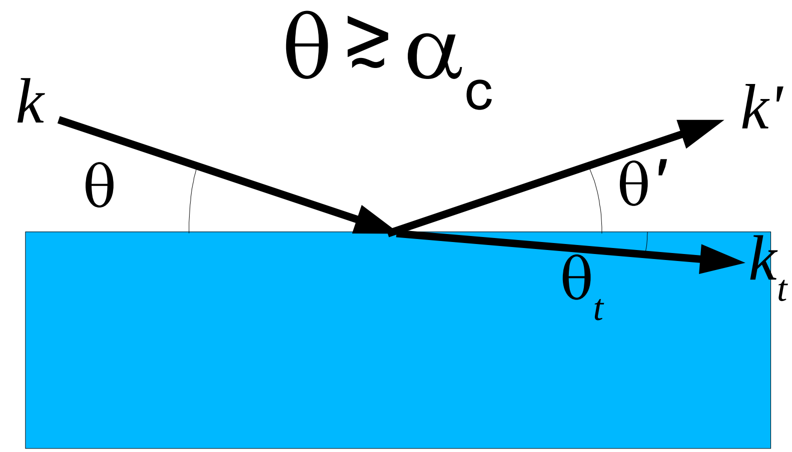
with

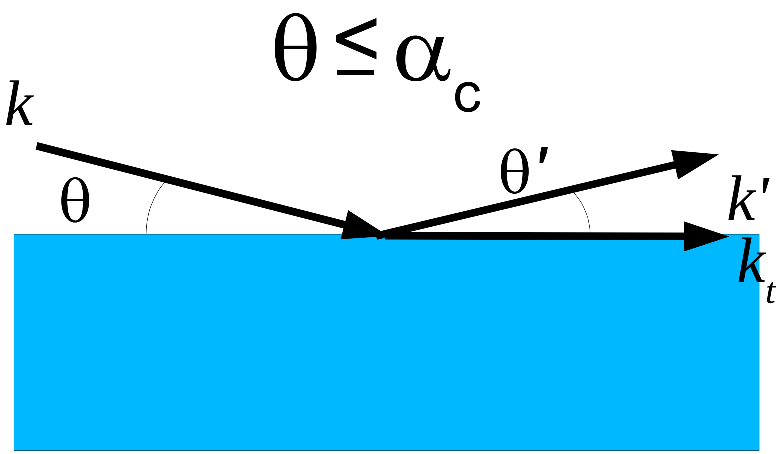
$$k_z = k\sin\theta$$

$$k_{t,z} = k_t \sin(\theta_t) = k\sqrt{n_t^2 - \cos^2\theta}$$

$$k = 2\pi/\lambda$$







Evanescent Wave for $\theta \leq \alpha_c$

- real part of $k_{t,z}$ is zero
- imaginary part still exists with finity penetration depth (see below)

$$k_{t,z}=k\sqrt{n_t^2-\cos^2(\theta)}=k\sqrt{(1-\delta+i\beta)^2-\cos^2(\theta)}\approx k\sqrt{1-2\delta+2i\beta-(1-\sin^2\theta)}$$

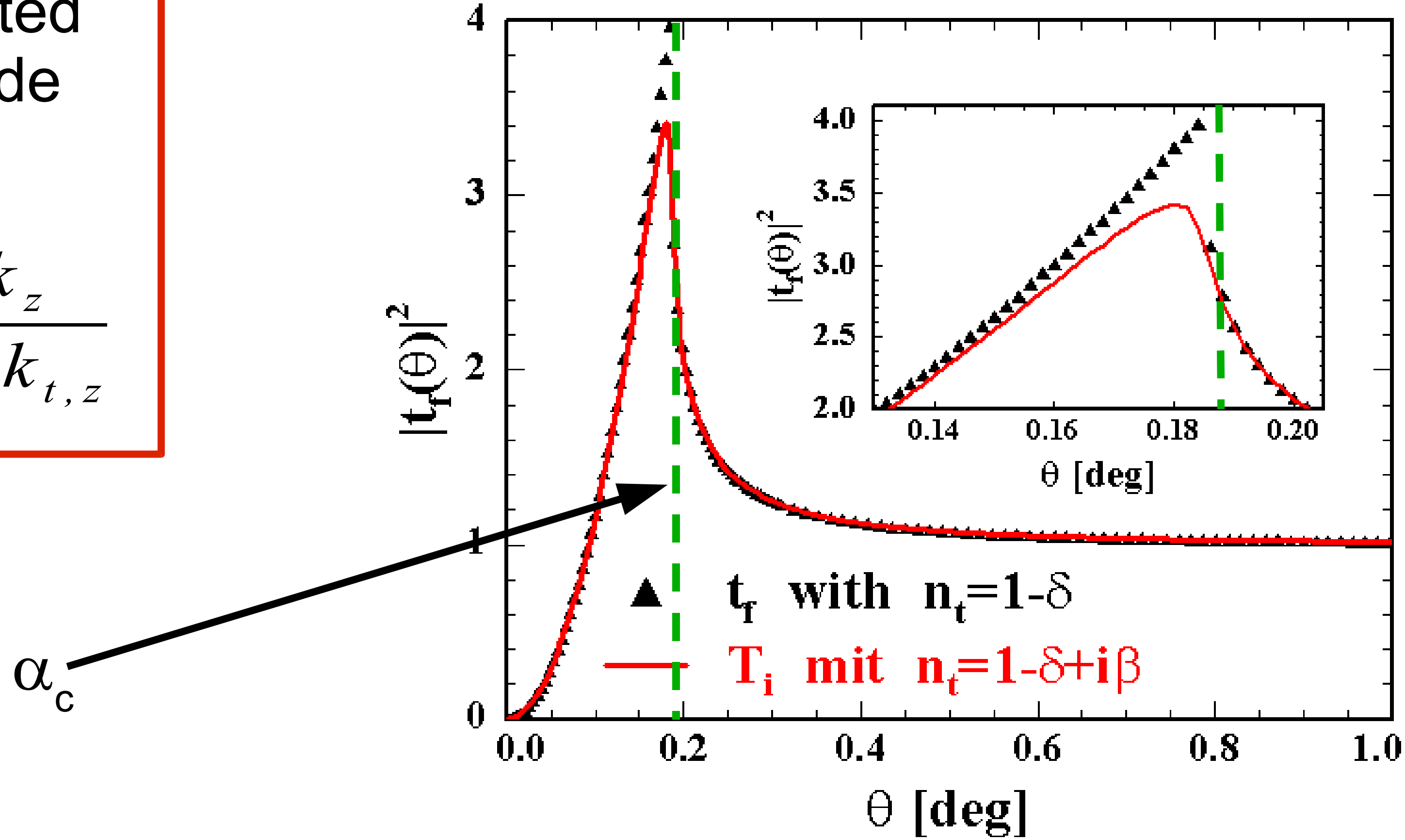
$$\approx k\sqrt{1-2\delta+2i\beta-1+\theta^2}\approx k\sqrt{\theta^2-2\delta+2i\beta}=k\sqrt{\theta^2-\alpha_c^2+2i\beta}=k_{t,z}$$

for small θ and δ and β

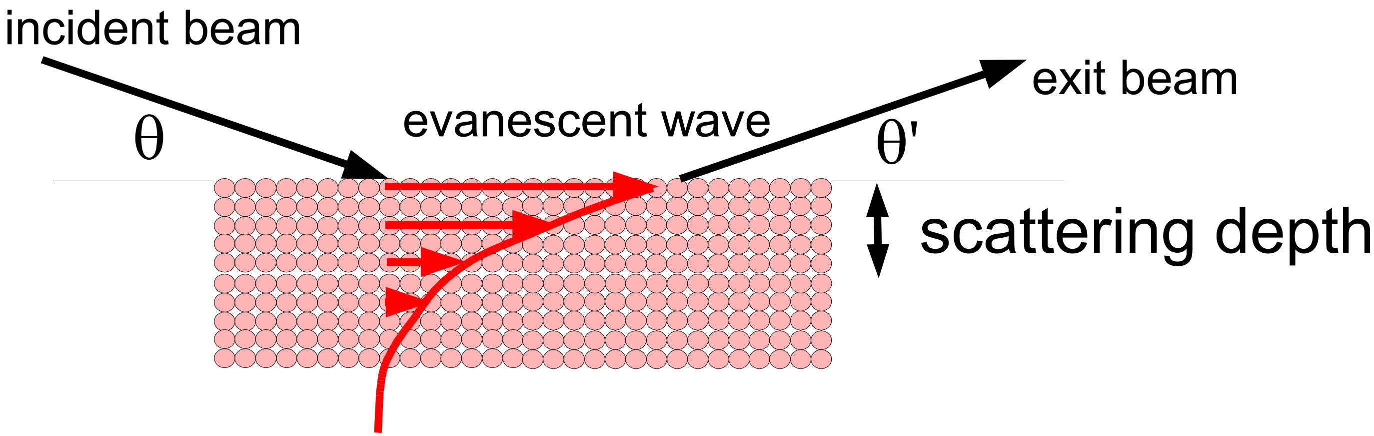
transmitted amplitude

$$t_f = \frac{2k_z}{k_z + k_{t,z}}$$

typical transmission coefficient @ 8keV photons

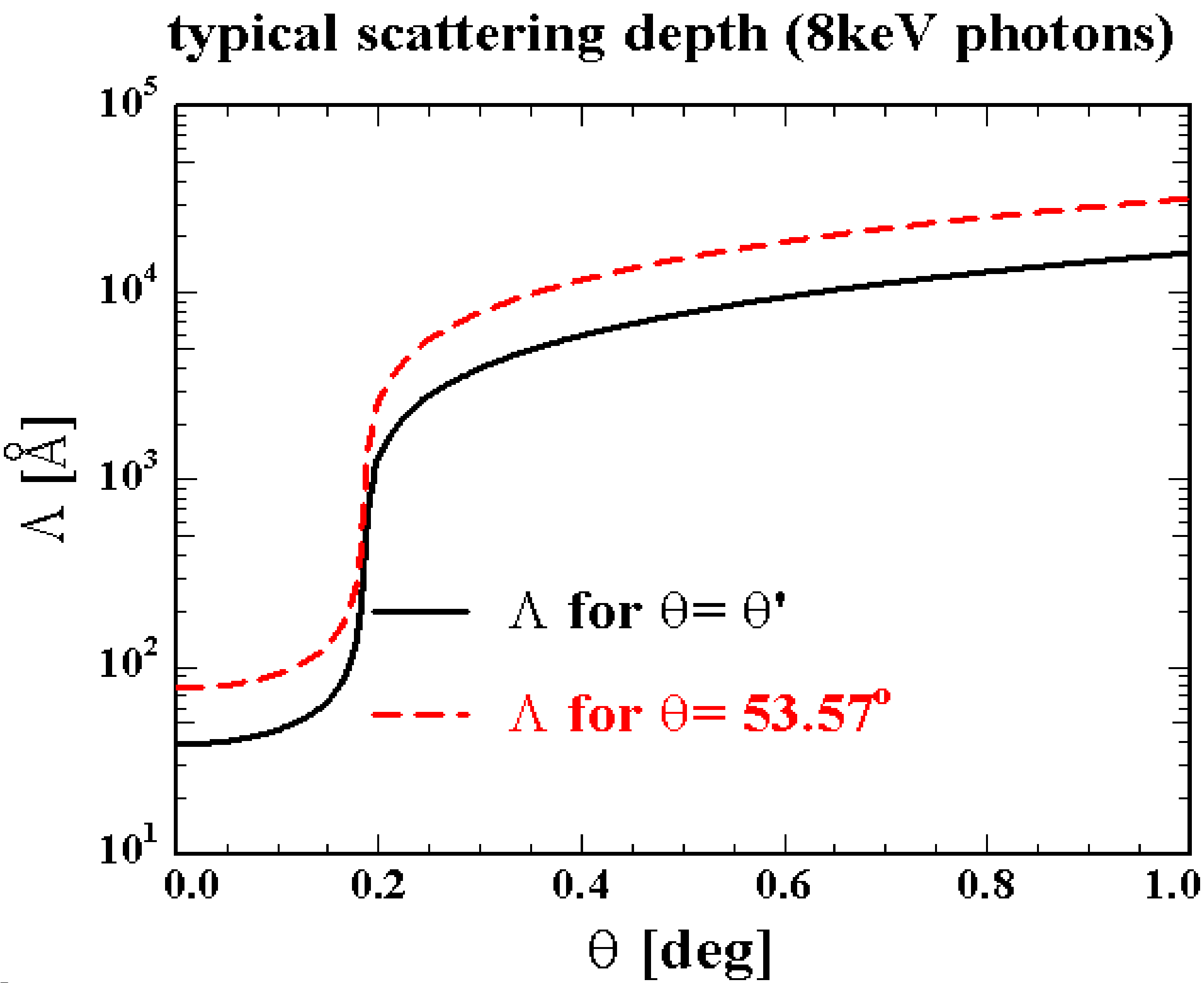


Amplification of the signal at the critical angle by a factor of 4



$$q_{zs} = k_{t,z}(\theta) + k_{t,z}(\theta')$$

$$\Lambda = \frac{1}{|Im\{q_{zs}\}|}$$

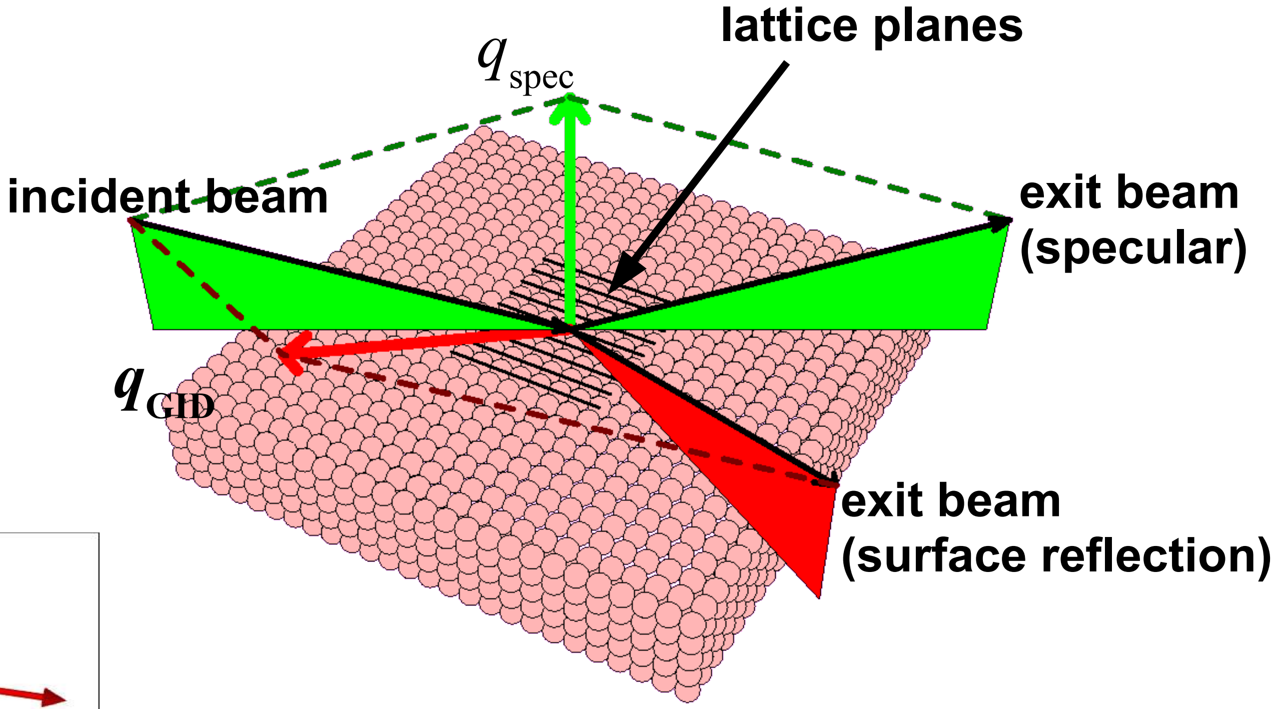


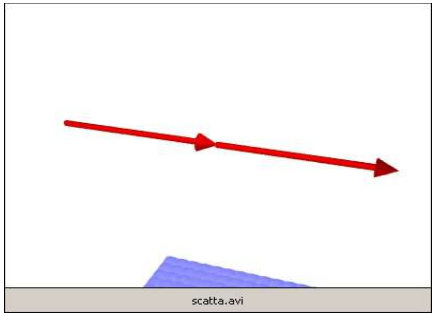
Can be used to tune the sensitivity to the surface:

small angle =>
only sensity to surface
large angle =>
sensity to bulk

Grazing Incidence Diffraction   The experiment

Excite lattice planes perpendicular to the surface with the use of the evanescent wave





reflected intensity scales with transmission functions

$$I(\boldsymbol{q}) \sim |t_f(\theta)|^2 |S(\boldsymbol{q})|^2 |t_f(\theta')|^2$$

$S(\boldsymbol{q})$: structure factor of the reflection

Example: Surface phase transition

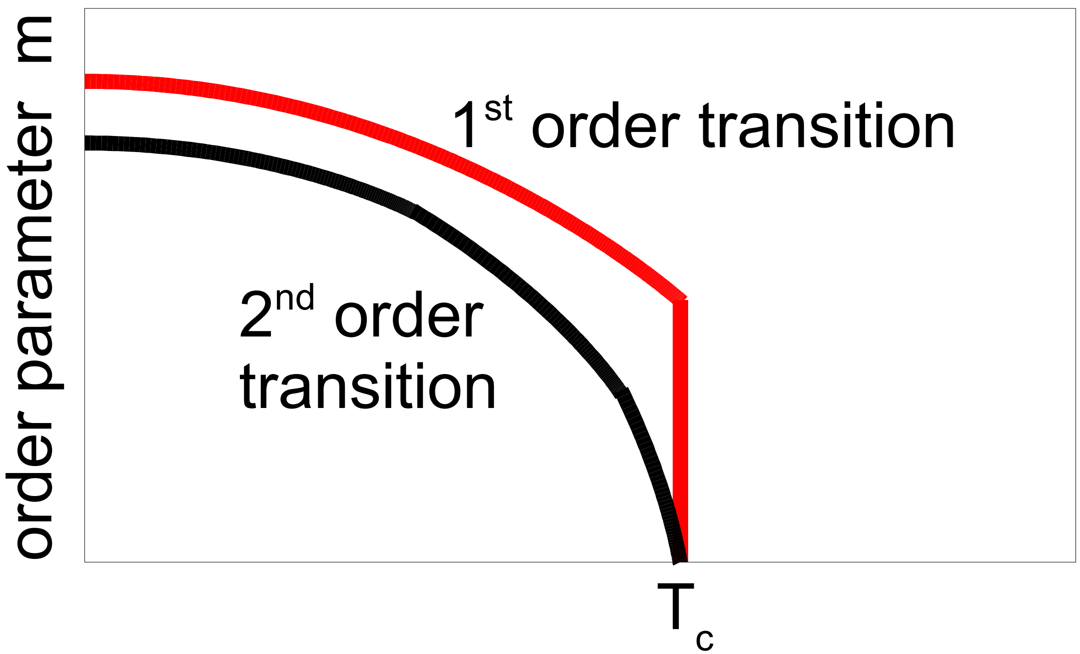
Phase transition

- Matter changes internal order with temperature
- usually: below phase transition temperature T_c => ordered

  above phase transition temperature T_c => disordered
- abrupt change of order :

  1st order transition
- continuous loss of order at increasing temperature :

  2nd order transition



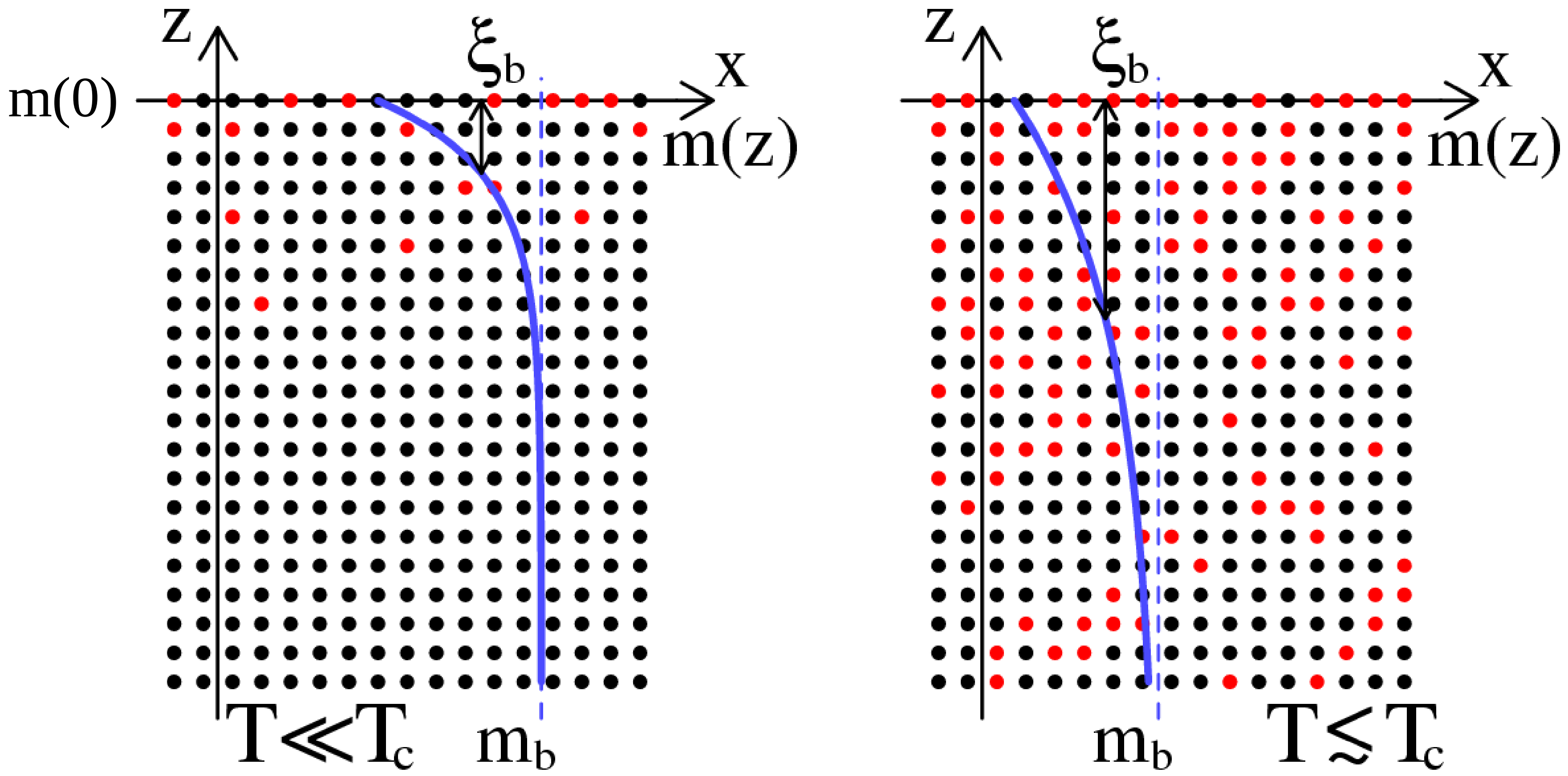
2nd order phase transitions: power laws of the order parameter with universal crictical exponents

$$m \sim \left(- \frac{T - T_c}{T_c} \right)^{\beta}$$

$\beta = 0.325$ for Ising model

Phase transition at the surface not identical to bulk (symmetry break at the surface)

Order parameter *m* depends on distance from surface : *m(z)*

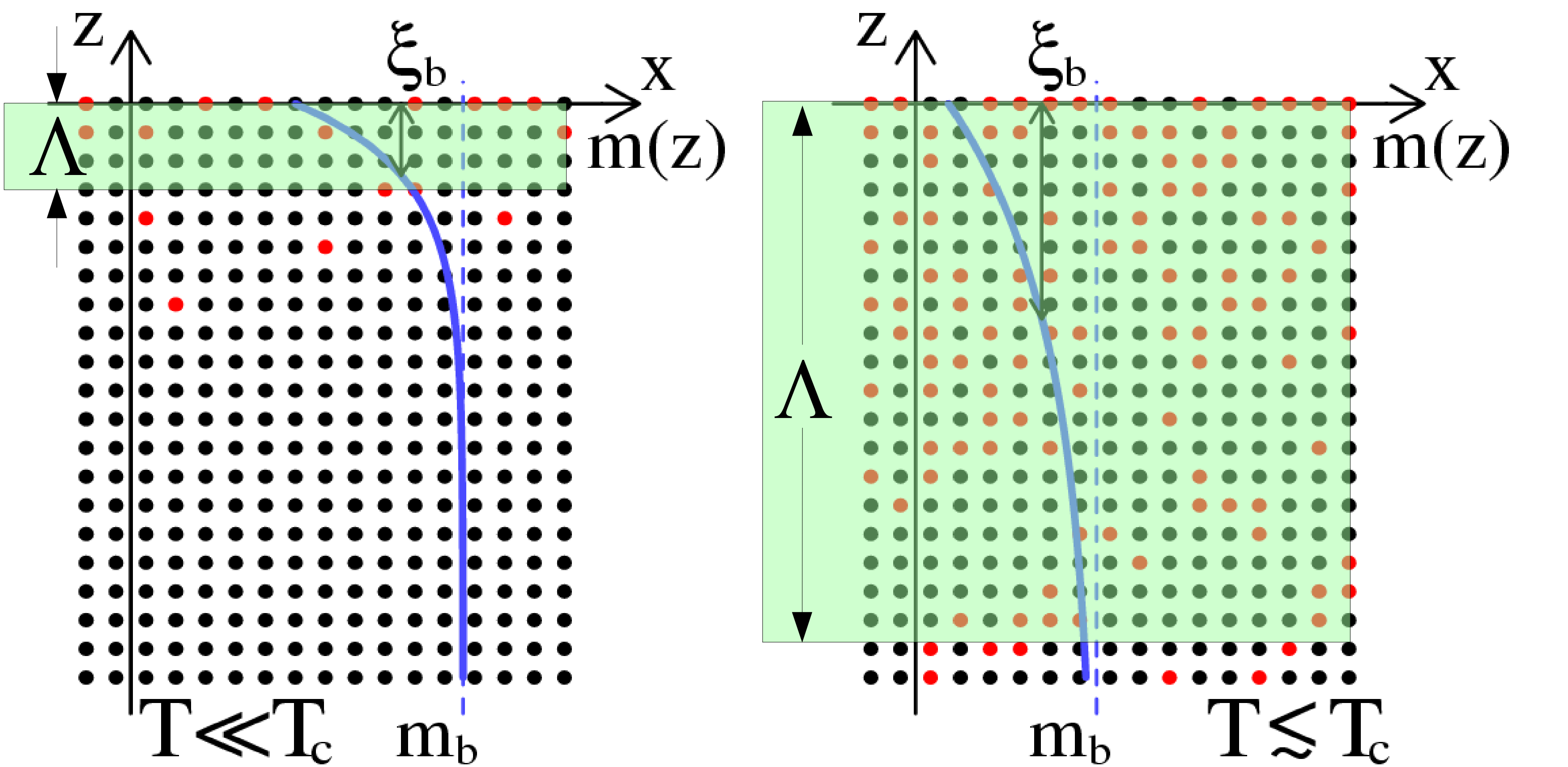


$$m(0) \sim \left(- \frac{T - T_c}{T_c} \right)^{\beta_{surf}}$$

$\beta_{surf} = 0.8$ for Ising model

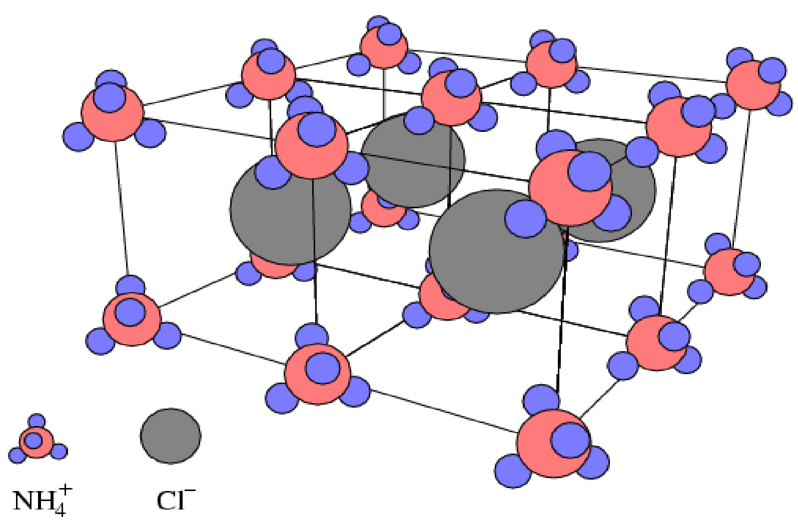
Using GID (changing scattering depth by changing the incident angle) the experiment can be sensitive to m(0) or m_{bulk}

Small incident angle : small scattering depth Λ => m(0)
Large incident angle : large scattering depth Λ => m_{bulk}



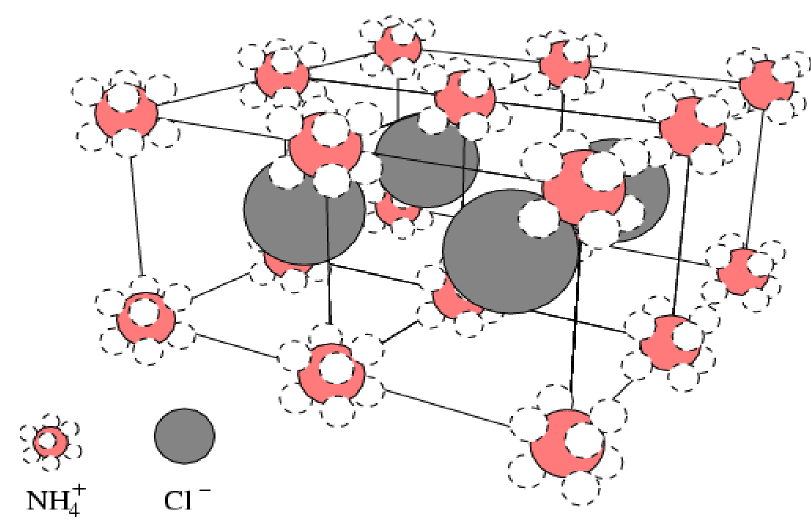
System Ammonium Chloride : deuterated NH_4Cl

$P\bar{4}3m$

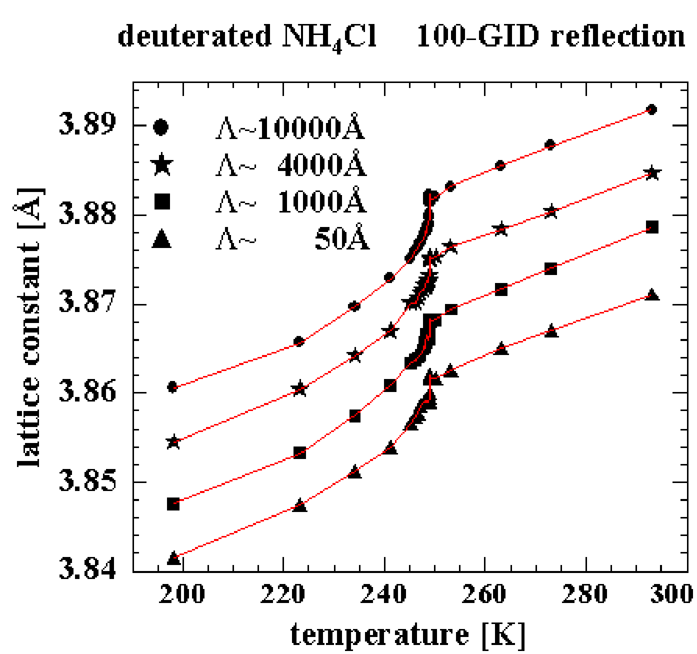


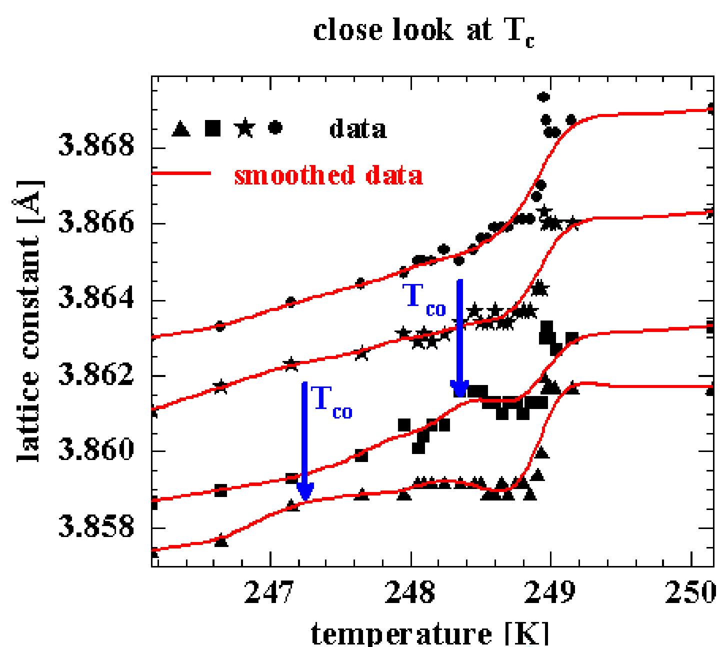
ordered low temperature phase

$Pm\bar{3}m$

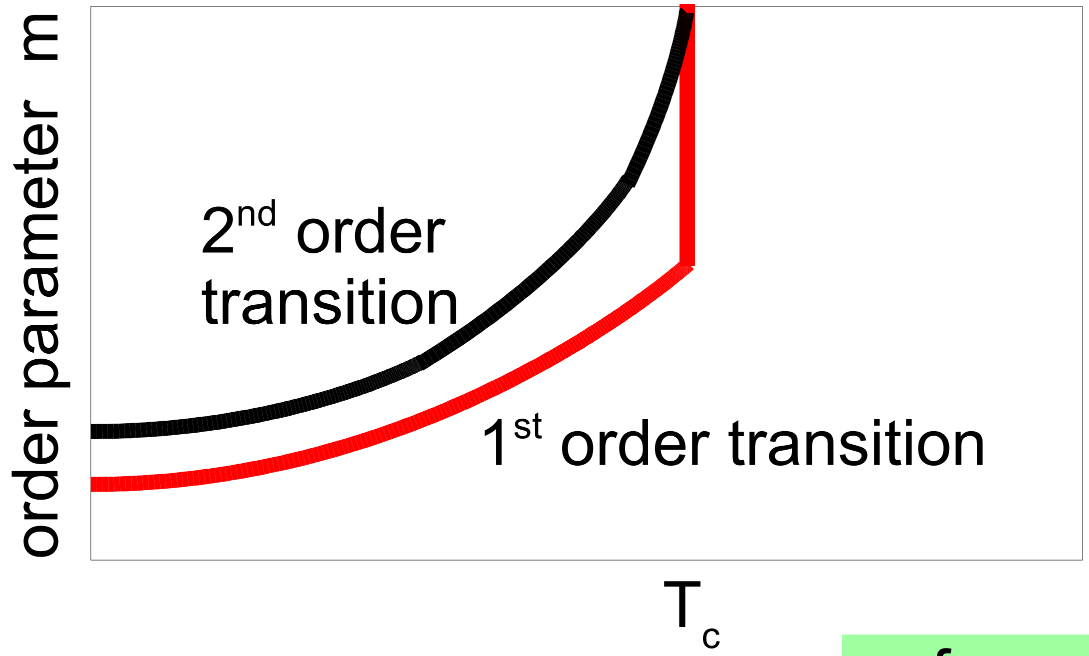


disordered high temperature phase



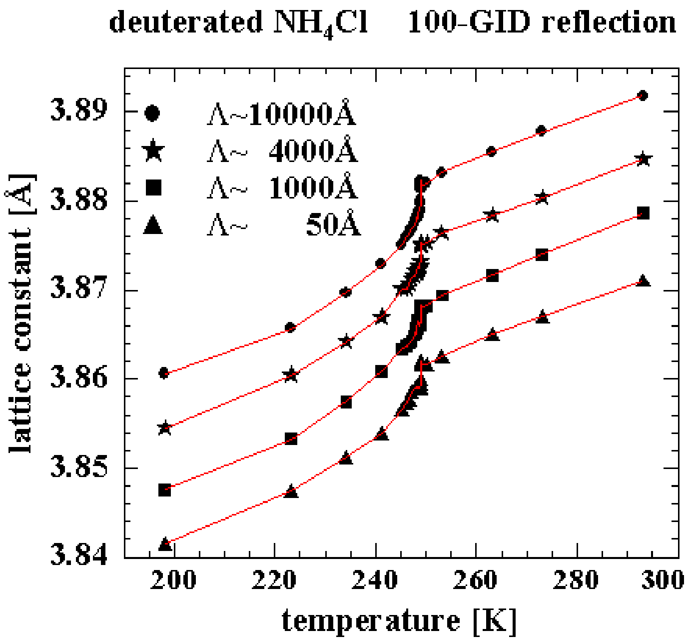


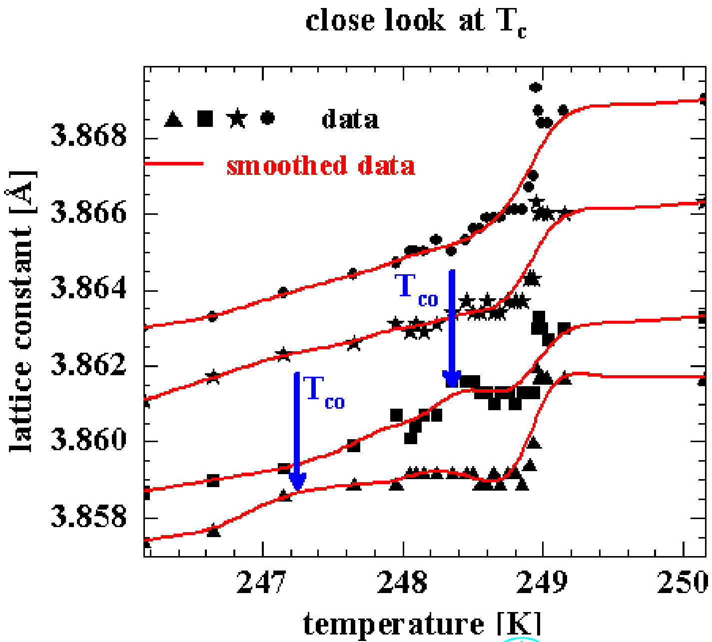
close to T_c :
change
of scattering
Λ dependent



Looks like 2^{nd} order

surface sensitive : 1^{st} order surface phase transition ?





close to T_c : change of scattering Λ dependent

Summary

- Grazing incidence diffraction can be used to investigate crystalline surface regions

- The surface-sensitivity can be tuned via the incident angle of the x-ray radiation.

- The scattered intensity is amplified if the incident angle is equal to the critical angle.