# 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

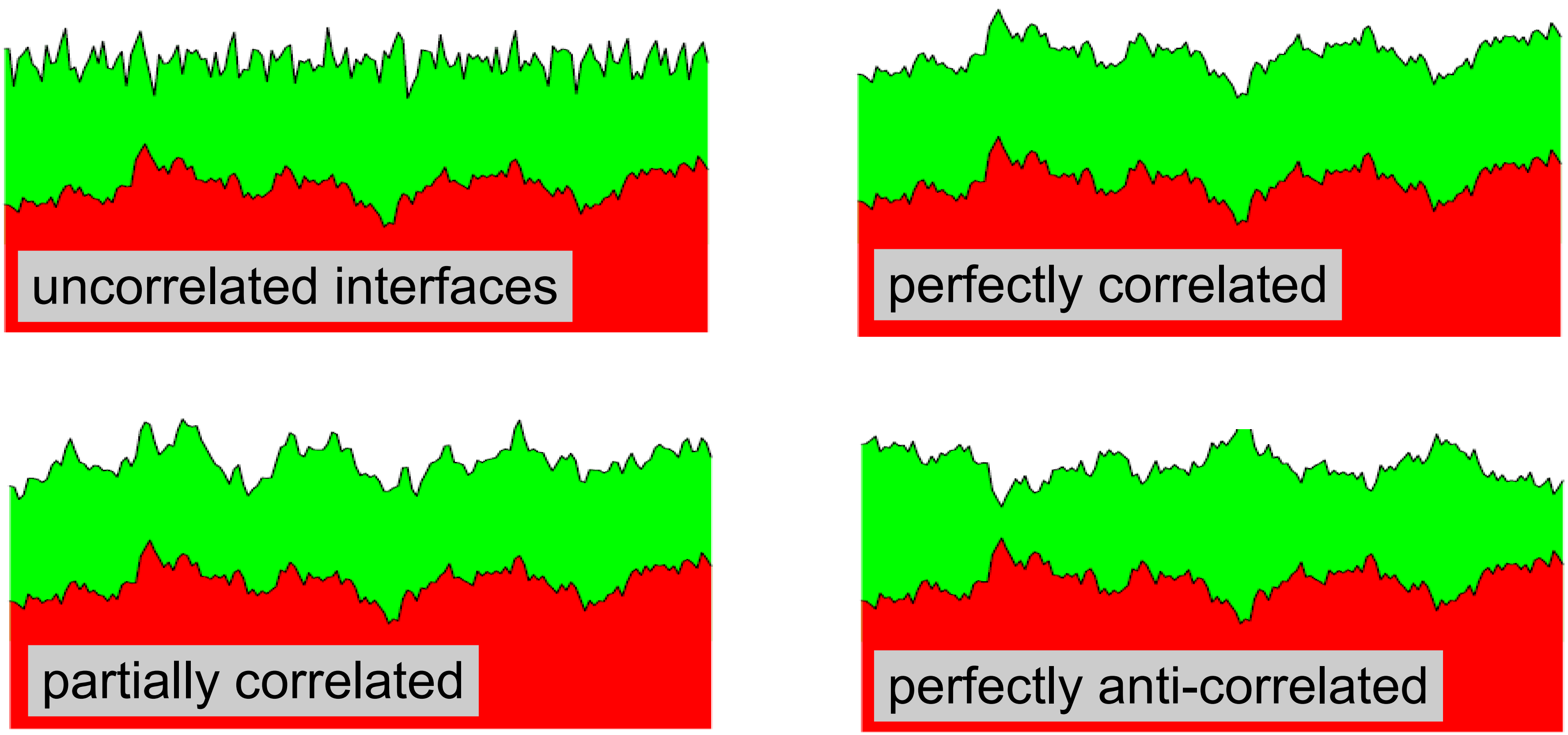
Reflectivity
- In Born  approximation
- Exact formalism (Fresnel)
- Examples

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

Diffuse Scattering
- Concepts of rough surfaces
- Correlation functions
- Scattering Born-approximation
- DWBA
- Examples

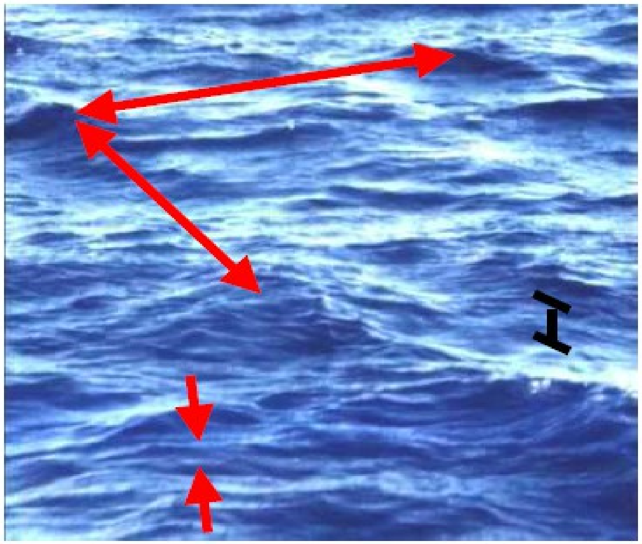
# X-ray Diffuse Scattering from Surfaces

- Interfaces and surfaces are usually NEVER perfectly smooth
- Rough interfaces can be described in terms of different models (fractal roughness, capillary waves ...)
- The different models are described by different parameters
- How is the roughness developing from interface to interface in a multilayer system



# Description of a Single Surface

e.g. macroscopically rough surface (water)

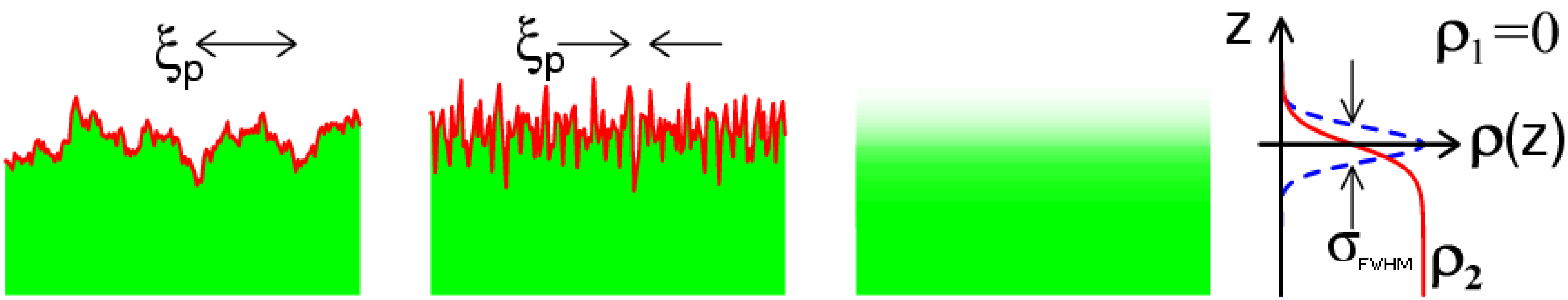


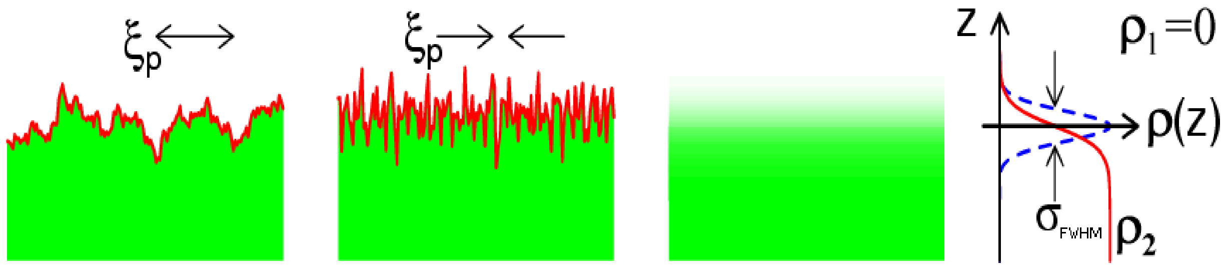
typical in-plane distance (long)

typical amplitude

typical in-plane distance (short)

1-dim cut






**How to describe the interface?**

1) Description via a real-space surface function $z(x,y)$

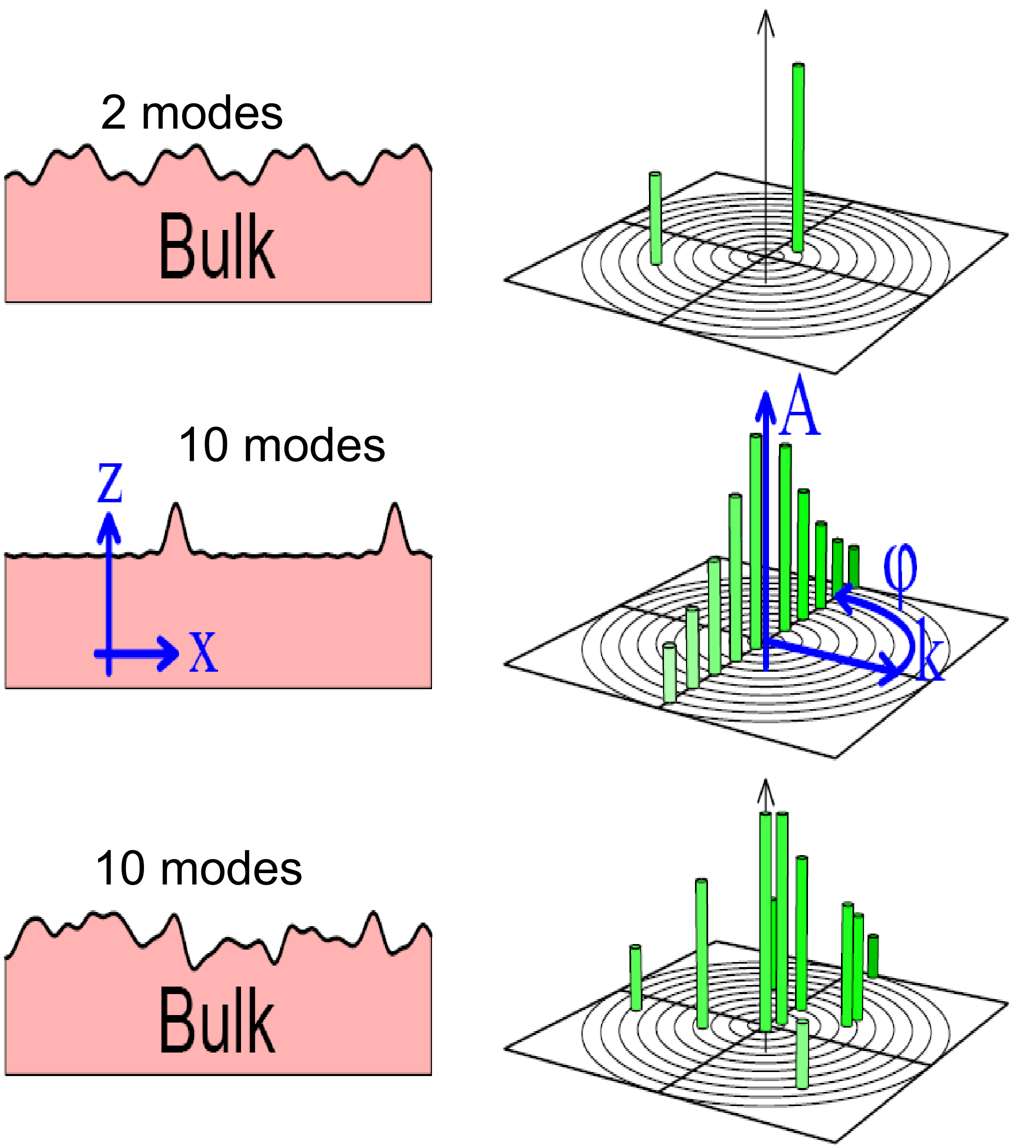
- is only useful for well-defined structures
- is useless for statistical surface

2) Description via a surface function in Fourier space

$$\tilde{z}(q_x, q_y) = \int z(x, y) \exp(i[q_x x + q_y y])\, dy dx = \mathcal{F}\{z(x, y)\}$$

- the description in Fourier space is equivalent to real-space
- what is the advantage ????

**Real-space** **Fourier-space**




Each oscillation (**so-called modes**) in real-space makes a peak in Fourier-space

Separation of amplitude & phase

$$\tilde{z}(q_x, q_y) = |\tilde{z}(q_x, q_y)| \exp[i\varphi(q_x, q_y)]$$

amplitude phase

Characteristics of the surface are determined by the amplitude

Special realization of the surface is determined by the phase (usually not of interest)

If the phase is not of interest, take absolute square:

$$\tilde{z}(q_x, q_y)\,\tilde{z}(q_x, q_y)^* = |\tilde{z}(q_x, q_y)|^2 = \tilde{C}(q_x, q_y)$$

$\tilde{C}(q_x,q_y)$ is the so-called Power Spectral Density (PSD)

The PSD is a measure of the number of waves of a particular wavelength

**Good points for the PSD :**

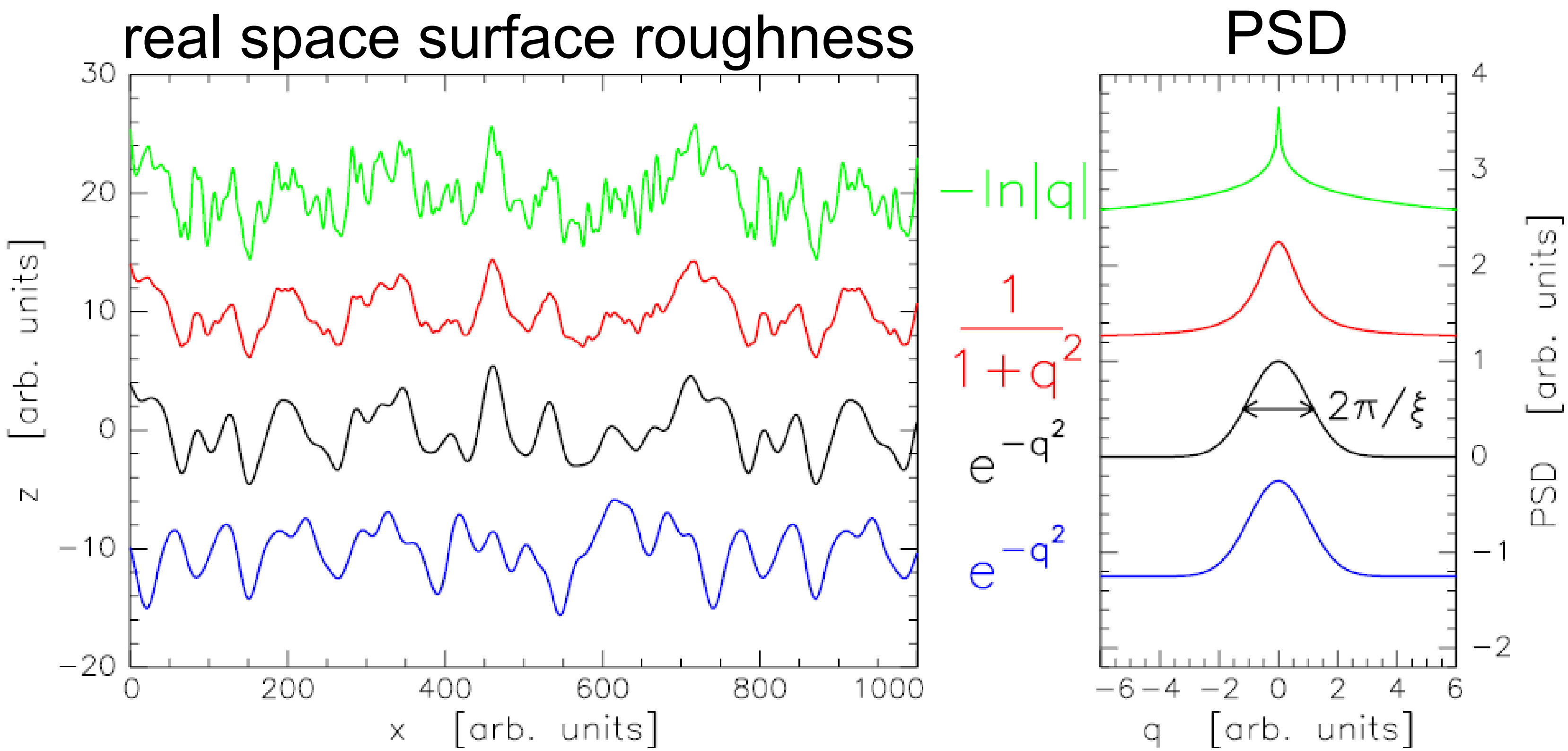
1) is independent from the special realization of the surface
2) is connected with physical properties e.g. dynamical susceptibility of liquid surfaces

$$\tilde{C}(\boldsymbol{q}, \omega) = 2\mathrm{k}_B T \frac{\Im\{\chi_{zz}(\boldsymbol{q}, \omega)\}}{\omega}$$

3) Fourierbacktransformation yields the so-called auto-correlation function $C(x,y)$

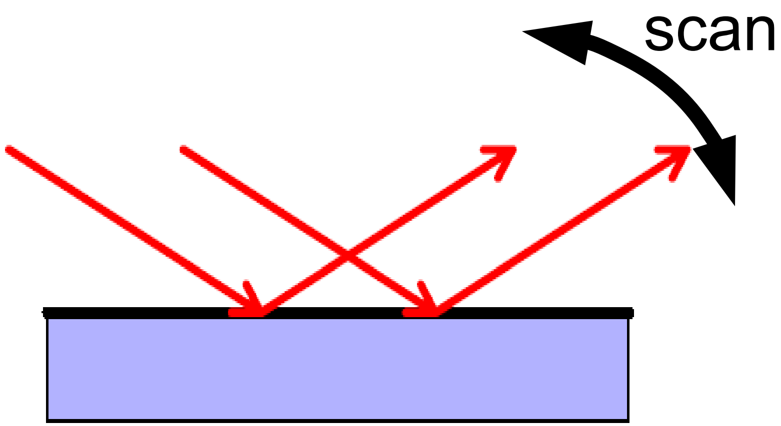
$$C(x, y) = \int z(X, Y)\, z(X+x, Y+y)\, dX dY = \int \tilde{C}(q_x, q_y) \exp(-i[q_x x + q_y y])\, dq_y dq_x$$

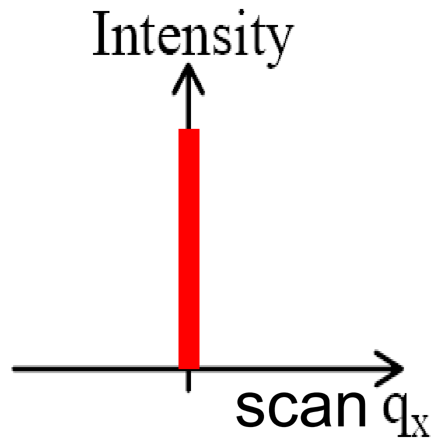
# Examples of statistical interfaces



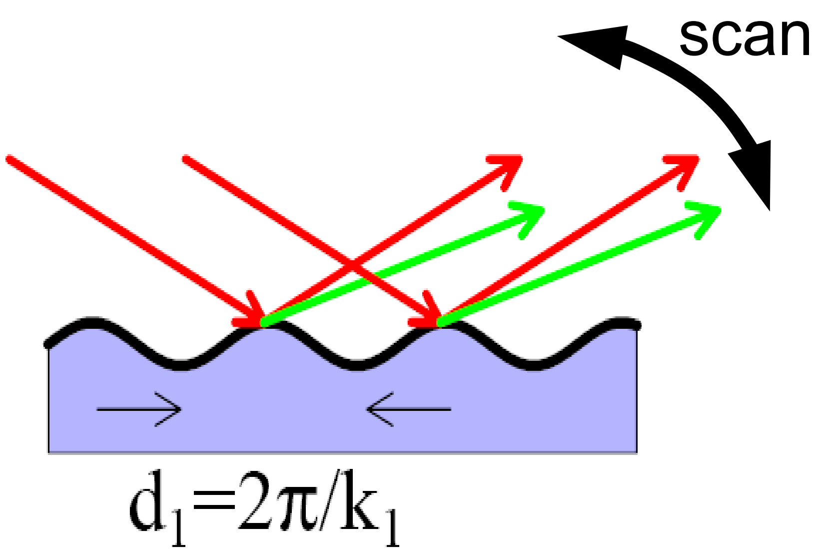

- Same rms-roughness $\sigma$ used for all surfaces
- Same in-plane correlation length $\xi$ used
- The top three surface are created with the same phase $\varphi(x)$

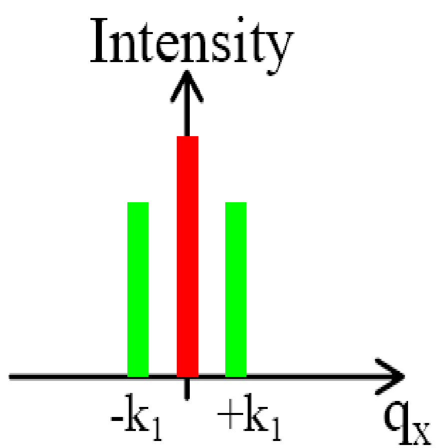
# Diffuse X-ray Scattering (Principle)



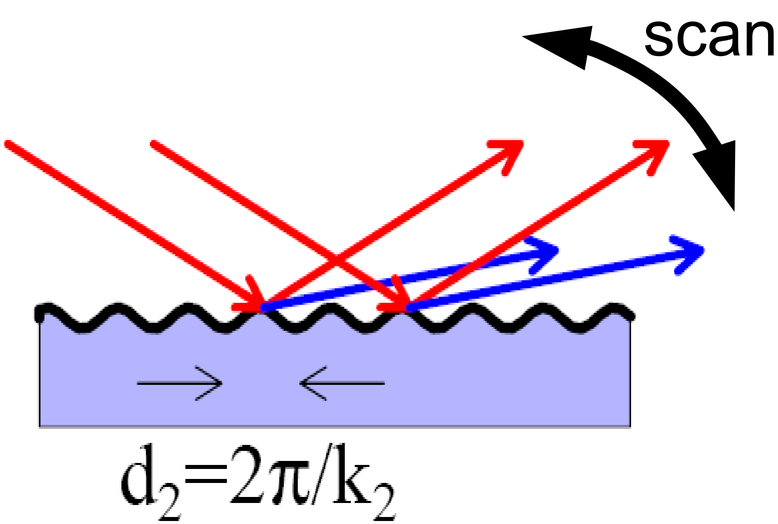



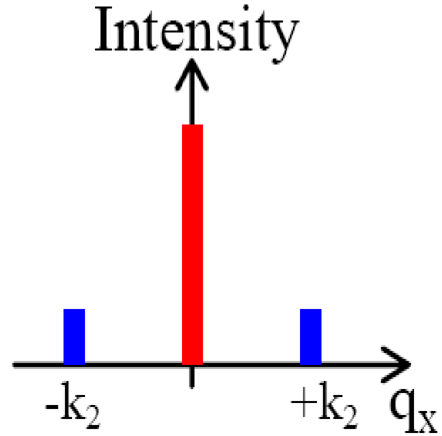

perfectly smooth:
only intensity in
specular direction
(qx = 0)



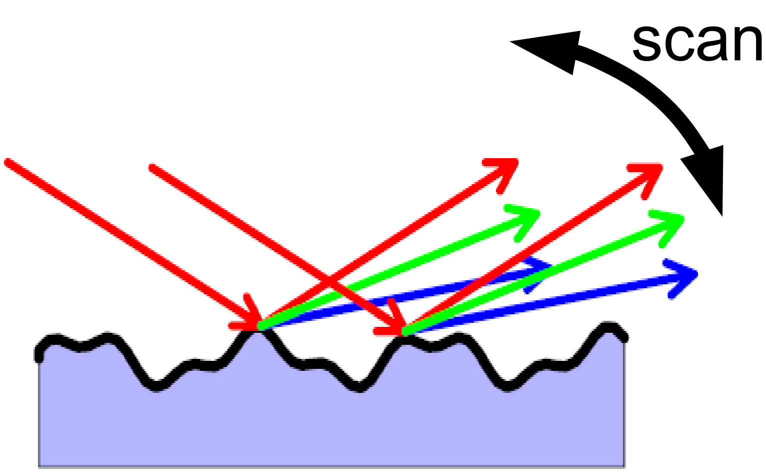



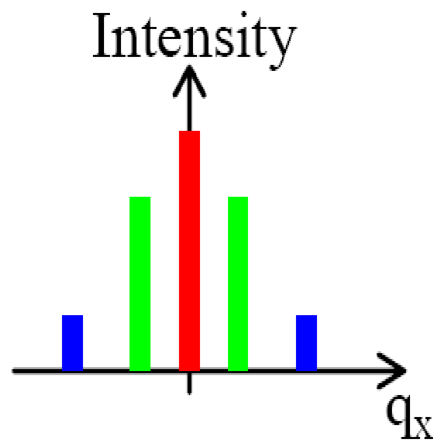

one mode:
side peaks at
(qx ≠ 0)




different wave vector of the mode shifts also qx

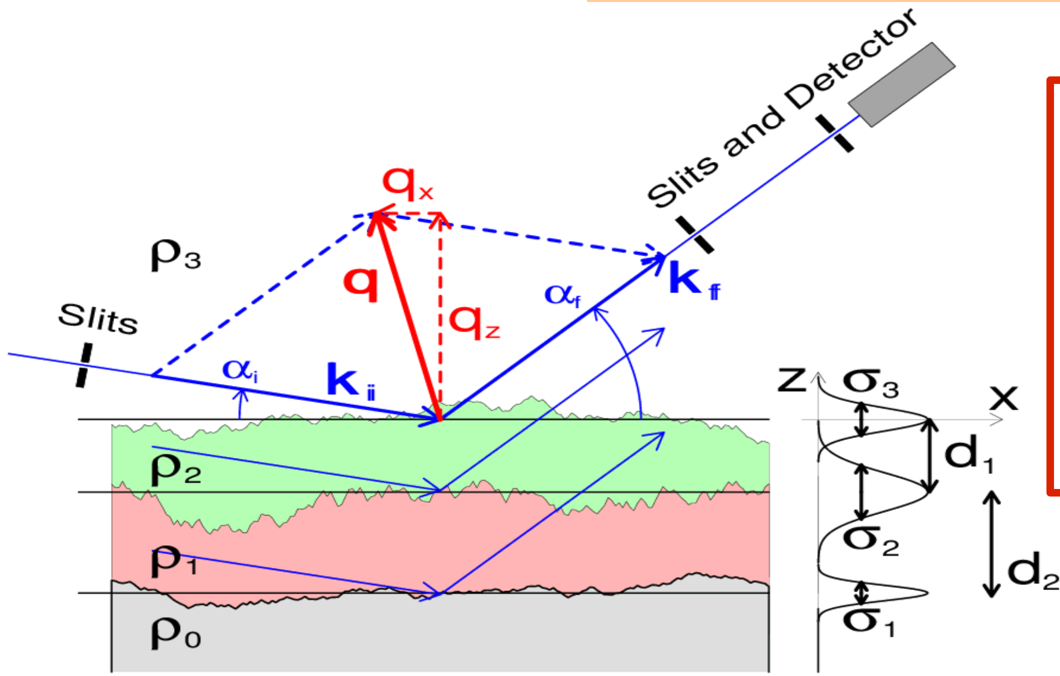



two modes: respective side peaks at ($qx \neq 0$)

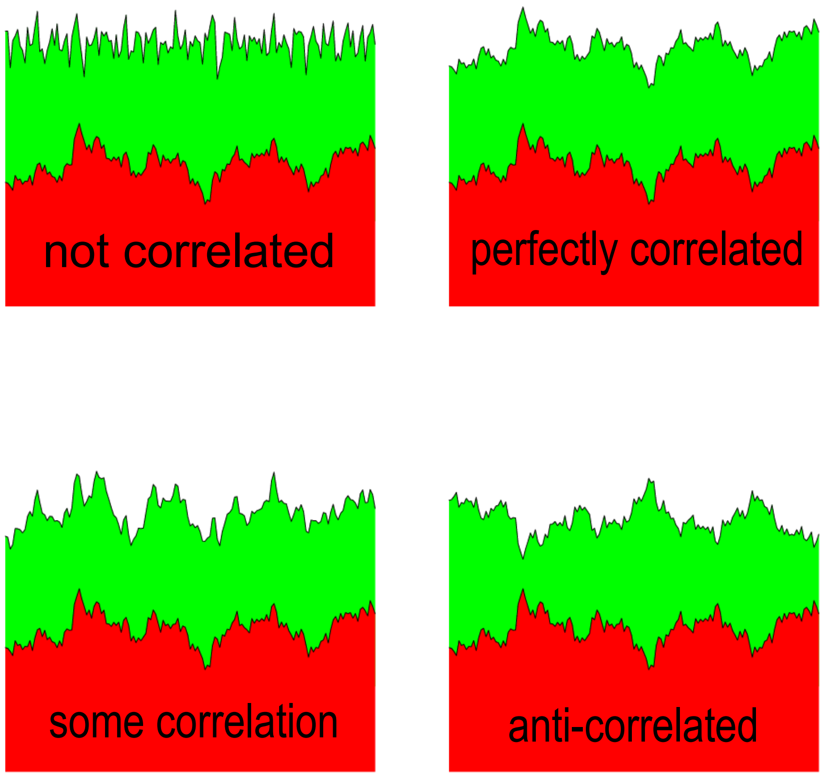
1) Rough surfaces are a collection of modes with different amplitudes, phases and wave vectors.
2) The modes create the respective scattering
   => diffuse scattering

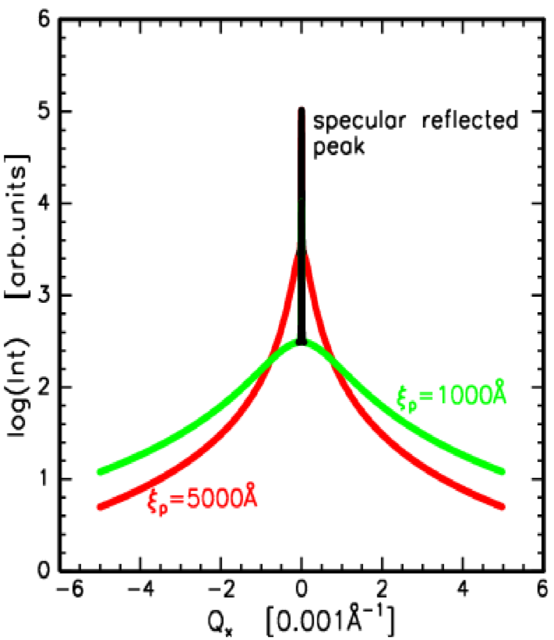
# Diffuse X-ray Scattering

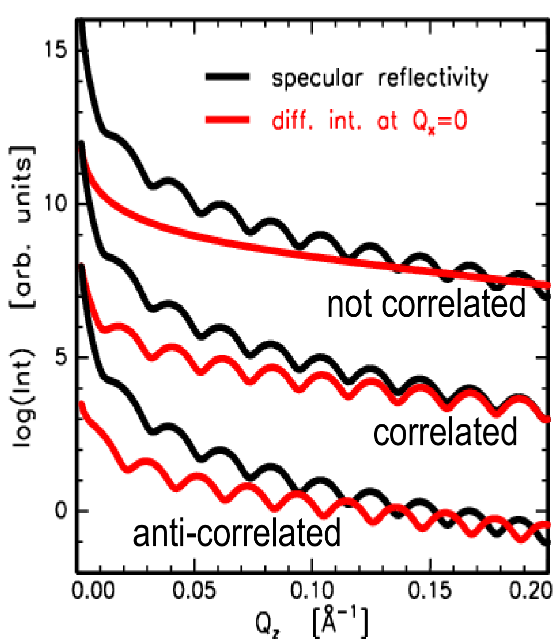



Experiment : incident angle θ ≠ exit angle θ'

often resolution in $q_y$ bad => Integrated Intensity in $q_y$



# Diffuse Scattering of one Rough Interface in Born Approximation

- multiple scattering effects are neglected
- refraction index is 1 (only the electron density is considered)
- wrong for small incident or exit angles (compared to critical angle)

$$I_{diff}^{BA}(\boldsymbol{q}) = \frac{4\pi}{q_z^2} \Delta\rho \exp\left(-q_z^2\sigma^2\right) \int \left( \exp\left[q_z^2 C(x,y)\right] - 1 \right) \cos\left(q_x x + q_y y\right) dx dy$$

The diffusely scattered intensity depends on:

- the incident and exit angles (via $q_x, q_y, q_z$)
- the contrast (the density difference at the surface) $\Delta\rho$
- the roughness $\sigma$
- the auto-correlation function $C(x,y)$

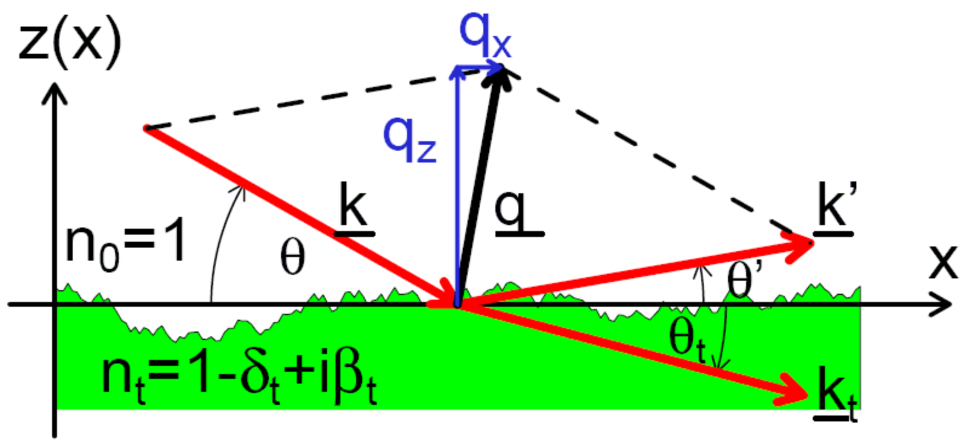
For small $q_z$ :

$$I_{diff}^{BA}(\boldsymbol{q}) \approx 4\pi \Delta\rho \exp\left(-q_z^2\sigma^2\right) \tilde{C}\left(q_x, q_y\right)$$

**In simplest approximation the diffuse scattering proportional to PSD**

# Diffuse Scattering of one Rough Interface
# Distorted Wave Born Approximation (DWBA)

- multiple scattering effects are taken into account via transmission functions
- refraction index is considered
- only valid vor small $\sigma q_z$




For a single surface:

$$I_{diff}^{DWBA}(\boldsymbol{q}) \approx |t_f(\theta)|^2 \, I_{diff}^{BA}(\boldsymbol{q}) \, |t_f(\theta')|^2$$

with

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

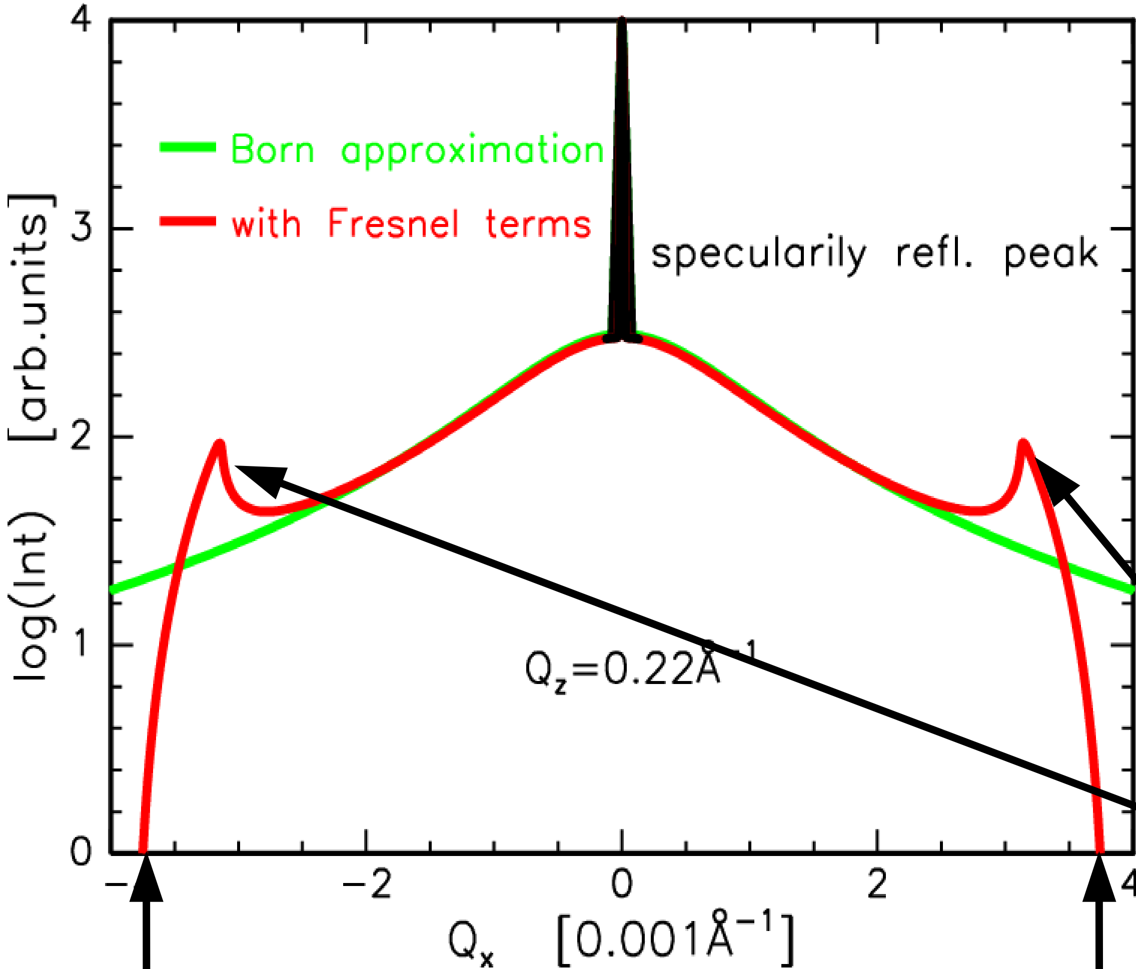
Fresnel transmission coefficient and

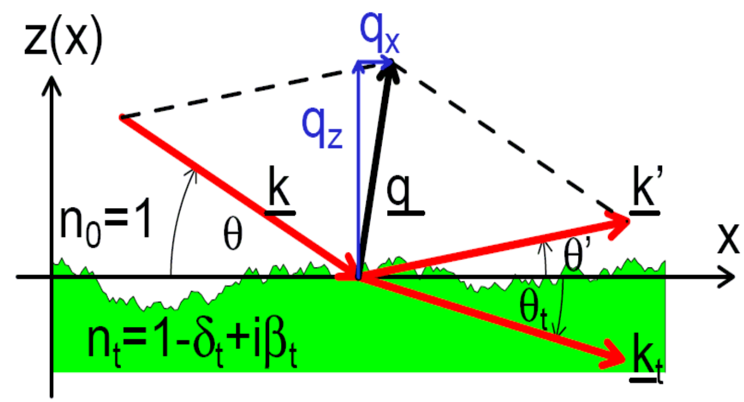
$$k_z = k \sin\theta$$

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

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

# Rocking scan (detector angle fixed, rotating sample)




Yoneda-wings (amplifications of the scattering at the critical angle)

incident angle θ = 0

exit angle θ' = 0