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# Basic Principles of X-ray Reflectivity in Thin Films

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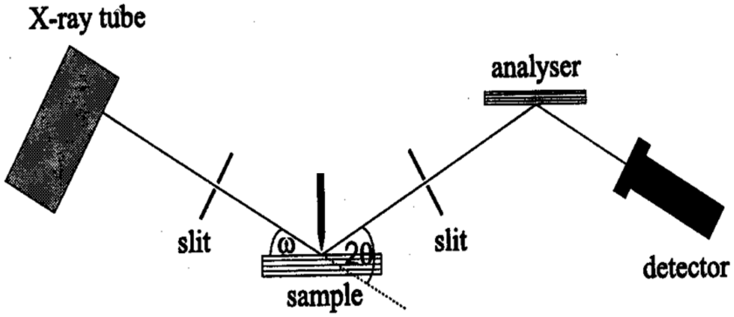
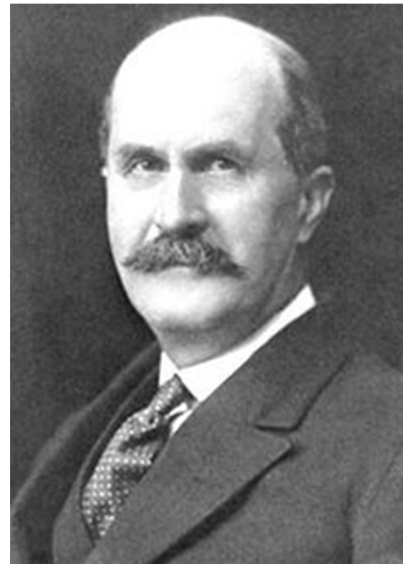
# Outline

- X-ray diffraction
- X-ray diffraction in thin films: high angle vs low angle
- XRR as structural characterization
- Diffuse scattering: specular vs off-specular reflectivity
- Summary

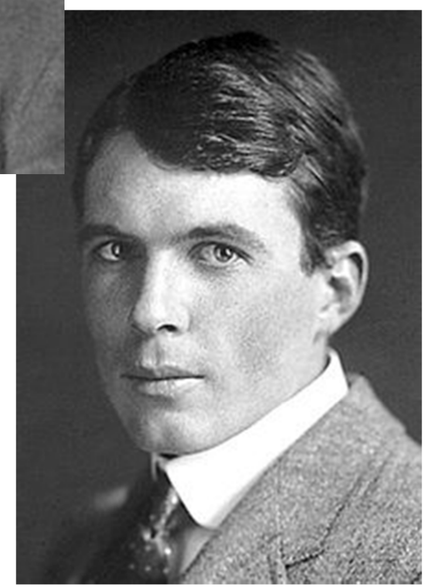
# X-ray diffraction




William Henry Bragg



William Lawrence Bragg



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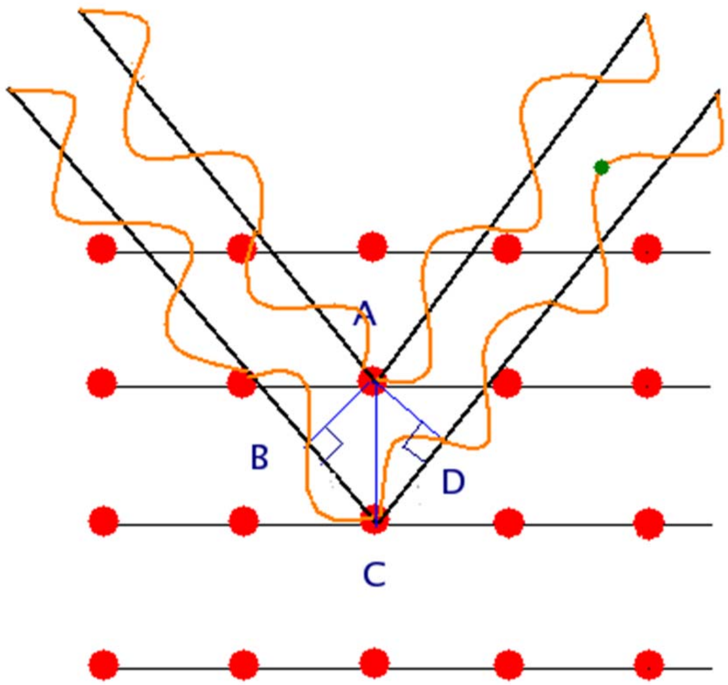
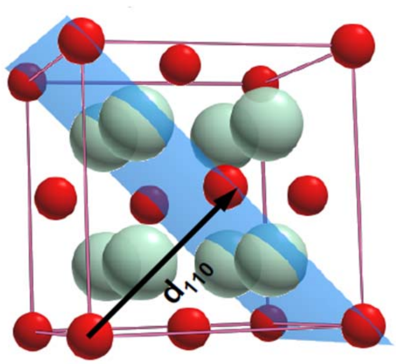
# X-ray diffraction

Bragg s law: angle where constructive interference of scattered X-rays produces a diffraction peak:

$$n\lambda = BC + CD = 2d_{hkl}\sin\theta$$

where $d_{hkl}$ is the vector drawn from the origin of the unit cell to intersect the crystallographic plane.

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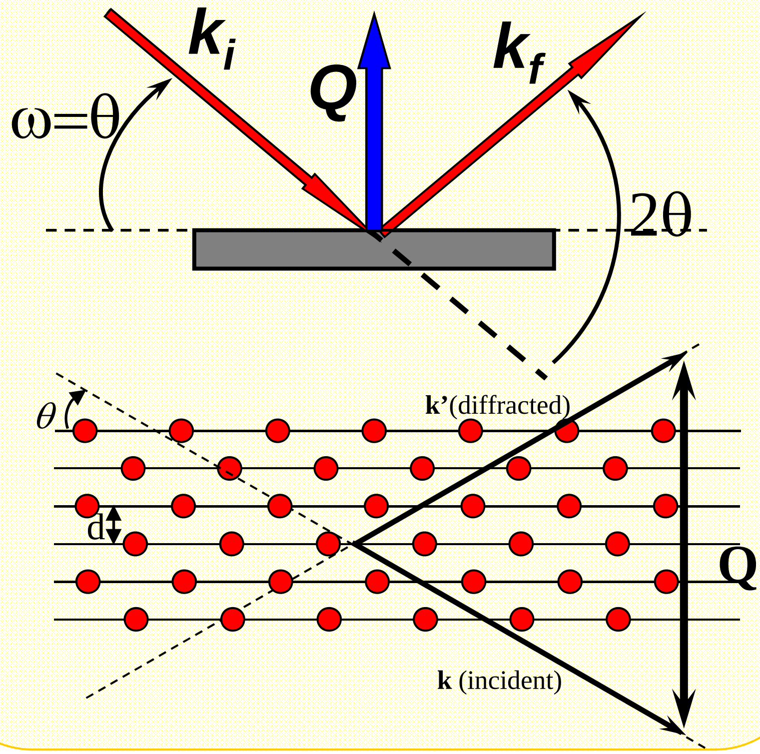
# High angle vs Low angle

*Probing ranges in x-ray diffraction on thin films*

$n\lambda = 2d\sin\theta$ → $\theta \sim 1/d$

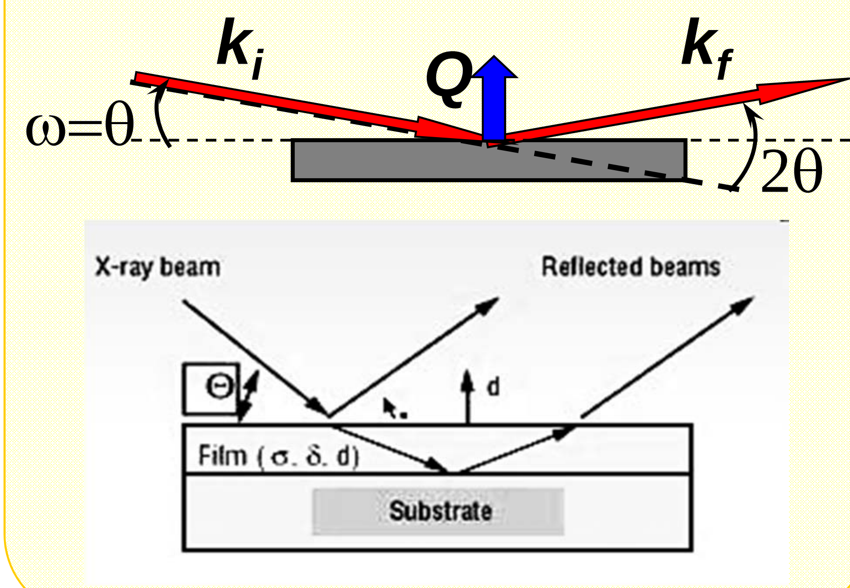
High $\boldsymbol{\theta}$ (high $\boldsymbol{Q}$) = Low $\boldsymbol{d}$

$\lambda = 2d_{hkl}\sin\theta$




Low $\boldsymbol{\theta}$ (low $\boldsymbol{Q}$) = High $\boldsymbol{d}$

$n\lambda = 2t\sin\theta$

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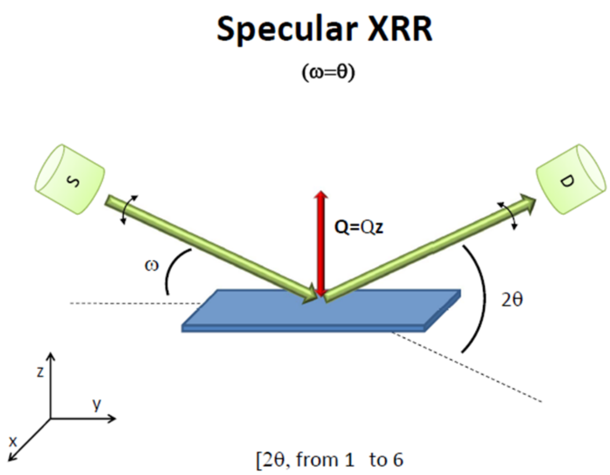
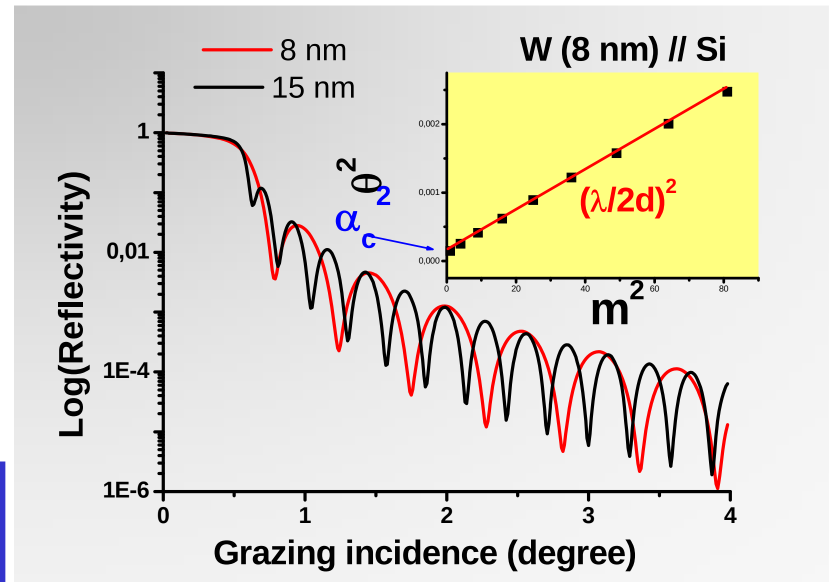
# X-ray Reflectivity




Kiessig fringes $$\theta^2 - \alpha_c^2 = m^2\left(\frac{\lambda}{2d}\right)^2$$

Reflectivity (background) $$R(\vec{Q}) = \frac{16\pi^2\rho_{el}^2}{q_z^4}\delta q_x \delta q_y \propto \frac{1}{q_z^4}$$

At every interface, a portion of x-rays is reflected. Interference of these partialy reflected x-ray beams creates a reflectometry pattern.

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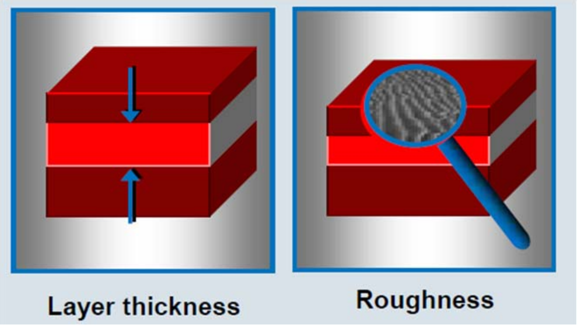
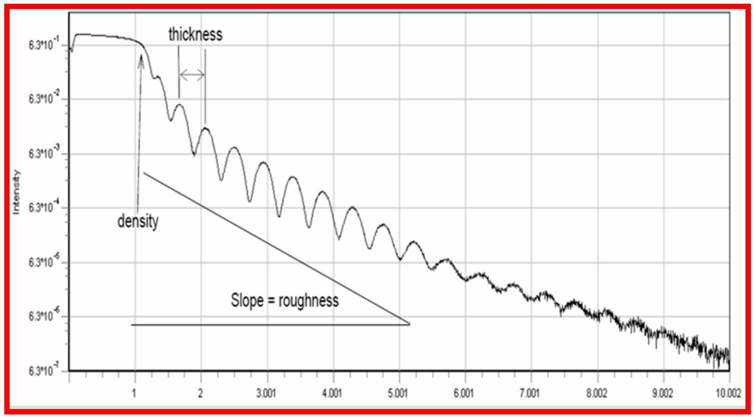
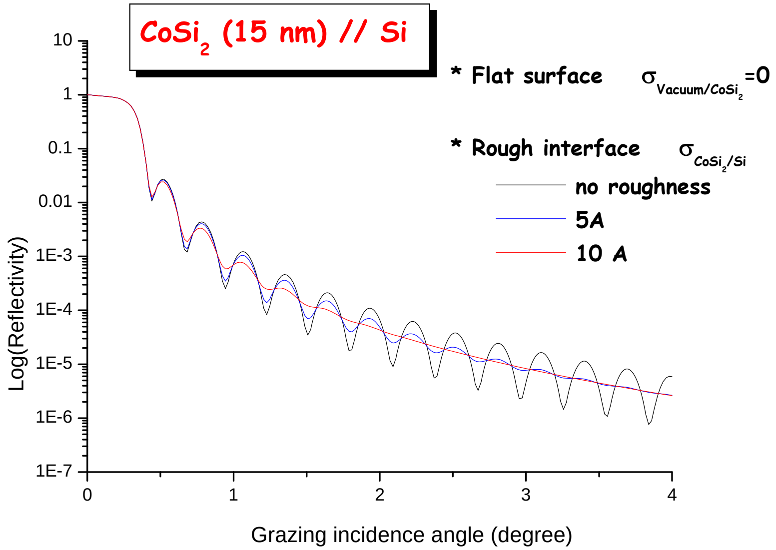
# X-ray Reflectivity

· X-ray reflectivity can be used for:
- Layer thickness of thin films and multilayers.
- Surface and interface roughness.
- Surface density gradients and layer density.

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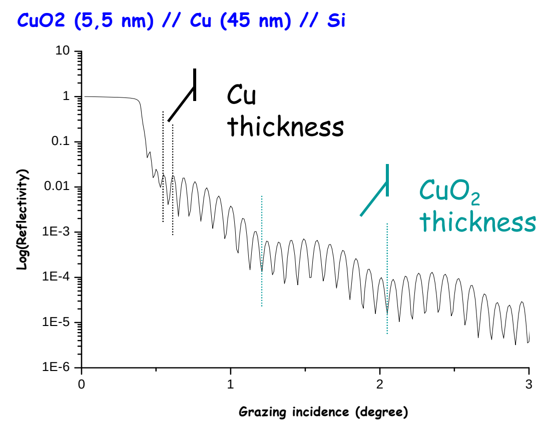
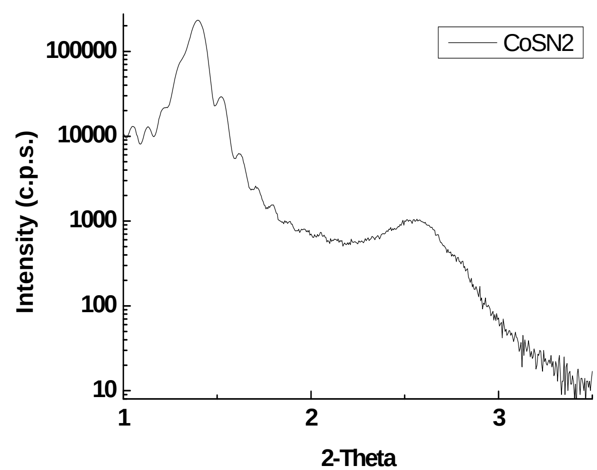
# X-ray Reflectivity

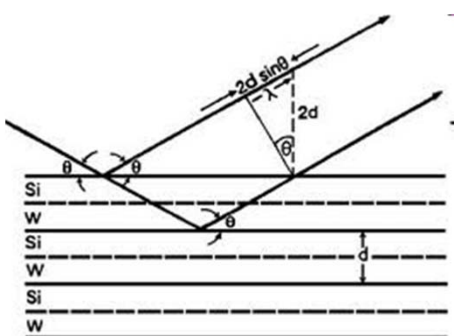
*Special case: bilayers and multilayers*




**Bilayer:** 2 oscillation frequencies are evidenced




**Multilayer:** n-1 Kiessig fringes between 2 Bragg Peaks

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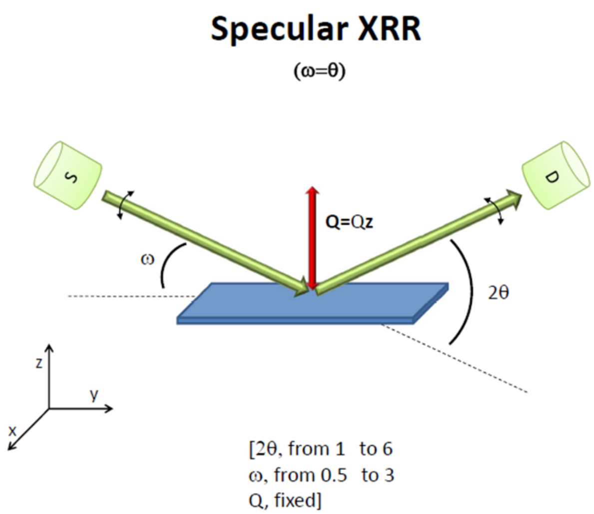
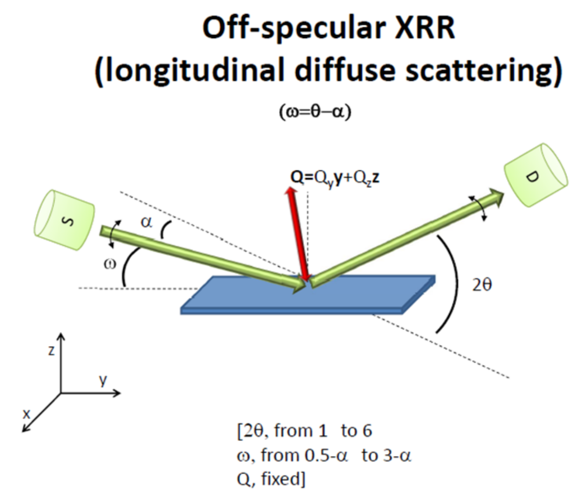
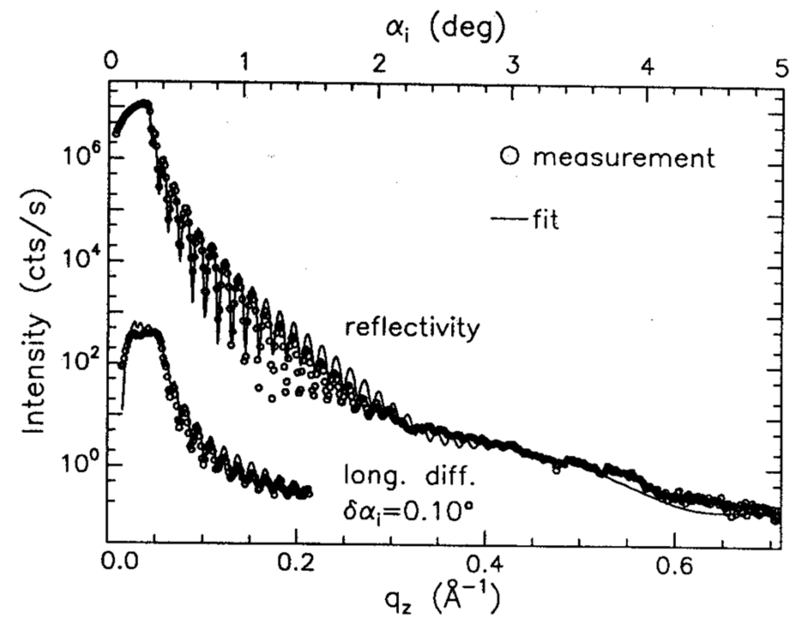
# Diffuse scattering

## Longitudinal diffuse scattering

*Specular vs off-specular reflectivity*




- Specular contribution of the diffuse scattering
- Same oscillations than reflectivity curve

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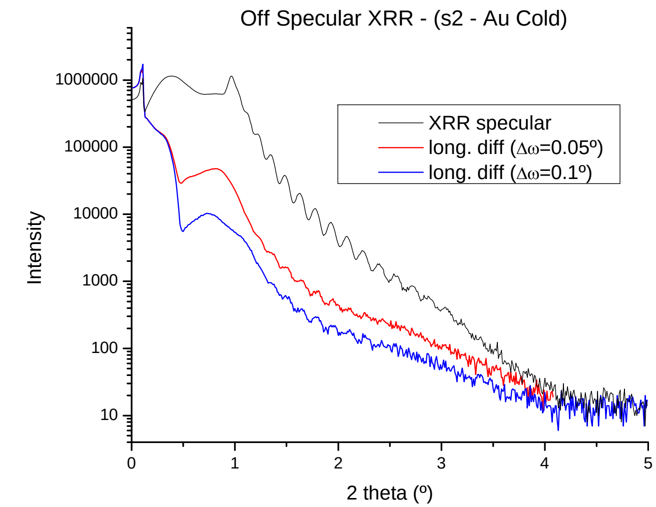
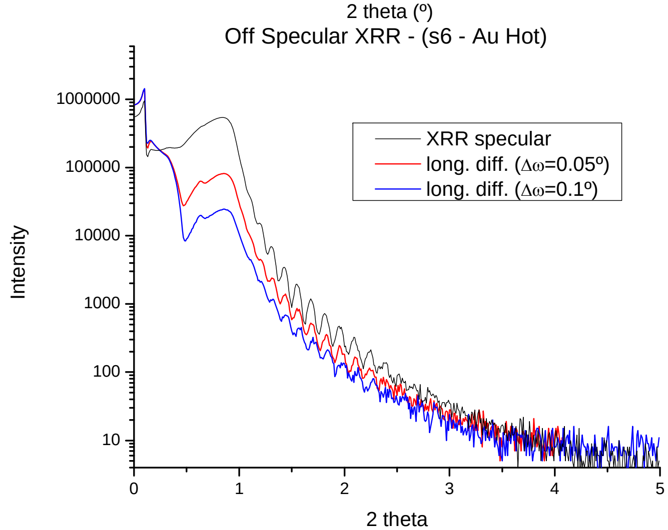
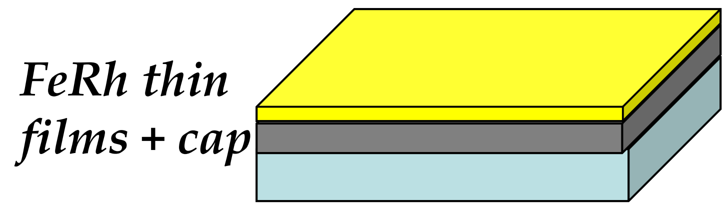
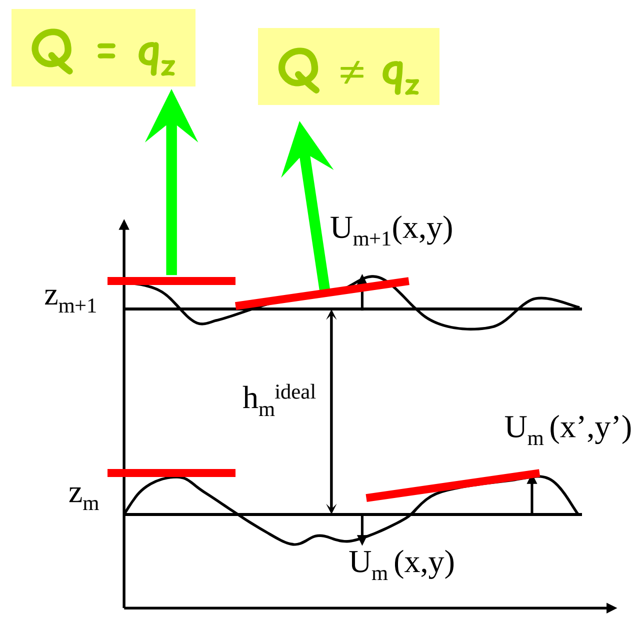
# Diffuse scattering

## Longitudinal diffuse scattering

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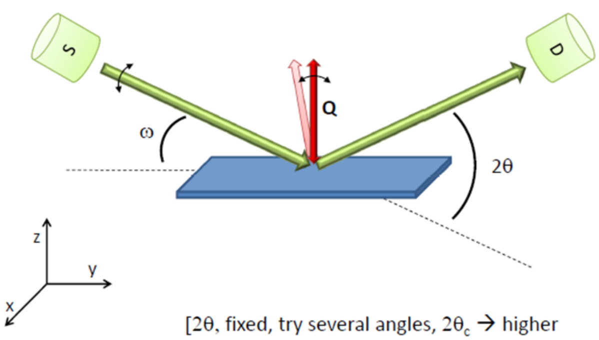
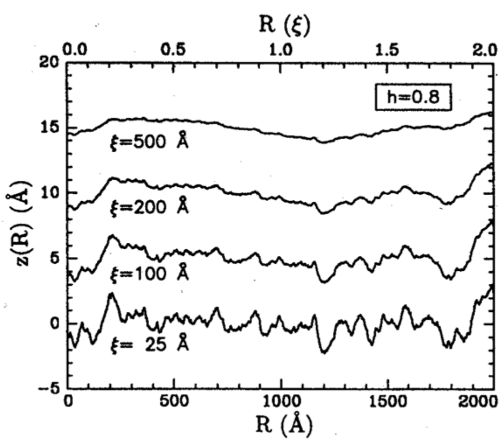
# Diffuse scattering

## Transverse diffuse scan (ω-rocking curve)

**ω-rocking**




[2θ, fixed, try several angles, $2\theta_c$ → higher ω, from θ-0.5 to θ+2 ]

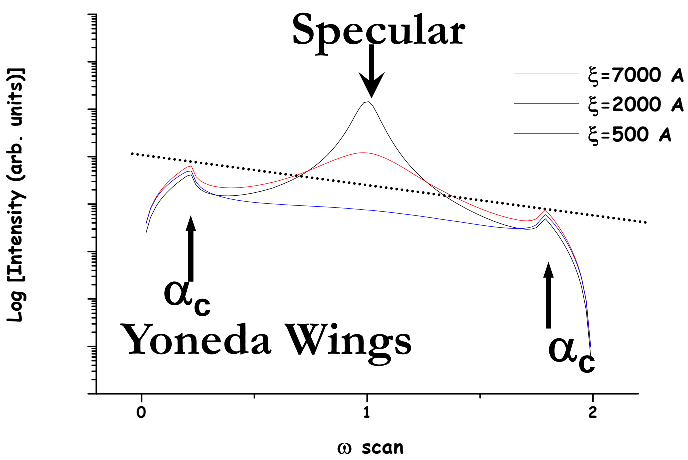



*Various ξ : Large lateral correlation ξ at interface*

⇓

*Specular peak*

*Yoneda wings : each time $\alpha_i$ or $\alpha_f$ = $\alpha_c$*

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# Summary

- At every interface, a portion of x-rays is reflected. Interference of these partialy reflected x-ray beams creates a reflectometry pattern.

- X-ray reflectivity is a useful techinque for structural characterization of thin films. Information about the thickness and the roughness of such samples can be obtained.

- Diffuse scattering of x-rays give also information about the roughness, correlation length (fractal parameters) in surfaces and interfaces.