Today's outline - October 21, 2021

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- Extinction and absorption

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Reading Assignment: Chapter 6.5; Chapter 7.1

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- Dumond diagrams and monochromators

Reading Assignment: Chapter 6.5; Chapter 7.1

Homework Assignment #05:
Chapter 5: 1,3,7,9,10
due Tuesday, November 02, 2021

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- Extinction and absorption
- Perfect crystal integrated intensity
- Comparison of intensities
- Absorption, energy, and order effects
- Standing waves
- Dumond diagrams and monochromators

Reading Assignment: Chapter 6.5; Chapter 7.1

Homework Assignment #05:
Chapter 5: 1,3,7,9,10
due Tuesday, November 02, 2021

Homework Assignment #06:
Chapter 6: 1,6,7,8,9
due Tuesday, November 16, 2021

Review of Darwin theory

Starting with a single layer, the Darwin theory of diffraction from a perfect crystal is developed giving the reflectivity $R(x)$ where $\epsilon = \Delta - g_0$, $i\eta = \pm\sqrt{\epsilon^2 - g^2}$, and $x = \epsilon/g$

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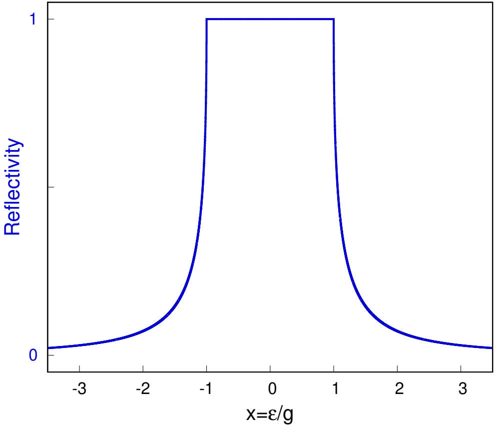

$$R(x) = |r|^2 = \begin{cases} (x - \sqrt{x^2-1})^2 & x \geq 1 \\ 1 & |x| \leq 1 \\ (x + \sqrt{x^2-1})^2 & x \leq -1 \end{cases}$$

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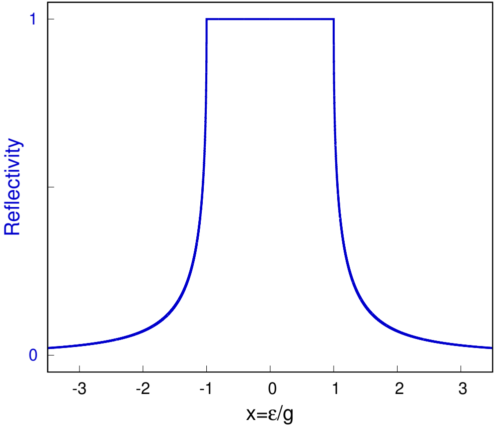

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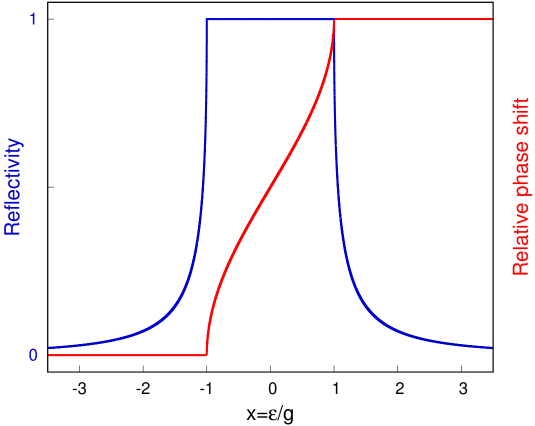

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the Darwin curve has 100% reflectivity across a width that varies inversely with the order, m, of the reflection

the relative phase between the scattered and transmitted waves varies from out of phase at $x = -1$ to in phase at $x = +1$

Extinction depth

An x-ray penetrating into a crystal scatters and thus is attenuated as it passes each plane of atoms by an amount $e^{-Re\{\eta\}}$

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$$\Lambda_{ext}(x=0) = \frac{d}{2g} = \frac{1}{4}\left(\frac{m}{d}\right)\frac{v_c}{r_0|F|}$$

Extinction depth for GaAs

The extinction depth depends on the structure factor and thus will vary significantly depending on the strength of the particular Bragg reflection

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for $\lambda = 1.54056\,\text{Å}$, $v_c = 180.7\,\text{Å}$, and $d_{400} = 1.41335\,\text{Å}$ the extinction depth is

$\Lambda_{ext}(400) = 0.74\,\mu\text{m}$

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For the weak (200) reflection of GaAs

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$$F_{GaAs}(200) = 4\times[f_{Ga}(200)-f_{As}(200)]$$

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$$\begin{aligned} F_{GaAs}(200) &= 4\times[f_{Ga}(200)-f_{As}(200)] = 4\times[f^0_{Ga}(200)+f'_{Ga}+if''_{Ga}-f^0_{As}(200)-f'_{As}-if''_{As}] \\ &= 4\times[19.69-1.28-0.78i-21.05+0.93+1.00i] \end{aligned}$$

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so that $\Lambda_{ext}(200) = 8.1\,\mu\text{m}$ and $\sin\theta/2\mu = 3.9\,\mu\text{m}$, which is 2 times smaller

Integrated intensity

Starting with the expression for the Darwin curve it is possible to integrate and compute the integrated intensity of the reflected x-rays

$$R(x) = \begin{cases} (x - \sqrt{x^2-1})^2 & x \geq 1 \\ 1 & |x| \leq 1 \\ (x + \sqrt{x^2-1})^2 & x \leq -1 \end{cases}$$

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$$\int_{-\infty}^{\infty} R(x) dx = 2 + 2 \int_{1}^{\infty} (x - \sqrt{x^2 - 1})^2 dx$$

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Comparing the integrated intensity from a perfect crystal with that which was calculated for a mosaic crystal

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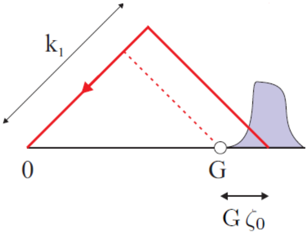
For the strong (400) reflection of GaAs this approximate ratio is $I_{SC}^{M}/I_{SC}^{P} \approx 6$ while for the weak (200) reflection it is $I_{SC}^{M}/I_{SC}^{P} \approx 0.2$

Harmonic suppression

The displacement of the Darwin curve varies inversely as the order, *m*, of the reflection.



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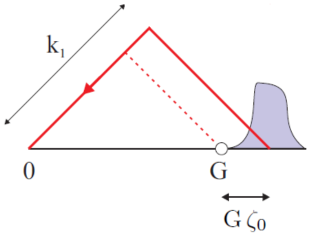

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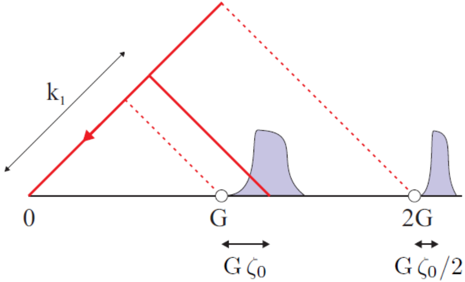
The displacement of the Darwin curve varies inversely as the order, *m*, of the reflection. The width varies as the inverse squared.



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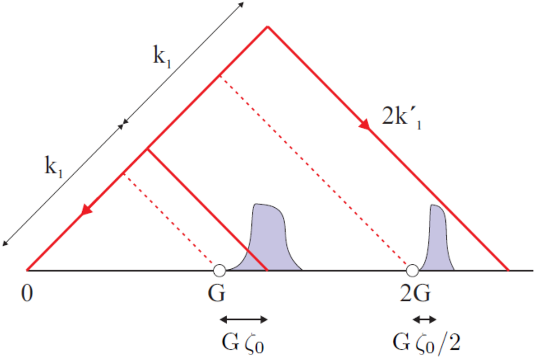

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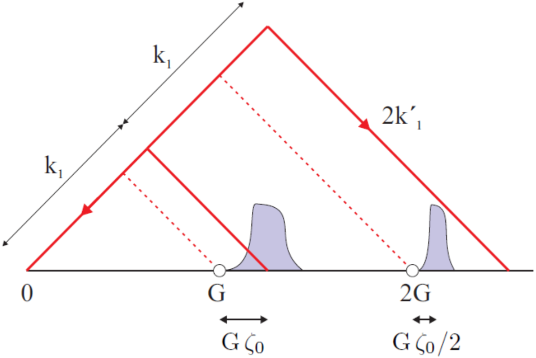

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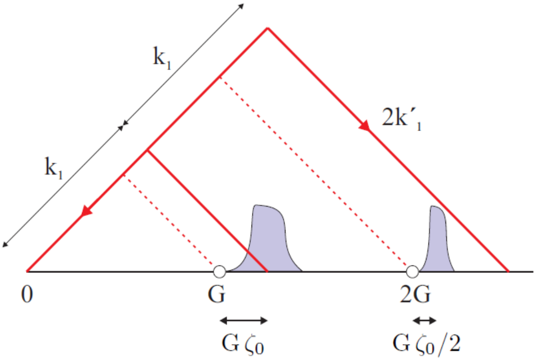
By tuning a bit off on the "high" side we get even more suppression. This is called "detuning".

Angular offset

We can calculate the angular offset by noting that the offset and width have many common factors.



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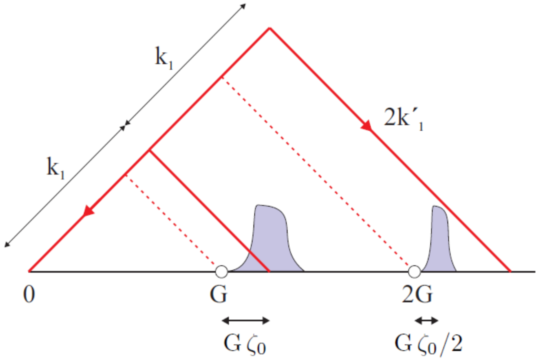

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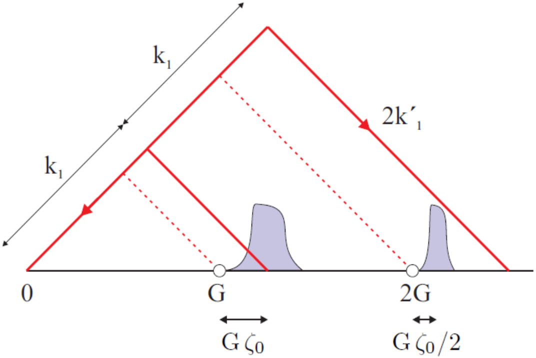

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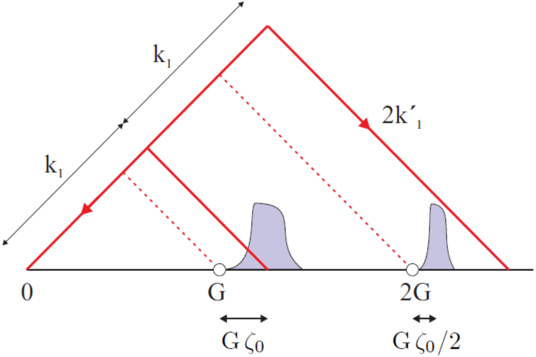

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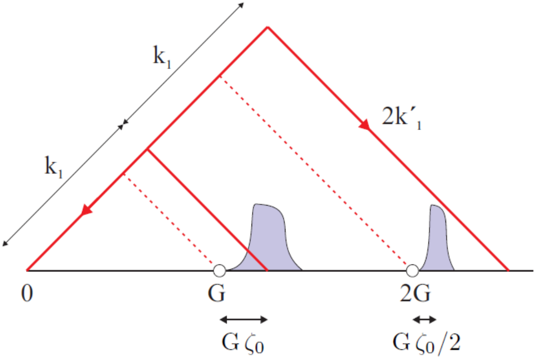

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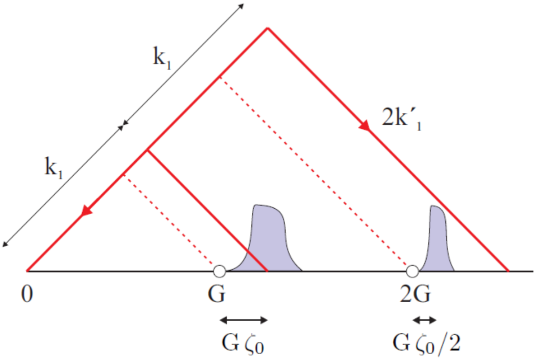

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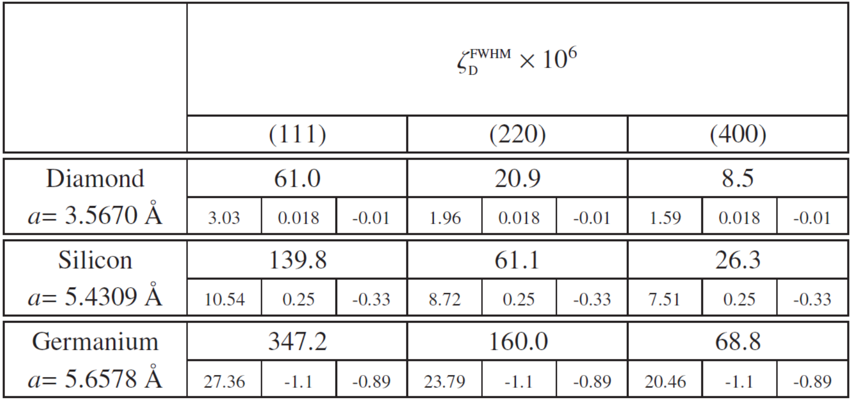
For the Si(111) at $\lambda = 1.54056$Å : $\omega_D^{total} = 0.0020^\circ$, $\Delta\theta^{off} = 0.0018^\circ$

Darwin widths



	$\zeta_D^{\mathrm{FWHM}} \times 10^6$								
	(111)			(220)			(400)		
Diamond a= 3.5670 Å	61.0			20.9			8.5		
	3.03	0.018	-0.01	1.96	0.018	-0.01	1.59	0.018	-0.01
Silicon a= 5.4309 Å	139.8			61.1			26.3		
	10.54	0.25	-0.33	8.72	0.25	-0.33	7.51	0.25	-0.33
Germanium a= 5.6578 Å	347.2			160.0			68.8		
	27.36	-1.1	-0.89	23.79	-1.1	-0.89	20.46	-1.1	-0.89

the quantities below the widths are $f^0(Q)$, f', and f'' (for $\lambda = 1.5405$ Å). For an angular width, multiply times $\tan\theta$ and for π polarization, multiply by $\cos(2\theta)$.

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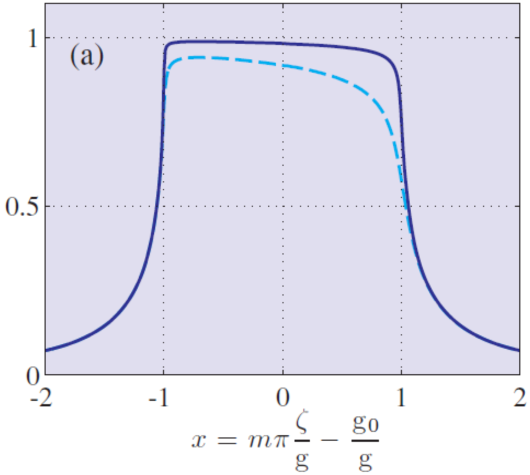
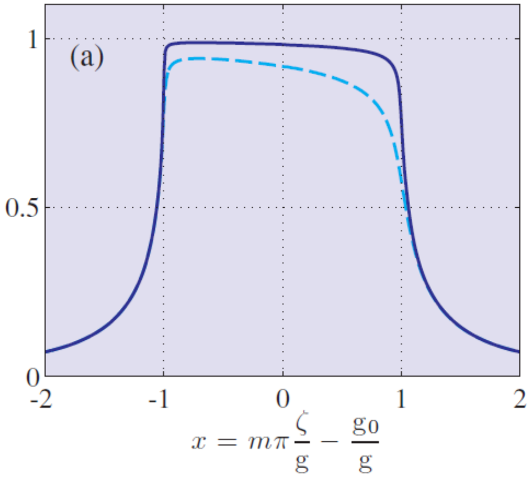
$$r(x_c) = \begin{cases} \frac{1}{x_c+\sqrt{x_c^2-1}} \approx x_c - \sqrt{x_c^2-1} & Re\{x_c\} \geq +1 \\ \frac{1}{x_c+i\sqrt{x_c^2-1}} \approx x_c - i\sqrt{x_c^2-1} & |Re\{x_c\}| \leq 1 \\ \frac{1}{x_c-\sqrt{x_c^2-1}} \approx x_c + \sqrt{x_c^2-1} & Re\{x_c\} \leq -1 \end{cases}$$

Absorption and the Darwin curve



Absorption and the Darwin curve



Silicon (111) Darwin curves

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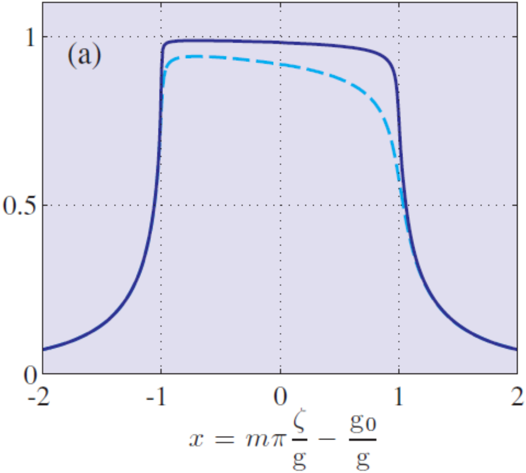

Silicon (111) Darwin curves

solid line is for $\lambda = 0.70926$ Å

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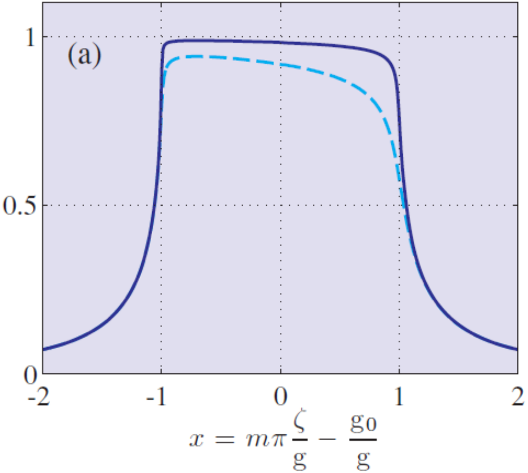

Silicon (111) Darwin curves

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dashed line is for $\lambda = 0.1.5405$ Å

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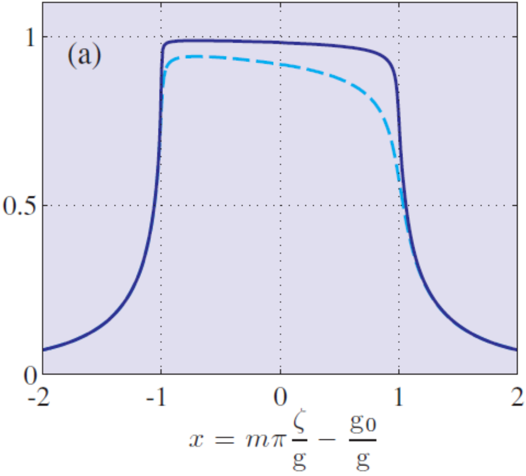

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absorption is highest at $x = +1$ since the standing wave field is in phase with the atomic planes

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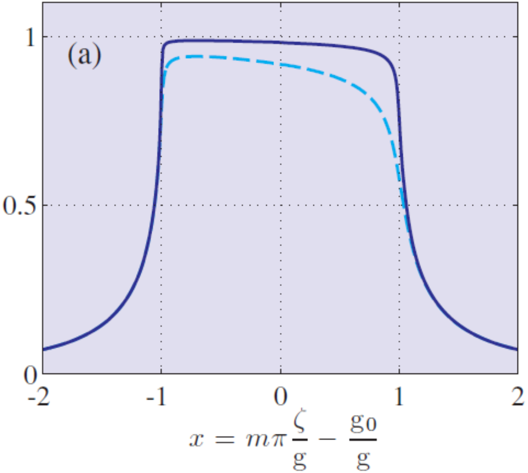

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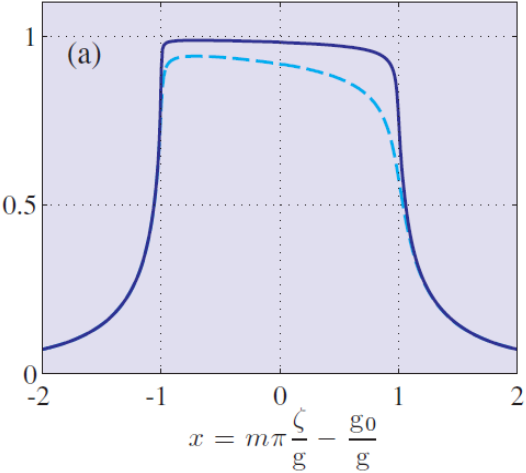

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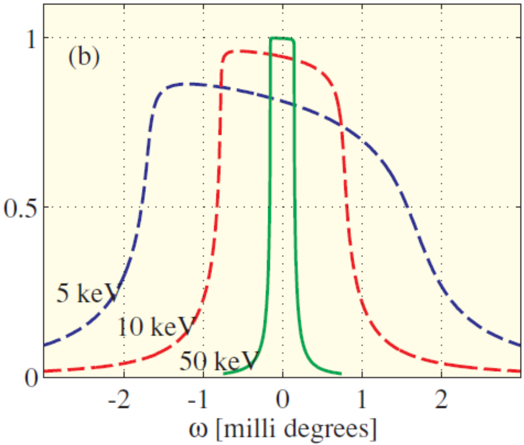
note that width of Darwin curve is independent of wavelength

Energy dependence



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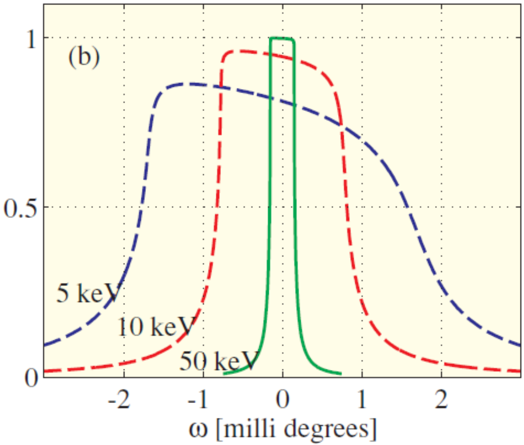

The angular Darwin width, w_D does depend on energy

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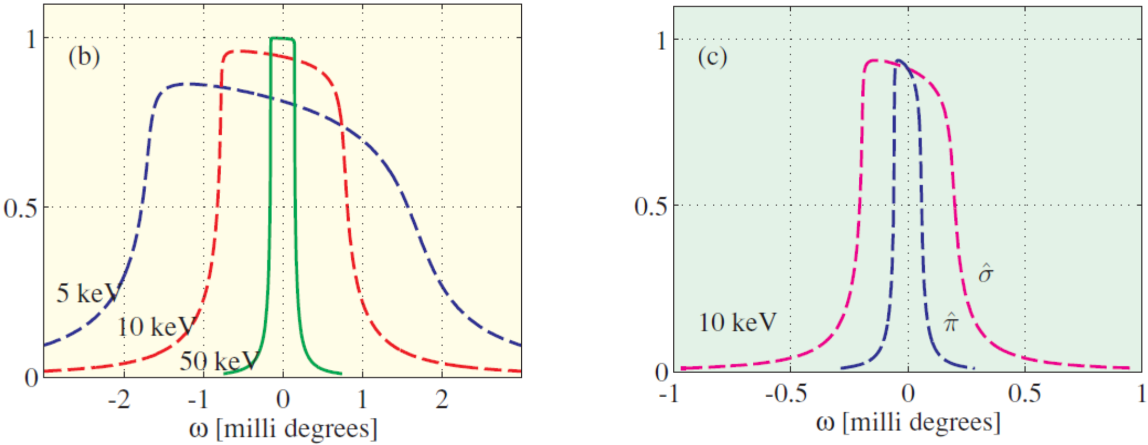

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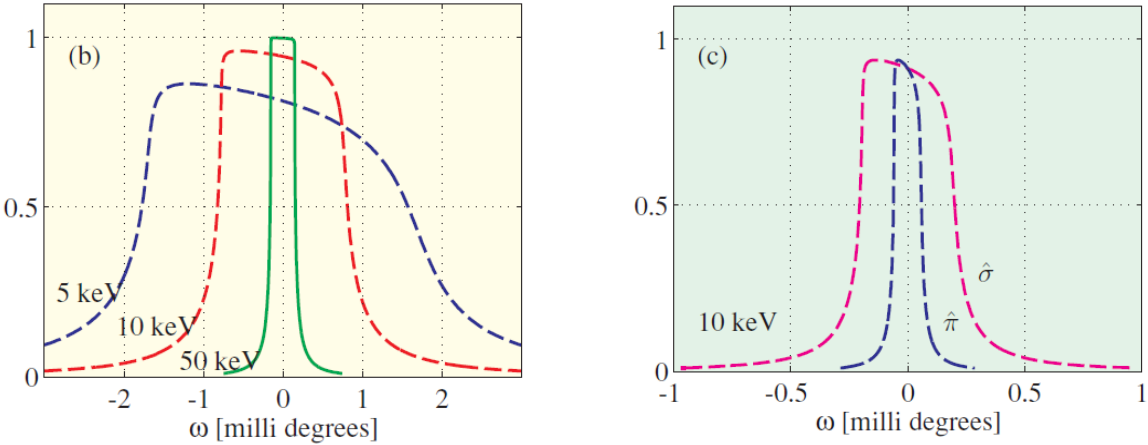
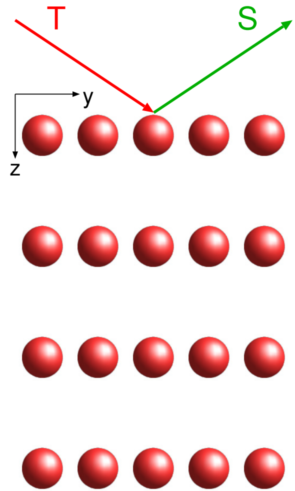


The angular Darwin width, w_D does depend on energy and polarization of the beam

Standing waves



When the Bragg condition is met for a perfect crystal, the total wavefield above the crystal is made up of the incident and diffracted wavefields, $T \propto e^{ik_y y} e^{ik_z z}$ and $S \propto e^{ik_y y} e^{-ik_z z}$

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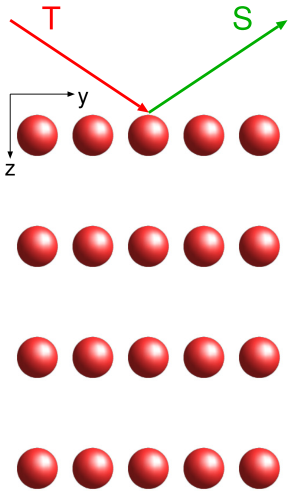

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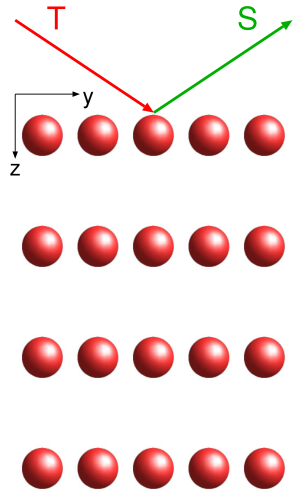

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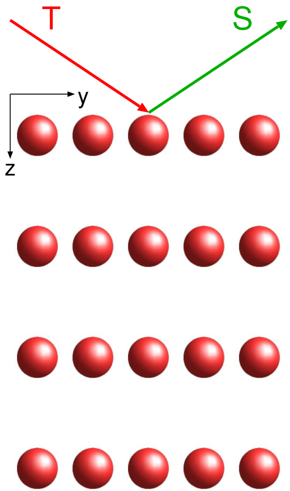

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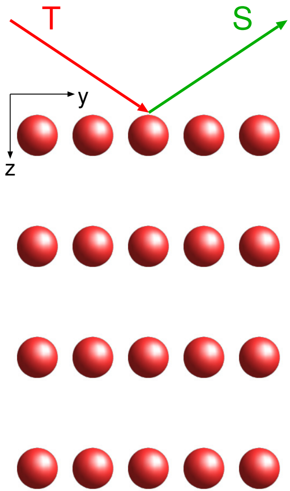

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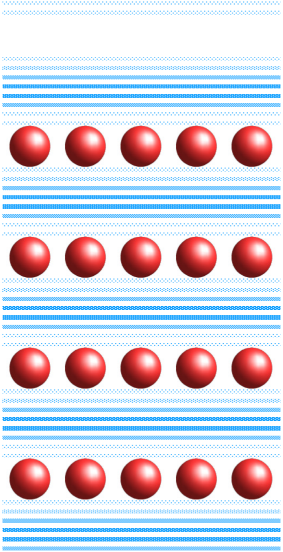

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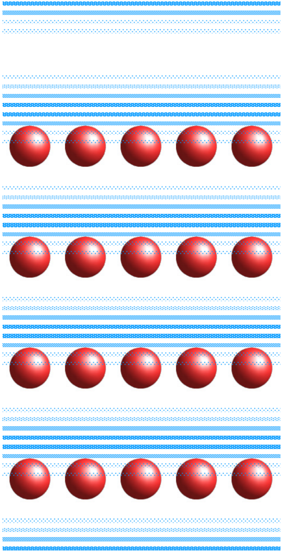

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as x varies along the Darwin curve, the phase of the standing wave at a position z varies by π

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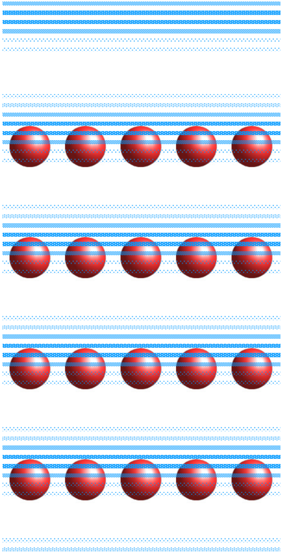

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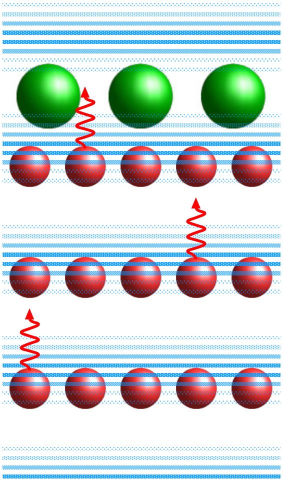
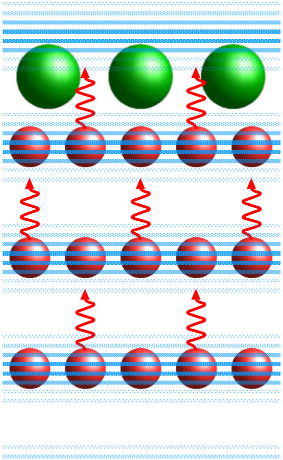
Standing wave experiments



Once a standing wave is established by diffraction from a perfect crystal, the nodes can be shifted in space by traversing the rocking curve

Standing wave experiments



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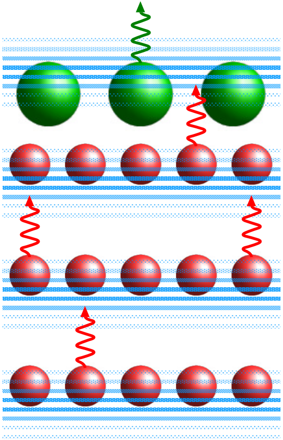
As the antinodes of the standing wave sweep past atoms in the crystal or on the surface, they will emit photoelectrons

Standing wave experiments



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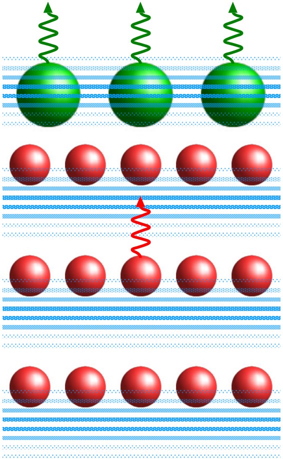

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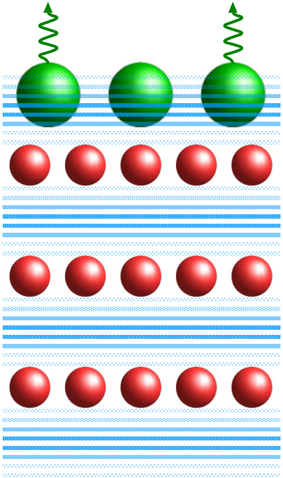

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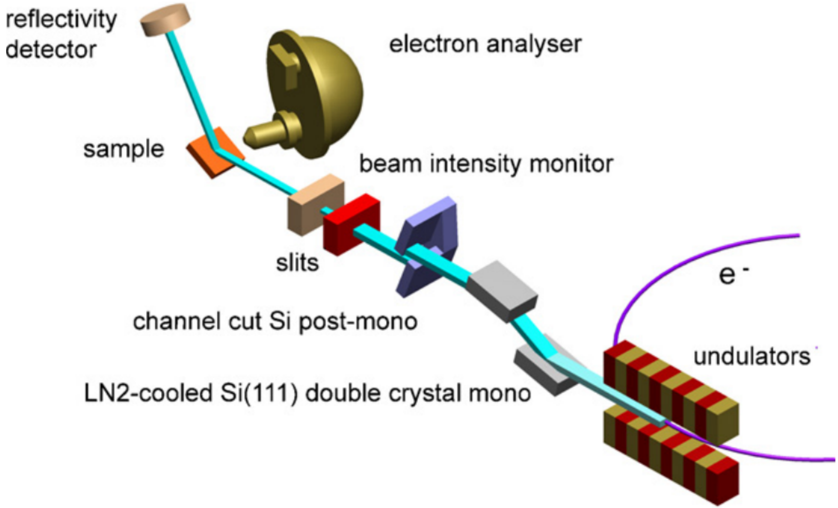
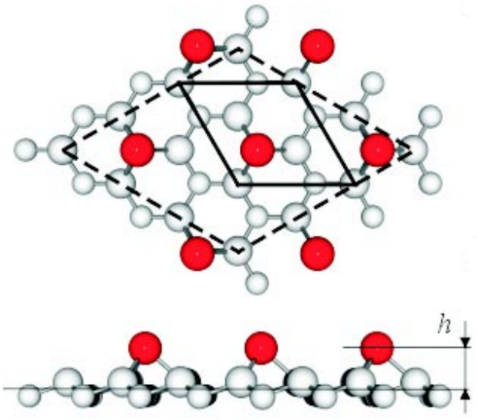
A high resolution monochromator is required for this kind of experiment

Beam line ID32 @ ESRF



Structure of Sn on Ge(111)

The low temperature 3 × 3 structure (dashed line) is well known but the room temperature $\sqrt{3} \times \sqrt{3}$ surface structure (solid line) is unresolved



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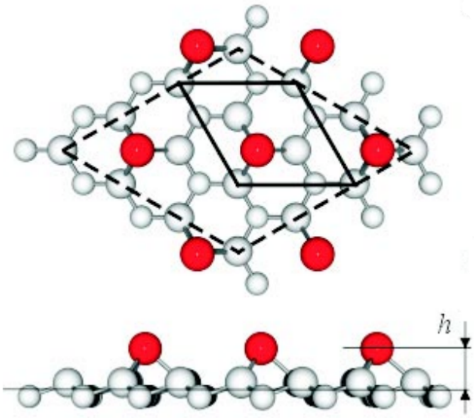

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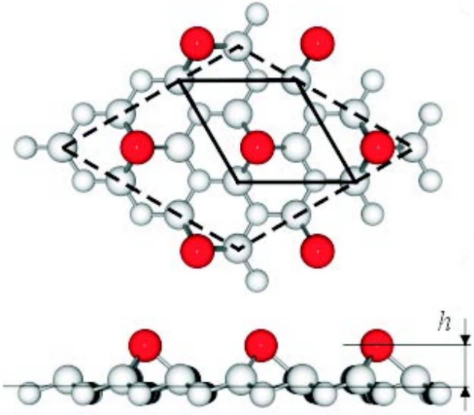

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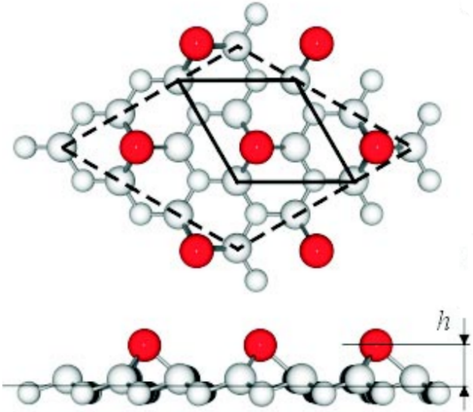
Above 0.2 ML, the $\sqrt{3} \times \sqrt{3}$ structure appears and then dominates



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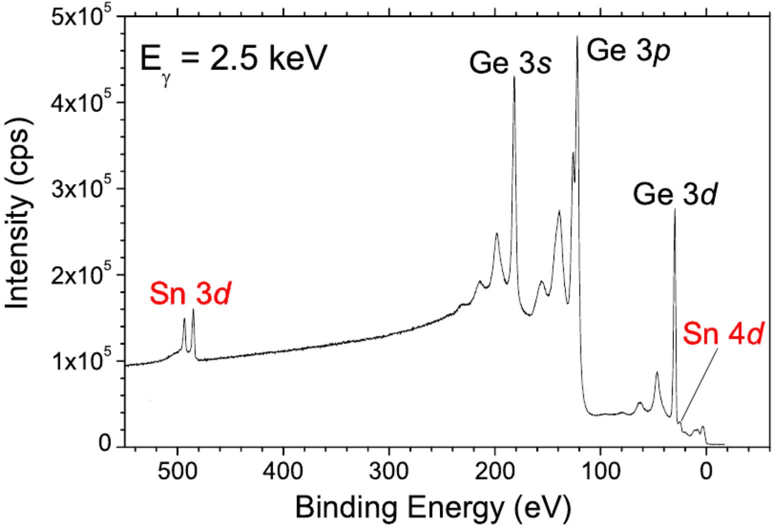

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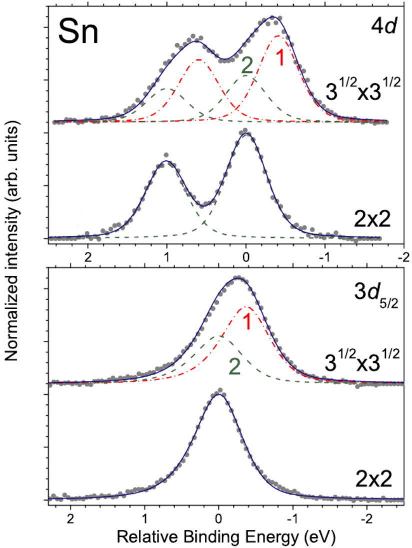

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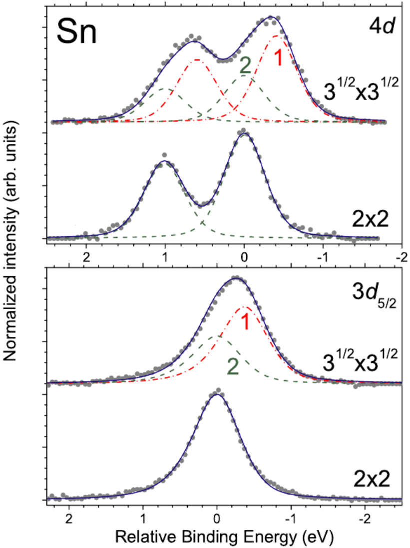

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The $\sqrt{3} \times \sqrt{3}$ structure shows two distinct chemical shifts, with the majority component, I_1, having a slightly lower binding energy than the minority component, I_2

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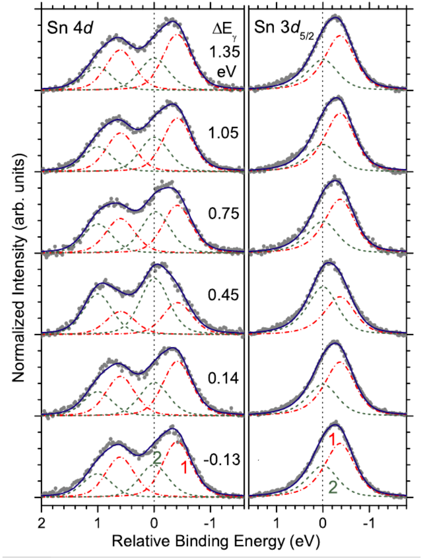
By varying the energy with a resolution of 500 meV, the standing wave is swept through the Sn layer



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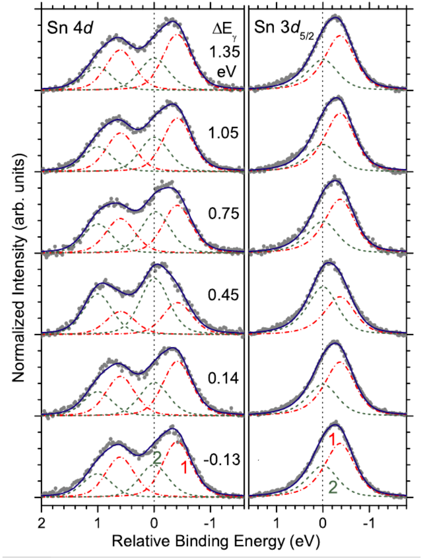

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At $\Delta E_\gamma = 0.45$ eV, the I_1/I_2 ratio almost completely inverts, showing that the two atom populations are at different heights above the surface

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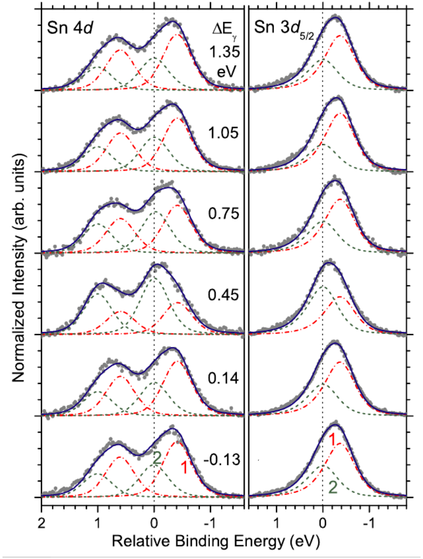
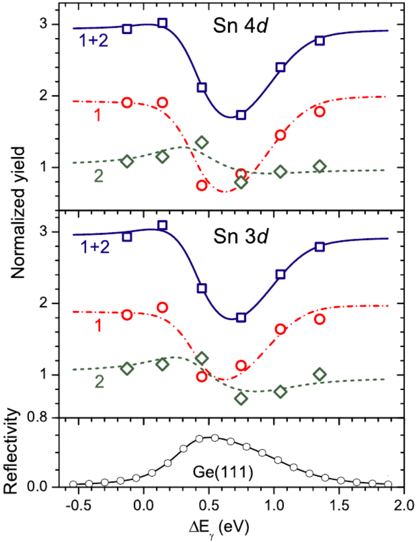


Structure of Sn on Ge(111)

The normalized peak intensities can be fitted to extract the relative positions of the two populations of atoms and their atomic ratio



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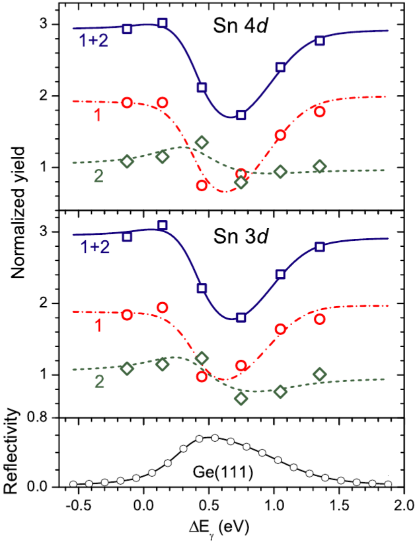

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Population 1 also has a lower binding energy, demonstrating that the binding energy is directly correlated to the height from the surface

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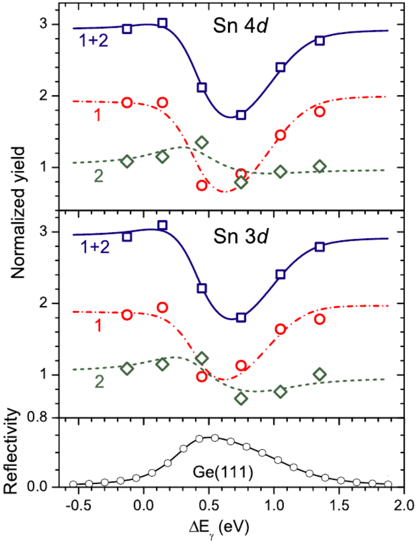

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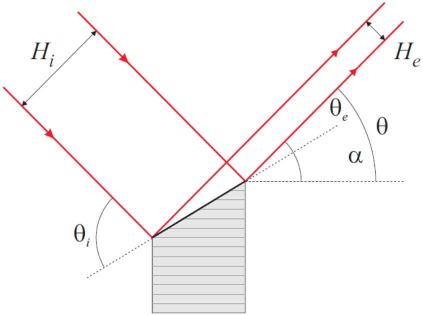
When the diffracting planes are not precisely aligned with the surface of the crystal the asymmetry angle, α, is the important parameter



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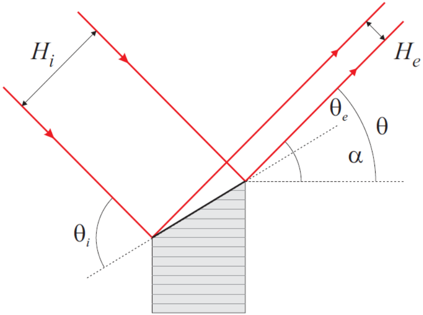

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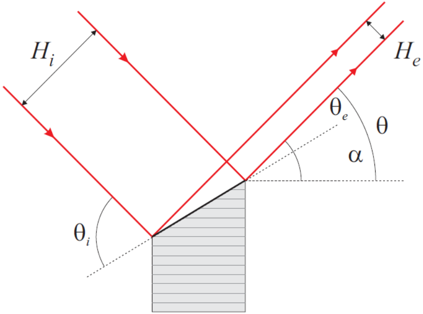

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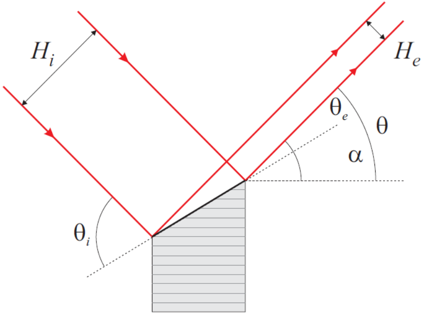

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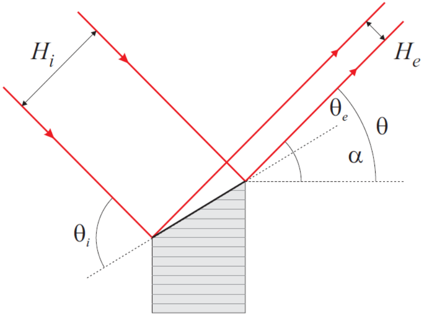

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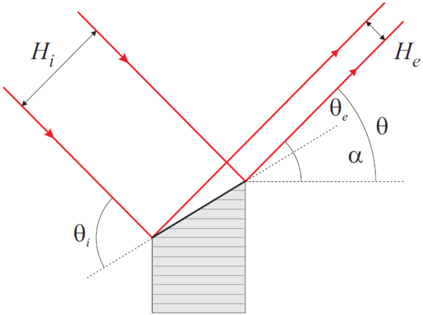

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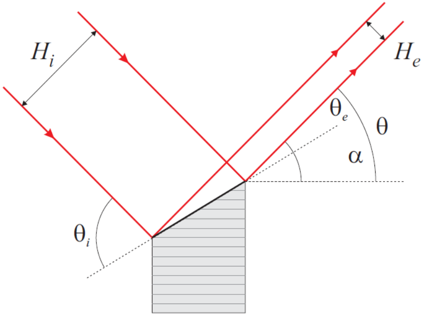

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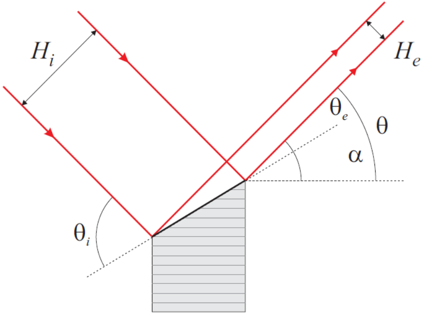

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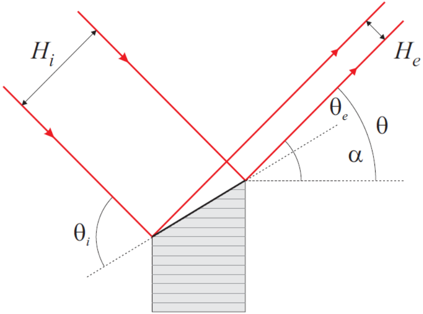

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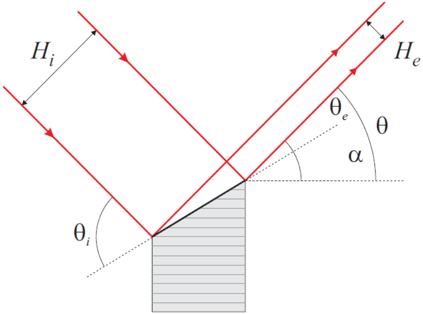

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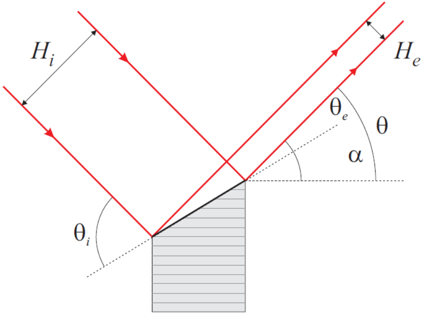

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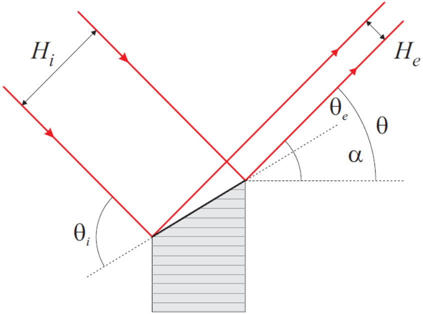

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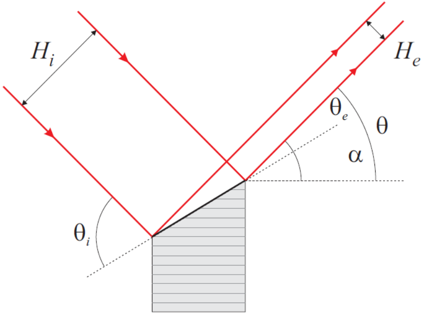

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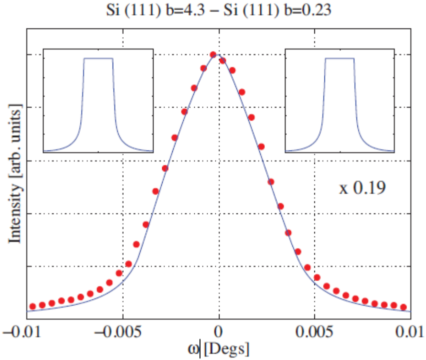

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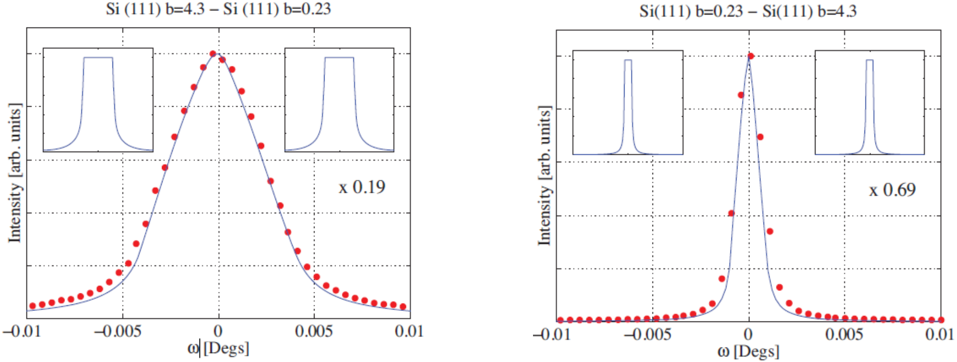

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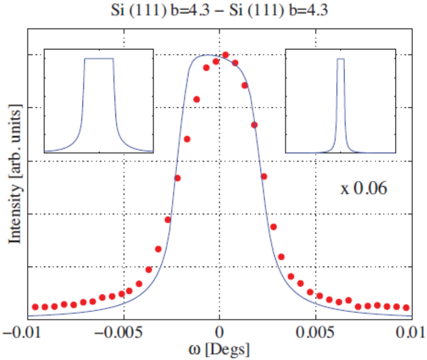

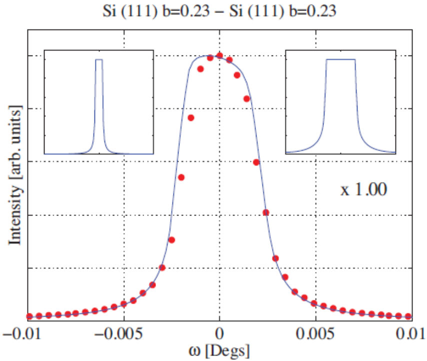

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