Today's outline - October 30, 2024

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- The Darwin curve

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- Extinction & absorption

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Reading Assignment: Chapter 7.2-3

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- The Darwin curve
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Reading Assignment: Chapter 7.2-3

Homework Assignment #05:
Chapter 5: 1,2,7,9,10
due Friday, November 01, 2024

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- The Darwin curve
- Extinction & absorption
- Standing waves
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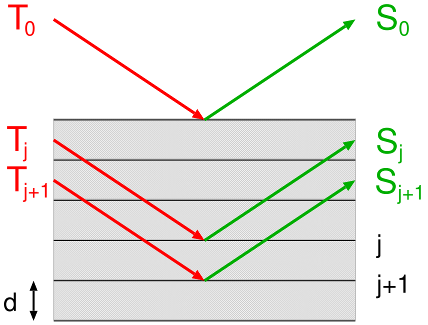
Reading Assignment: Chapter 7.2-3

Homework Assignment #05:
Chapter 5: 1,2,7,9,10
due Friday, November 01, 2024

Homework Assignment #06:
Chapter 6: 1,6,7,8,9
due Monday, November 11, 2024

Reflectivity of a perfect crystal

In order to calculate the absolute reflectivity curve, solve for S_0 and T_0 using the solution and the recursive relations.



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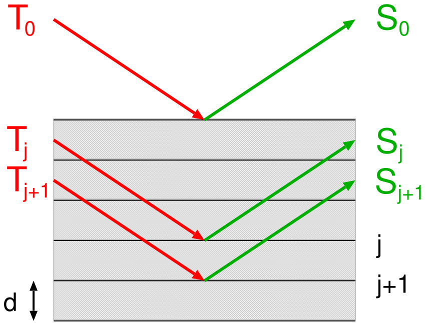

$$S_{j+1} = e^{-\eta} e^{im\pi} S_j$$

$$S_j = -igT_j + (1 - ig_0) S_{j+1} e^{i\phi}$$

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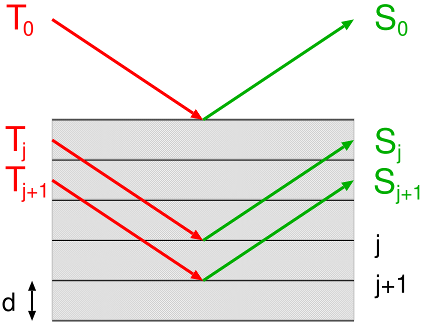

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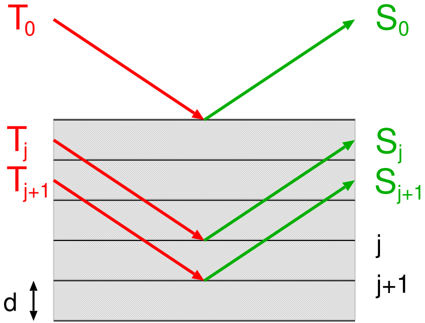

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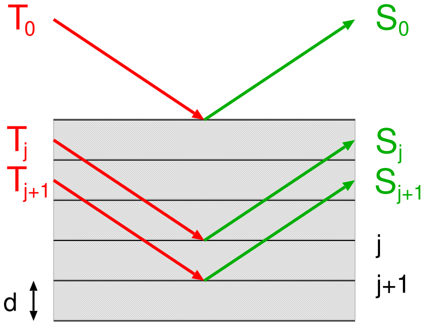

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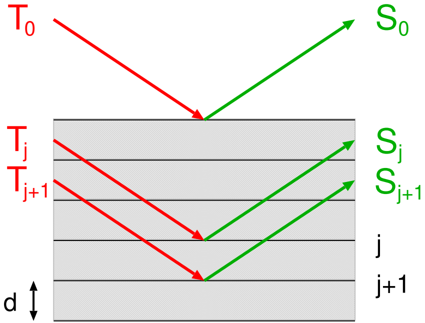

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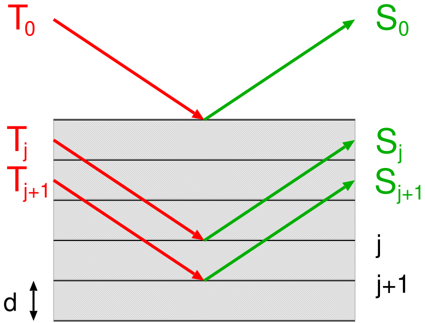

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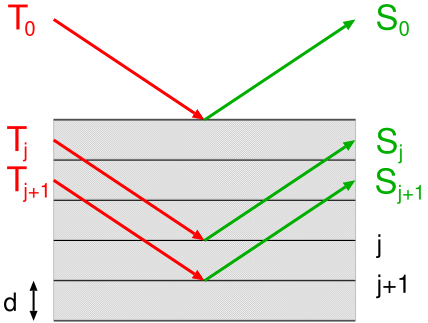

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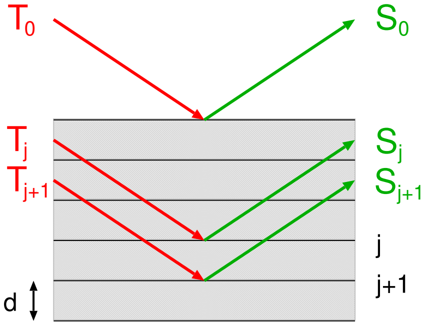

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Darwin reflectivity curve

$$r = \frac{S_0}{T_0} = \frac{g}{i\eta + (\Delta - g_0)}$$

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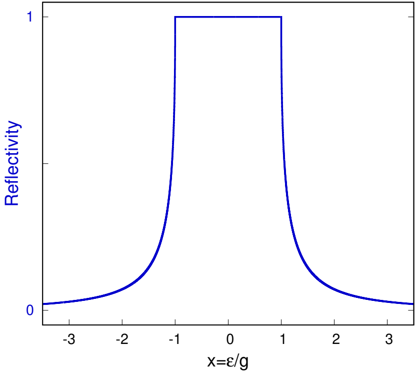

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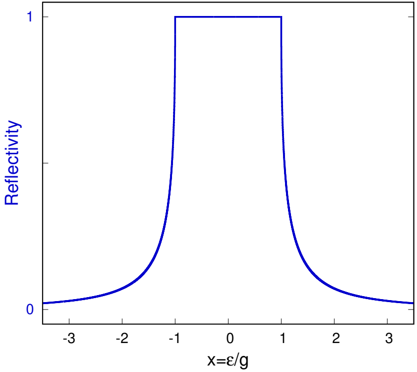

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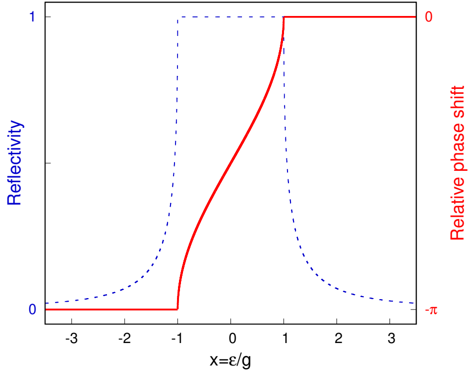

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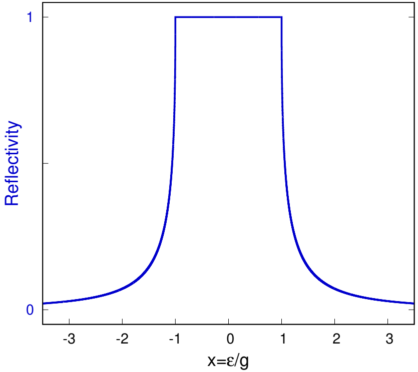
the relative phase between the scattered and transmitted waves varies from out of phase at $x = -1$ to in phase at $x = +1$

Darwin width



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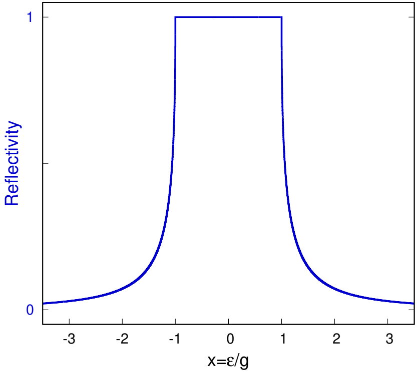

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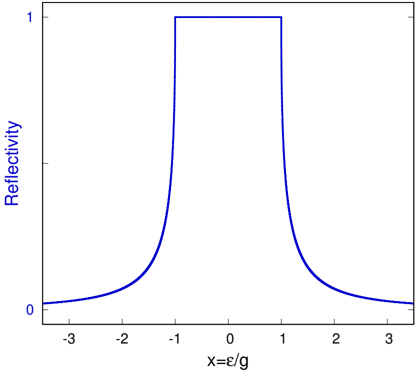

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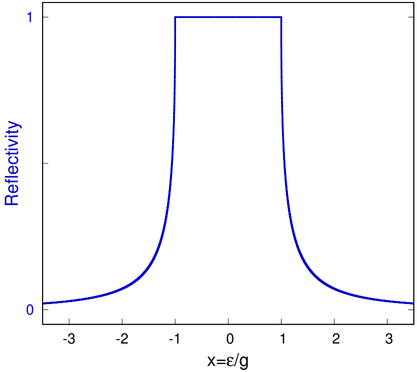

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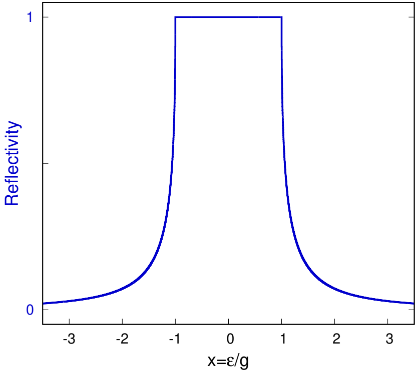

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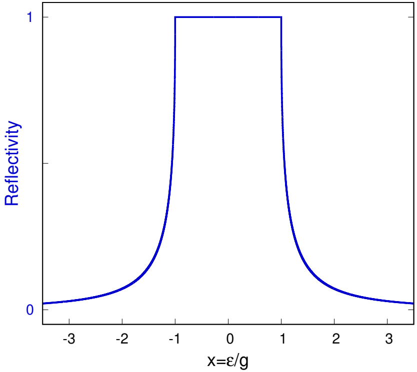

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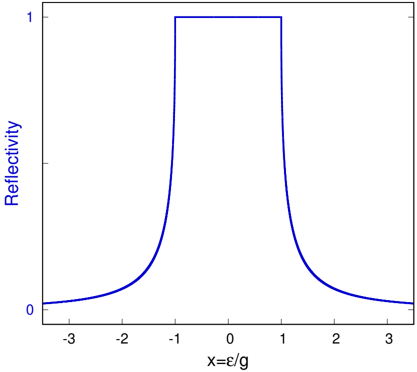

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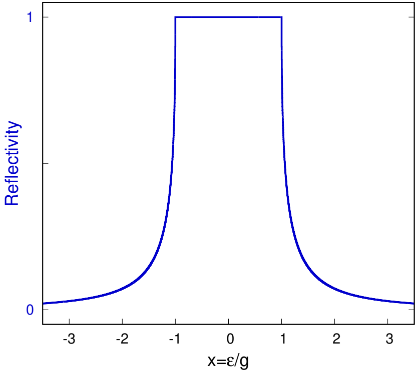

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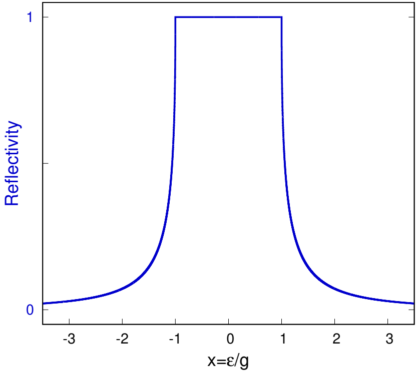

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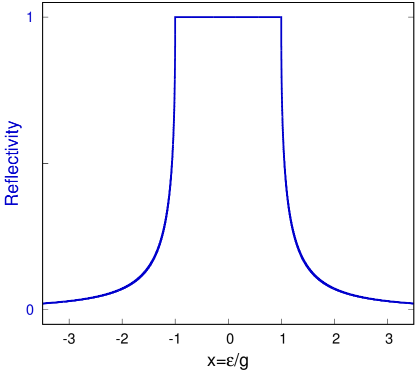

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$$e^{-N_{eff} Re\{\eta\}} = e^{-1/2} \quad \longrightarrow \quad N_{eff} = \frac{1}{2Re\{\eta\}}$$

multiplying by the layer spacing, d, gives the extinction depth

$$\Lambda_{ext} = N_{eff}\, d = \frac{d}{2Re\{\eta\}}$$

recalling that $\eta = g\sqrt{1-x^2}$, implies that Λ_{ext} varies across the Darwin reflectivity curve

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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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so that $\Lambda_{ext}(200) = 8.1\,\mu m$ and $\sin\theta/2\mu = 3.9\,\mu m$, 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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converting into an integrated intensity in terms of the variable ζ

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$$I_{SC}^{P} = \Phi_0 A_0 \frac{8\lambda^2 r_0|F|}{6\pi v_c \sin^2\theta} \tan\theta \left(\frac{1 + |\cos 2\theta|}{2}\right) e^{-M}$$

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Intensity comparison

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

Perfect crystal

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Mosaic crystal

$$I_{SC}^{M} = \frac{\Phi_0 A_0 \lambda^3 r_0^2 |F|^2}{2\mu v_c^2 \sin 2\theta} \left(\frac{1 + \cos^2 2\theta}{2} \right) e^{-2M}$$

Intensity comparison

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

Perfect crystal

$$I_{SC}^{P} = \frac{8\Phi_0 A_0 \lambda^2 r_0 |F|}{3\pi v_c \sin 2\theta} \left(\frac{1 + |\cos 2\theta|}{2} \right) e^{-M}$$

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Taking the ratio of these two intensities shows that the intensity from a mosiac crystal is significantly different than from a perfect crystal

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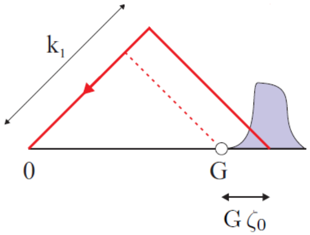
For the strong (400) reflection of GaAs this approximate ratio is $I_{SC}^{M}/I_{SC}^{P} \approx 6$ while for the weak (200) reflection it is $I_{SC}^{M}/I_{SC}^{P} \approx 0.2$

Harmonic suppression

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



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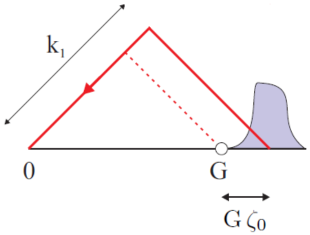

$$\zeta_0 = \frac{g_0}{\pi} = \frac{2d^2|F_0|r_0}{\pi m v_c}$$

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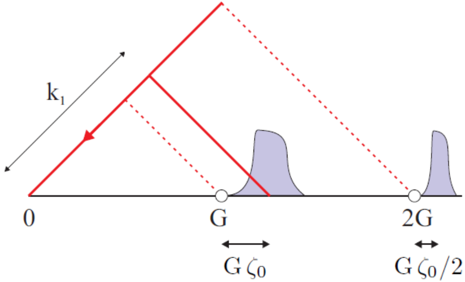
The displacement of the Darwin curve varies inversely as the order, m, of the reflection. The width varies as the inverse squared.



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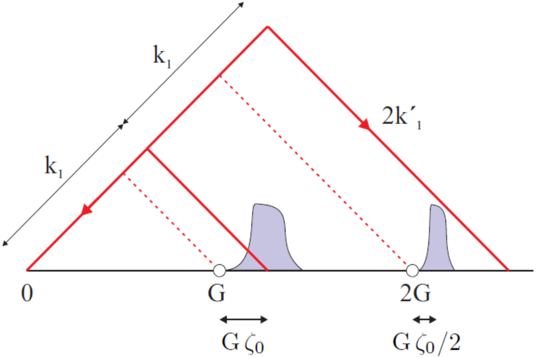

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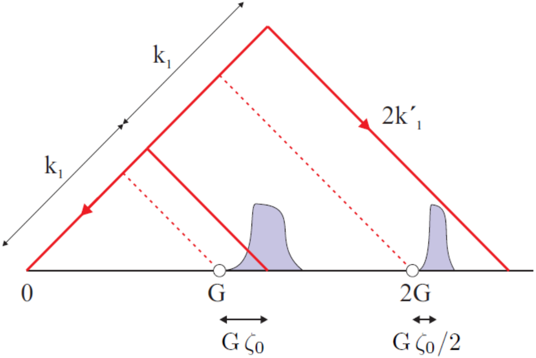

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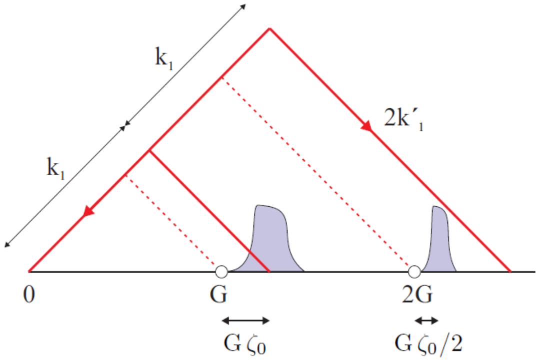
By tuning to the center of a lower order reflection, the high orders can be effectively suppressed.

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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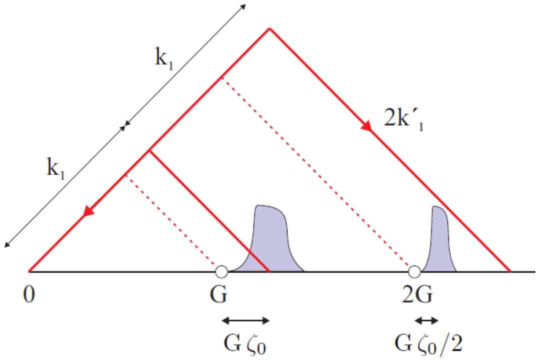

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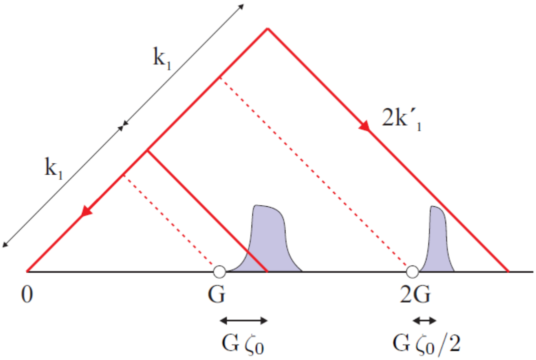
We can calculate the angular offset by noting that the offset and width have many common factors. Converting this to an angular offset.



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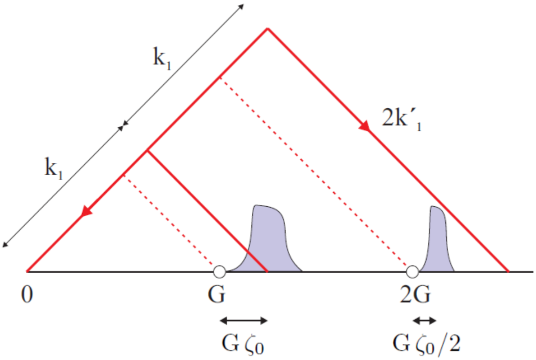

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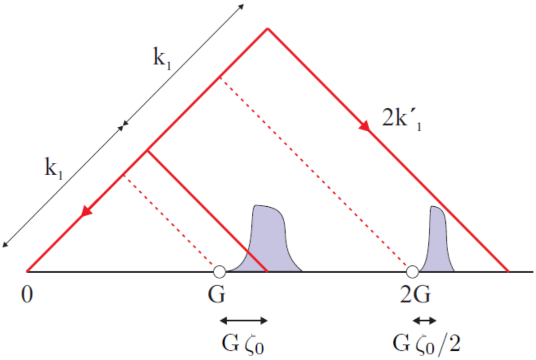

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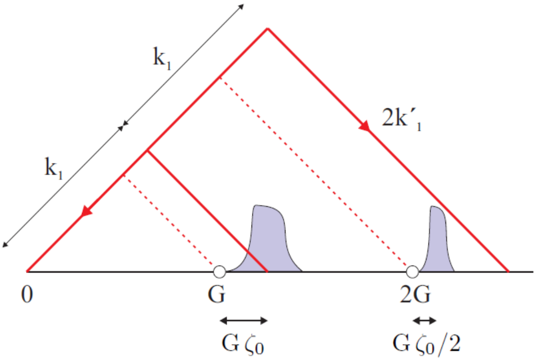

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For the Si(111) at $\lambda = 1.54056\text{Å}$: $\omega_D^{total} = 0.0020^\circ$, $\Delta\theta^{off} = 0.0018^\circ$

Darwin widths

	$\zeta_D^{FWHM} \times 10^6$								
	(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 $\lambda = 1.5405\,\text{Å}$). For an angular width, multiply times $\tan\theta$ and for π polarization, multiply by $\cos(2\theta)$.

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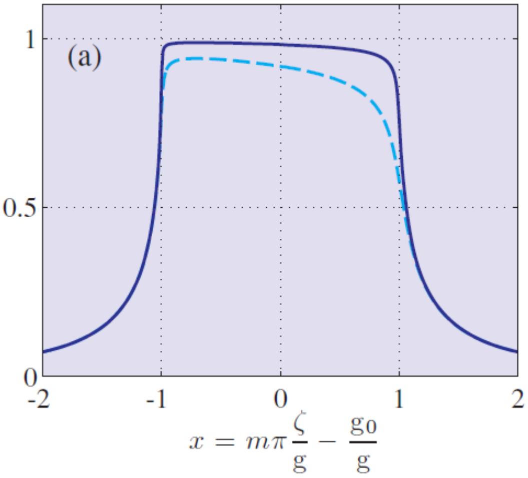
$$x_c = m\pi\frac{\zeta}{g} - \frac{g_0}{g}$$

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

Absorption and the Darwin curve



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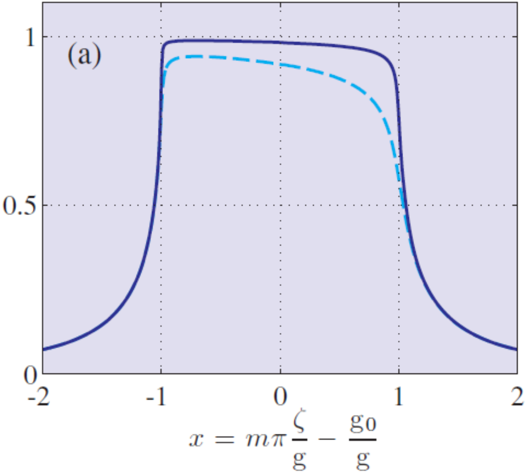

Silicon (111) Darwin curves

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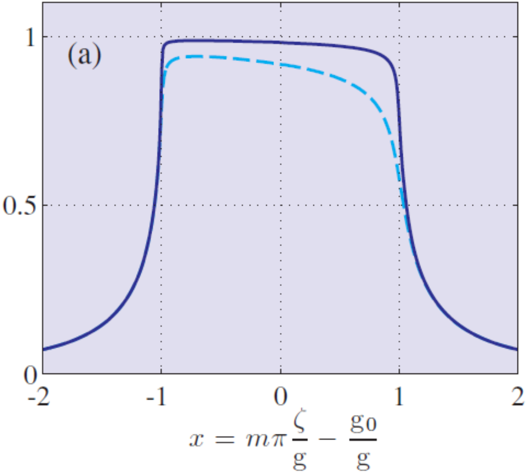

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solid line is for $\lambda = 0.70926$ Å

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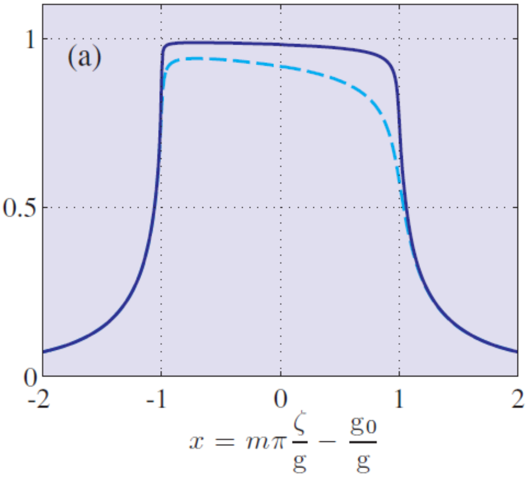

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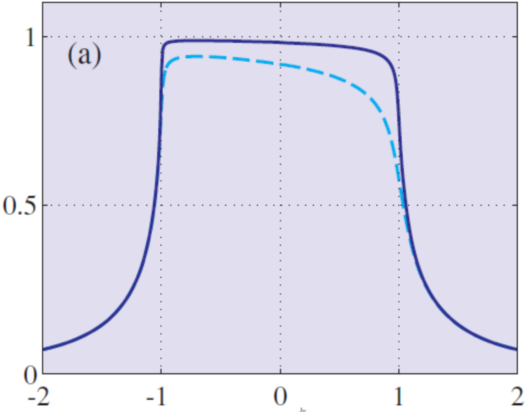

$$x = m\pi\frac{\zeta}{g} - \frac{g_0}{g}$$

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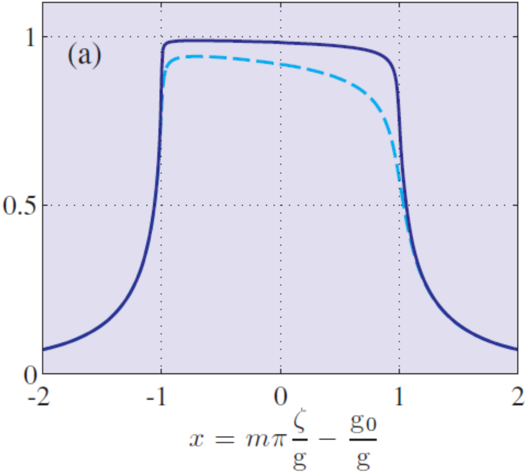

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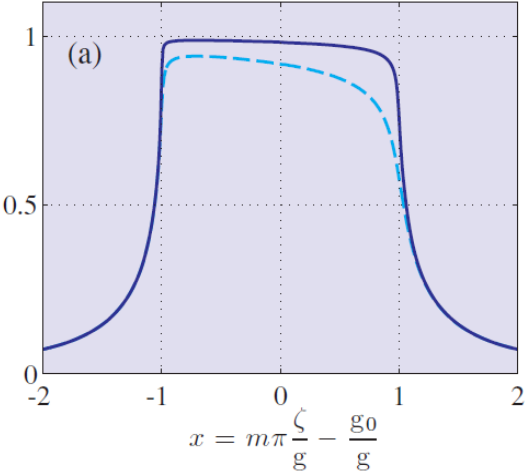

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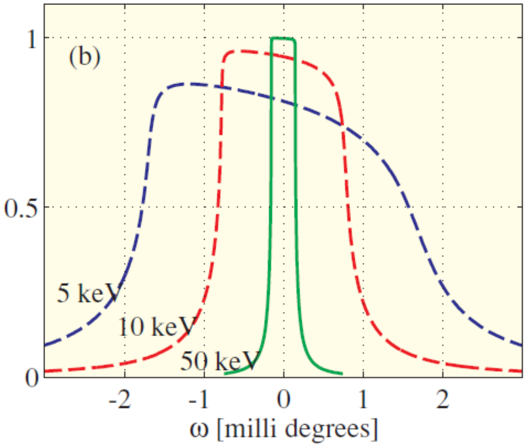
note that width of Darwin curve is independent of wavelength

Energy dependence



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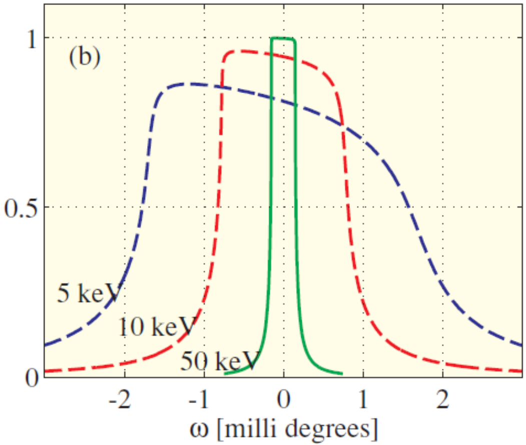

The angular Darwin width, w_D does depend on energy

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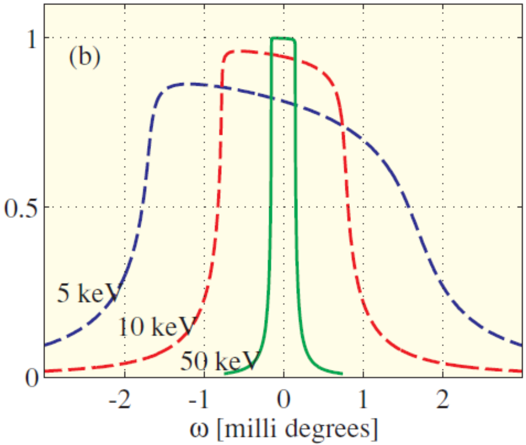

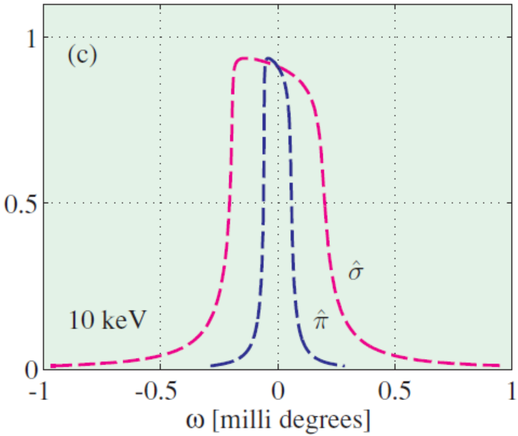

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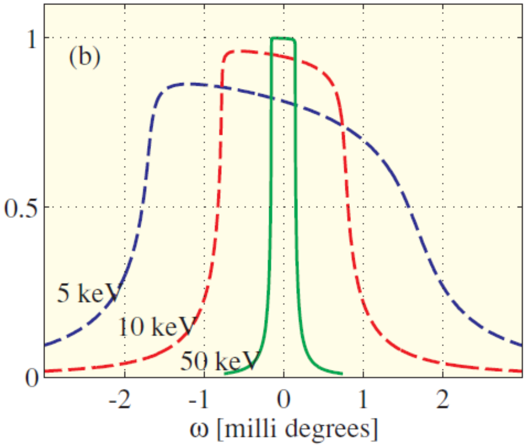
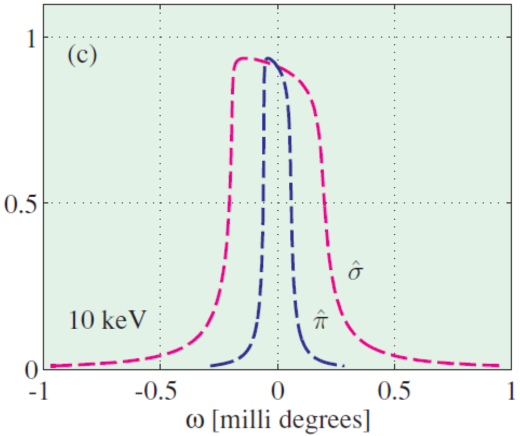
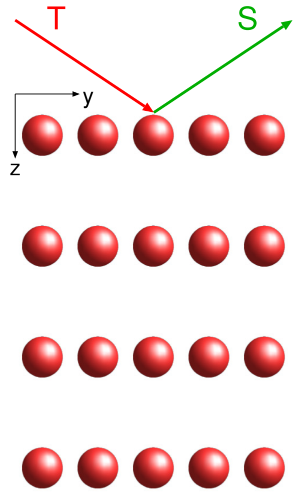




The angular Darwin width, w_D does depend on energy and polarization of the beam

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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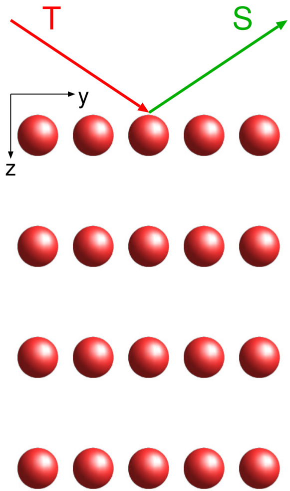

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at the crystal surface, $z = 0$ the amplitudes are given by T_0, and S_0 and the total wavefield for $z < 0$ is

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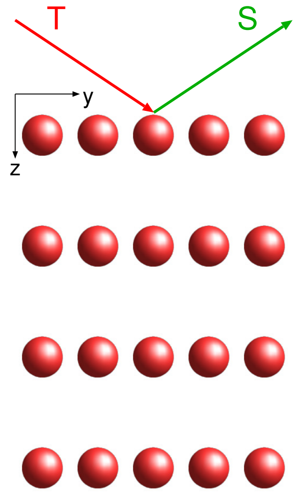

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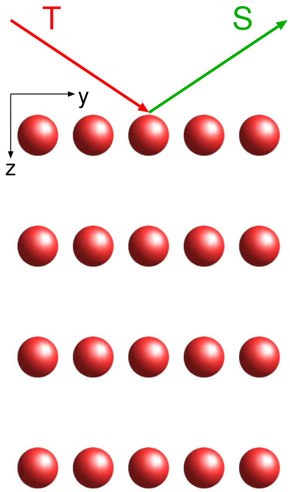

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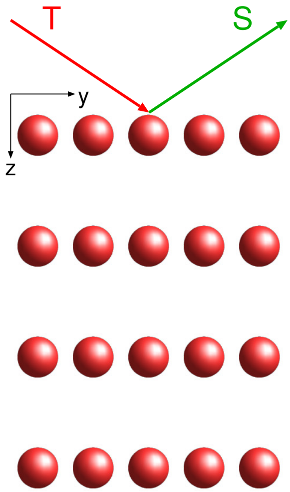
$$I(z,x) = T_0^2\left[e^{ik_z z} + |r|e^{i\phi}e^{-ik_z z}\right]\left[e^{-ik_z z} + |r|e^{-i\phi}e^{+ik_z z}\right]$$

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 $S \propto e^{ik_y y} e^{-ik_z z}$

at the crystal surface, $z = 0$ the amplitudes are given by T_0, and S_0 and the total wavefield for $z < 0$ is

$$A_{tot} = T_0 e^{ik_y y} \left[e^{ik_z z} + r e^{-ik_z z} \right], \quad r(x = \epsilon/g) = |r(x)| e^{i\phi}$$

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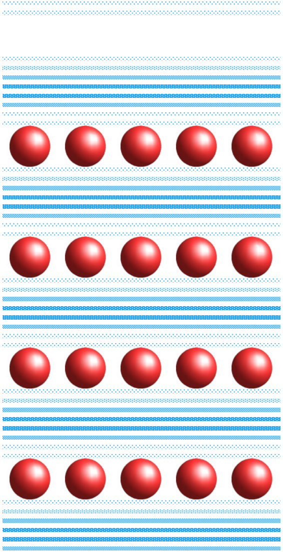
Standing waves



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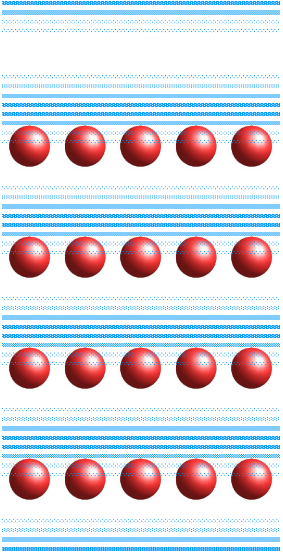

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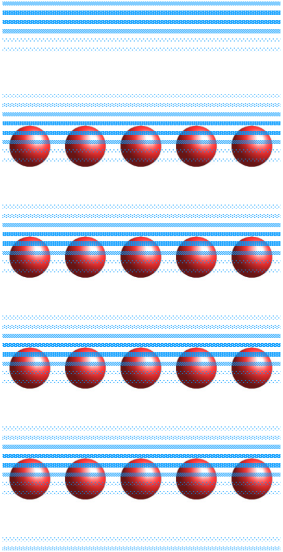
as x varies along the Darwin curve, the phase of the standing wave at a position z varies by π

Standing waves



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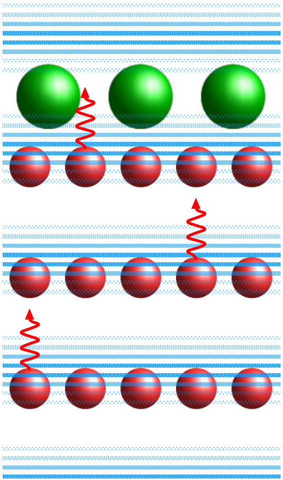
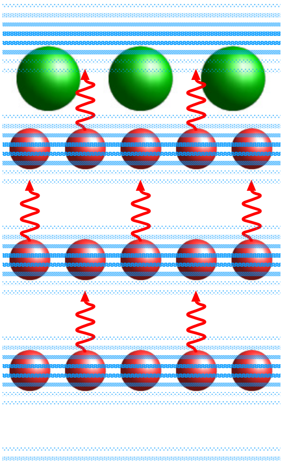
Standing wave experiments



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

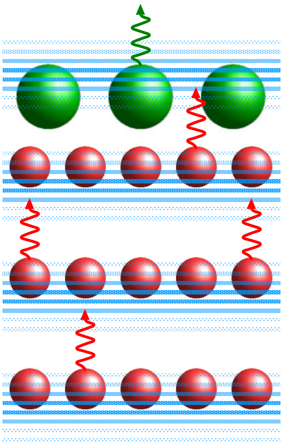
Standing wave experiments



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

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

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

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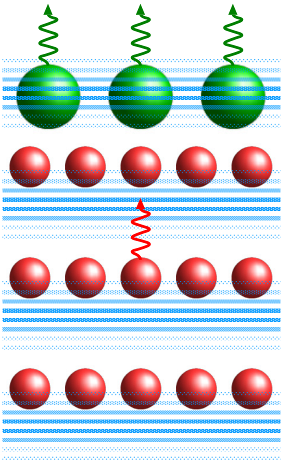
An electron or flourescence spectrometer is used to detect the signals and determine bond distances

Standing wave experiments



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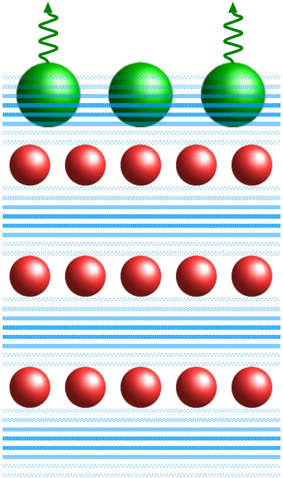

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A high resolution monochromator is required for this kind of experiment