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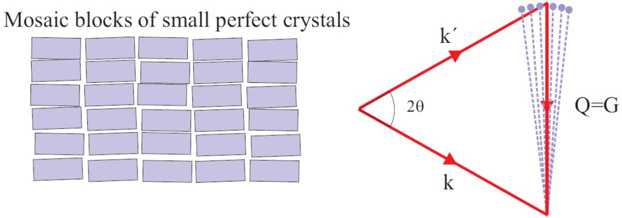
Homework Assignment #05:
Chapter 5: 1, 3, 7, 9, 10
due Wednesday, November 02, 2016

Friday, October 28 APS visit is cancelled!

Kinematical vs. dynamical diffraction



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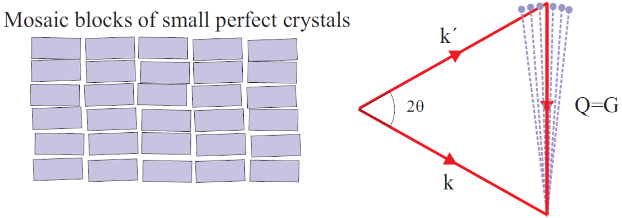

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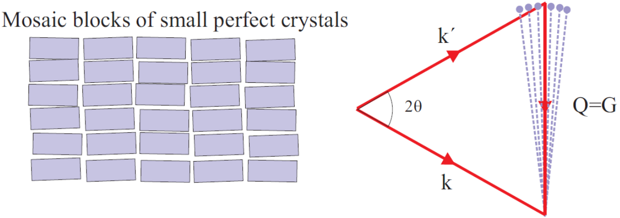

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For a perfect crystal, such as those used in monochromators, things are very different and we have to treat them specially using dynamical diffraction theory.

This theory takes into account multiple reflections, and attenuation of the x-ray beam as it propagates through the perfect crystal.

Bragg & Laue geometries

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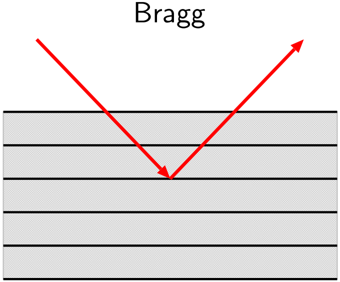
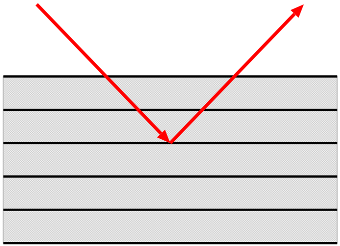


symmetric

Bragg & Laue geometries

Bragg



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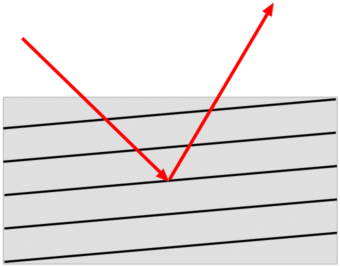

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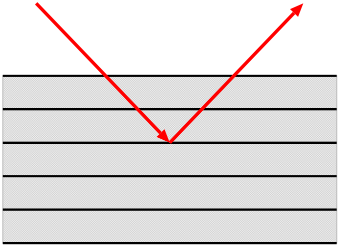

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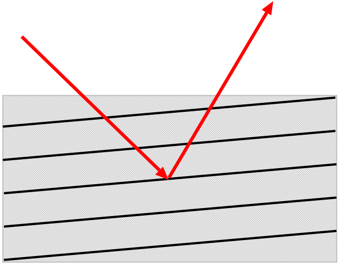

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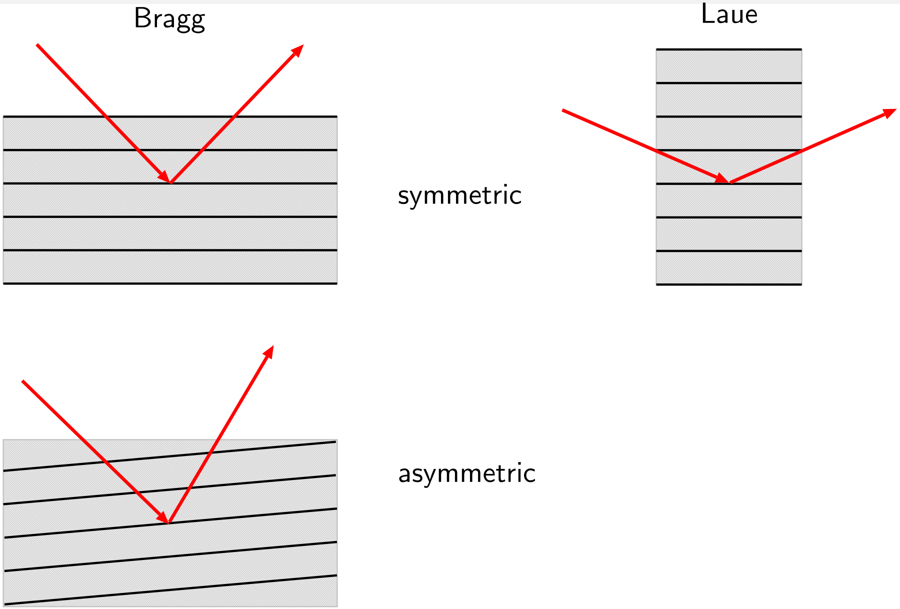

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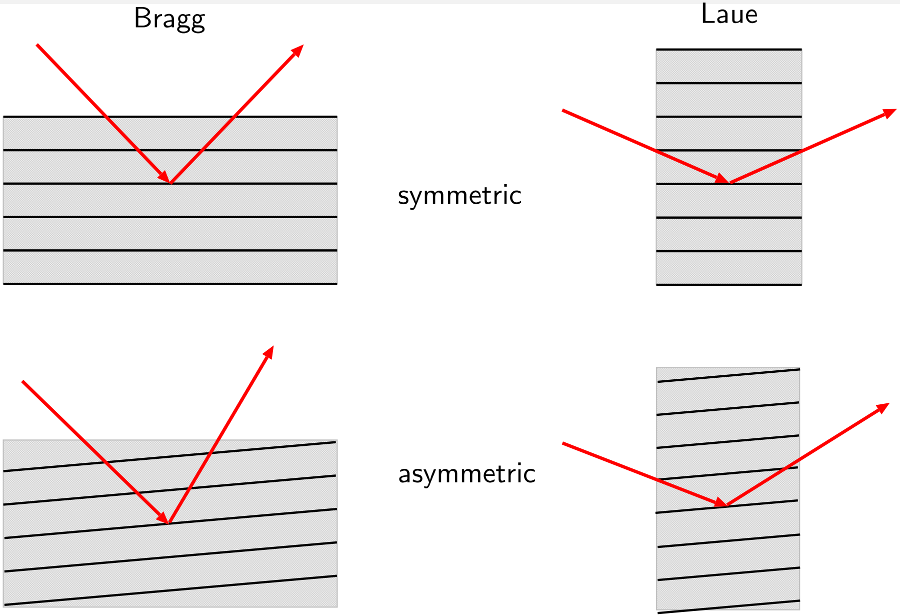

Scattering geometry

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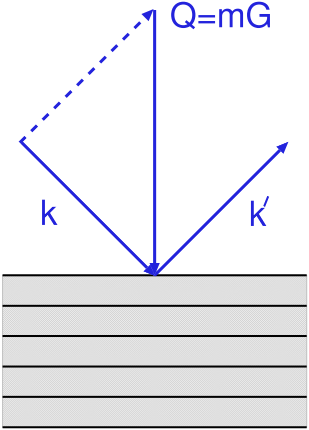

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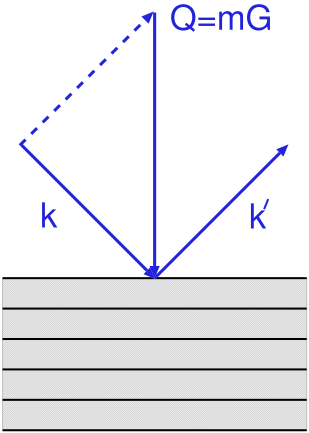
Consider symmetric Bragg geometry

We expect the crystal to diffract in an energy bandwidth defined by Δk



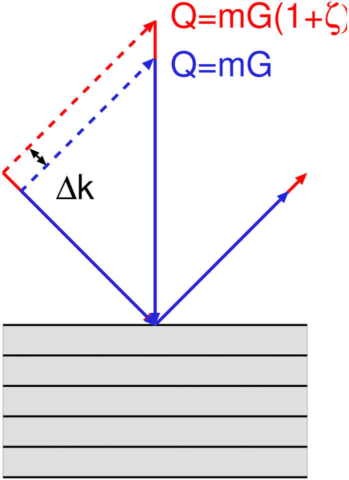
Consider symmetric Bragg geometry

We expect the crystal to diffract in an energy bandwidth defined by Δk

This defines a spread of scattering vectors such that

$$\zeta = \frac{\Delta Q}{Q} = \frac{\Delta k}{k}$$

called the relative energy or wavelength bandwidth



Dynamical diffraction - Darwin approach

The Darwin approach treats a perfect crystal as an infinite stack of atomic planes.

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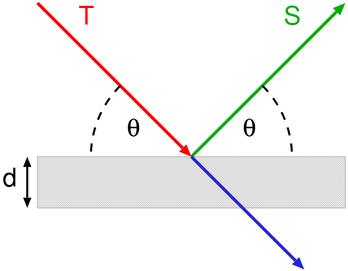

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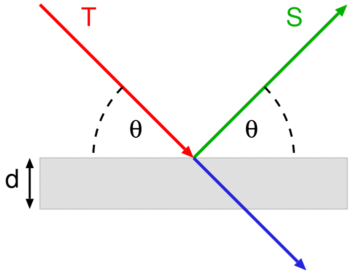
Considering a single thin slab with electron density ρ and thickness $d \ll \lambda$, the reflected and transmitted waves are



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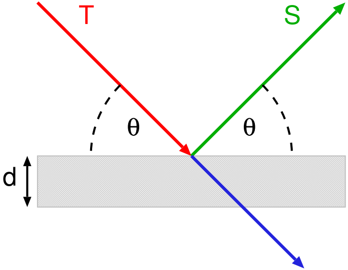

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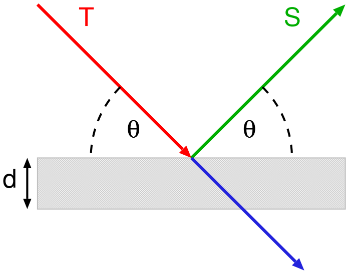

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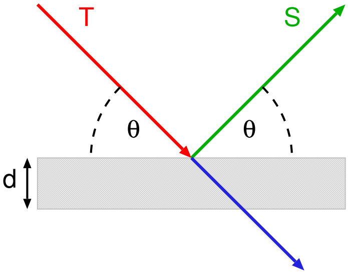

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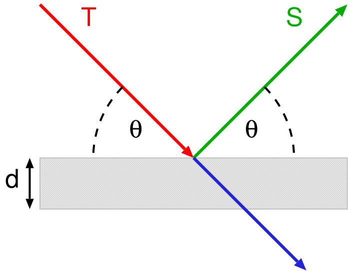

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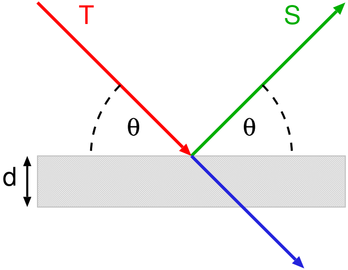

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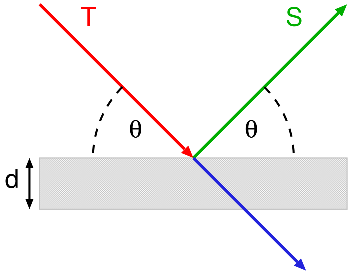

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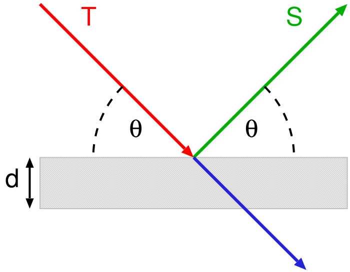

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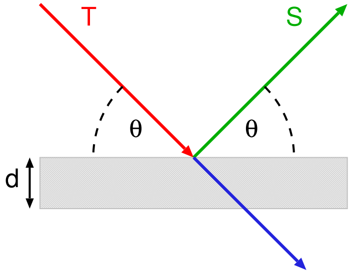

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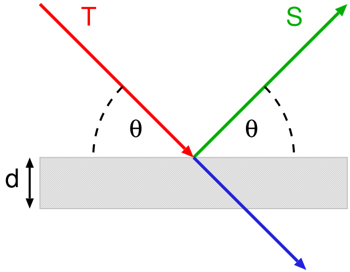

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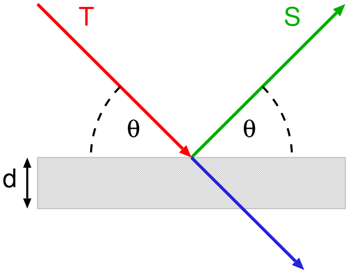

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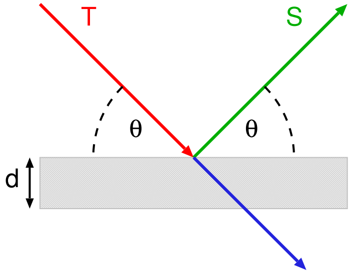
where F_0 is the forward scattering factor at $Q = \theta = 0$



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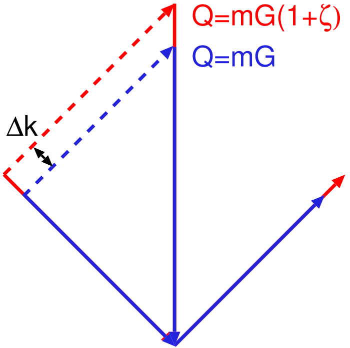


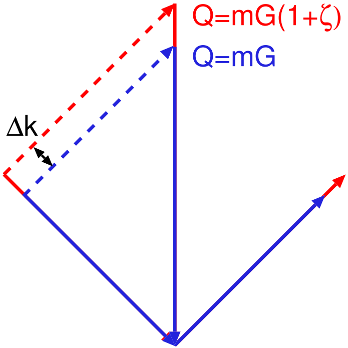
where the x-rays pass through each layer twice

these N unit cell layers will give a reciprocal lattice with points at multiples of $G = 2\pi/d$ we are interested in small deviations from the Bragg condition:

$$\zeta = \frac{\Delta Q}{Q} = \frac{\Delta k}{k} = \frac{\Delta \mathcal{E}}{\mathcal{E}} = \frac{\Delta \lambda}{\lambda}$$

Multiple Layer Reflection

$$r_N(Q) = -ig \sum_{j=0}^{N-1} e^{i(Qd-2g_0)j}$$



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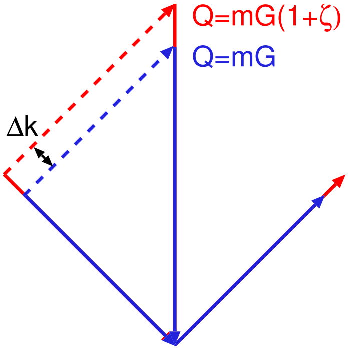

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$$Qd - 2g_0$$

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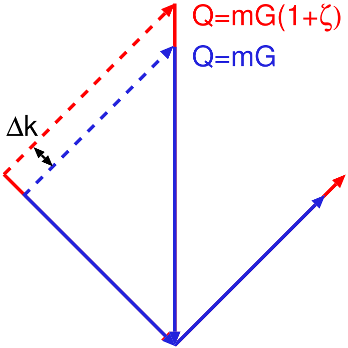

The term in the phase factor now becomes

$$Qd - 2g_0 = mG(1+\zeta)\frac{2\pi}{G} - 2g_0$$

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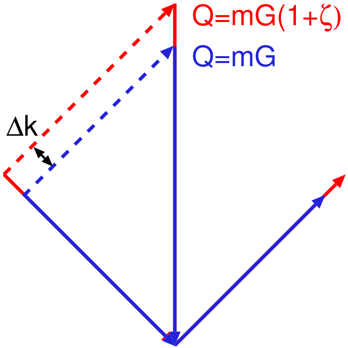

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$$\begin{aligned} Qd - 2g_0 &= mG(1+\zeta)\frac{2\pi}{G} - 2g_0 \\ &= 2\pi(m + m\zeta - \frac{g_0}{\pi}) \end{aligned}$$

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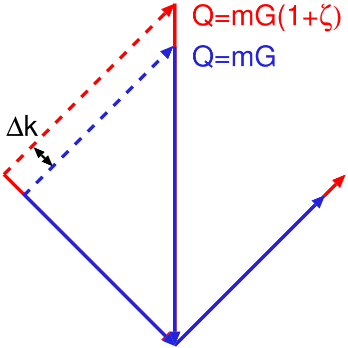

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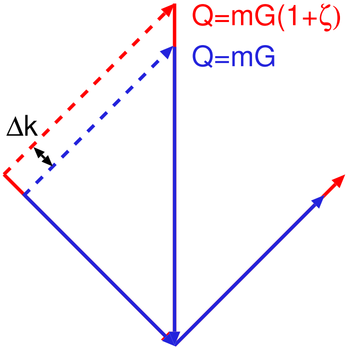

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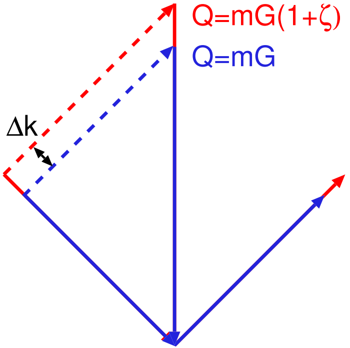

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$$\zeta_0 = \frac{g_0}{\pi} = \frac{2d^2|F_0|}{\pi m v_c} r_0$$

This describes a shift of the Bragg peak *away from the reciprocal lattice point*, the maximum being at $\zeta = \zeta_0/m$

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This describes a shift of the Bragg peak *away from the reciprocal lattice point*, the maximum being at $\zeta = \zeta_0/m$

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This geometric series can be summed as usual

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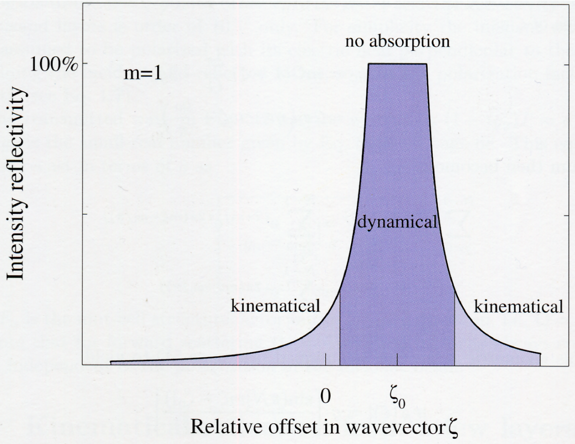
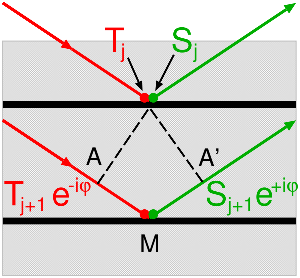


Difference equation review



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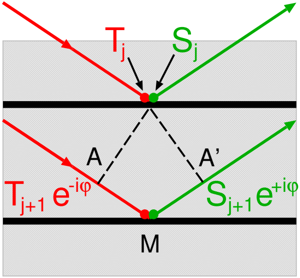

$$g = \frac{\lambda r_0 \rho d}{\sin\theta}, \qquad g_0 = \frac{|F_0|}{|F|} g$$

$$\Delta = m\pi\zeta, \qquad \zeta = \frac{\Delta\lambda}{\lambda}$$

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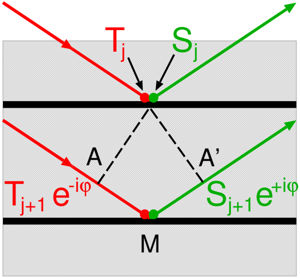

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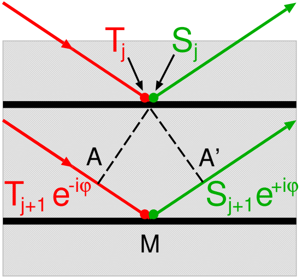

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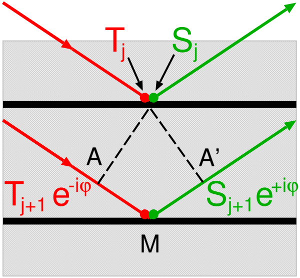

$$T_{j+1} = e^{-\eta} e^{im\pi} T_j$$
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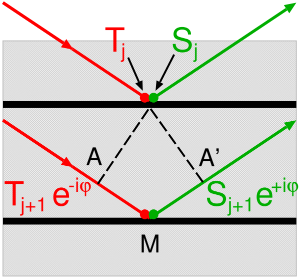

$$T_{j+1} = e^{-\eta} e^{im\pi} T_j$$
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$$i\eta = \pm\sqrt{(\Delta - g_0)^2 - g^2}$$

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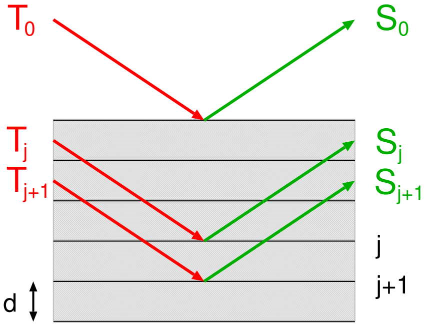
Reflectivity of a perfect crystal

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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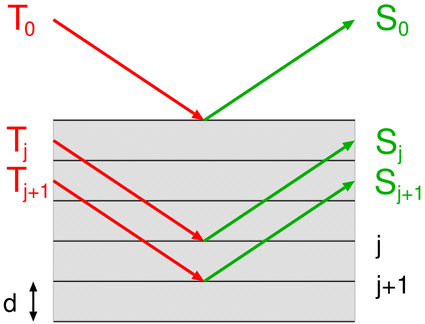

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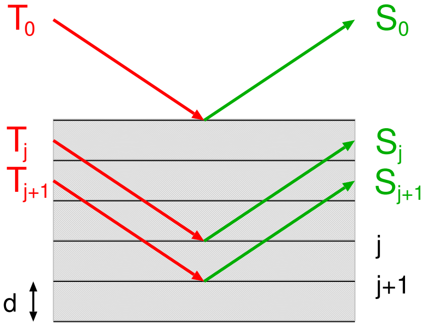

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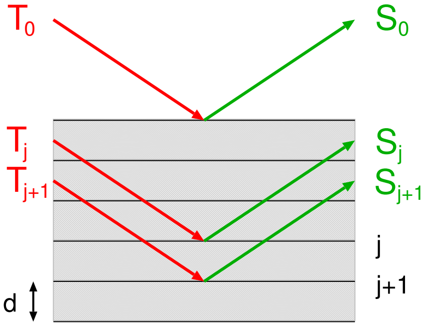

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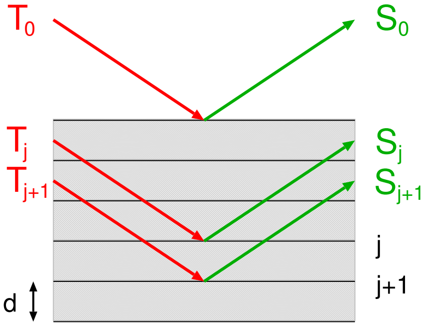

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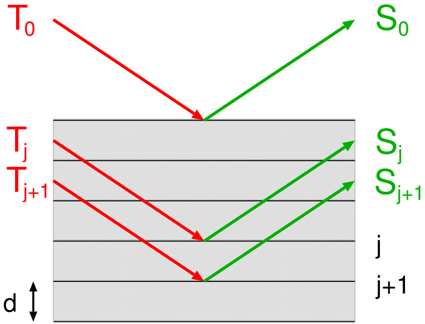

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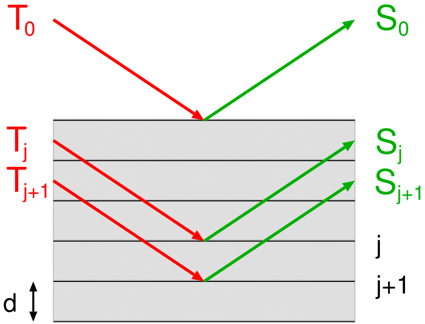

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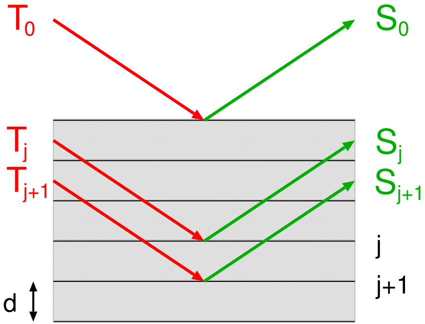

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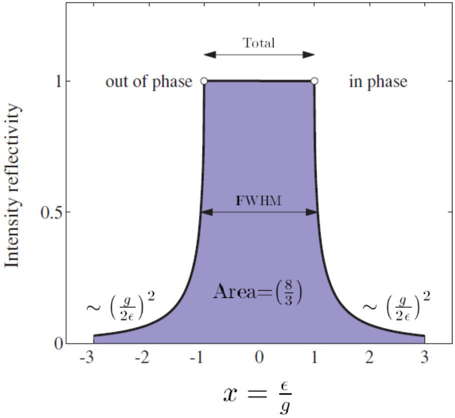
Darwin reflectivity curve

$$r = \frac{S_0}{T_0} = \frac{g}{i\eta + \epsilon} = \frac{g}{\epsilon \pm \sqrt{\epsilon^2 - g^2}}, \quad \epsilon = \Delta - \mathrm{g}_0 = \mathrm{m}\pi\zeta - \pi\zeta_0$$



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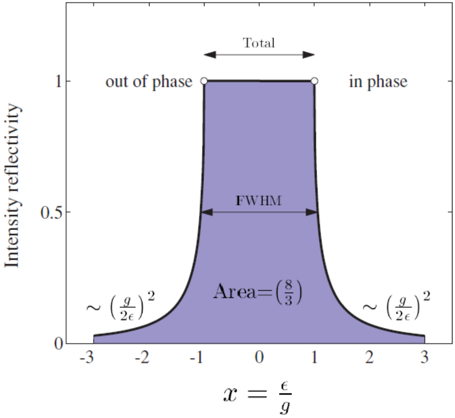
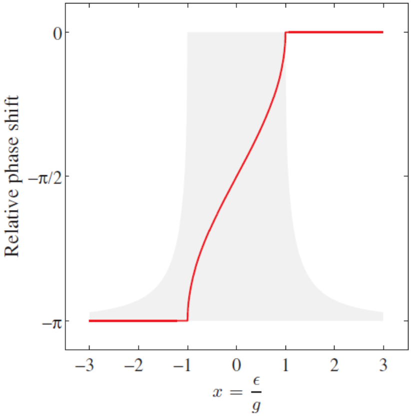
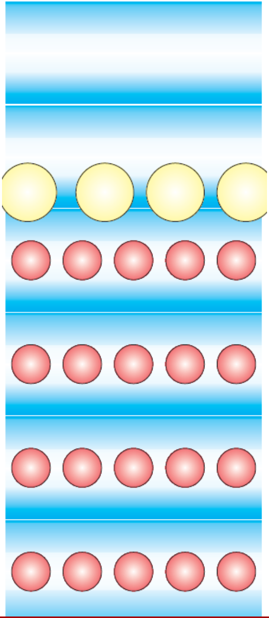


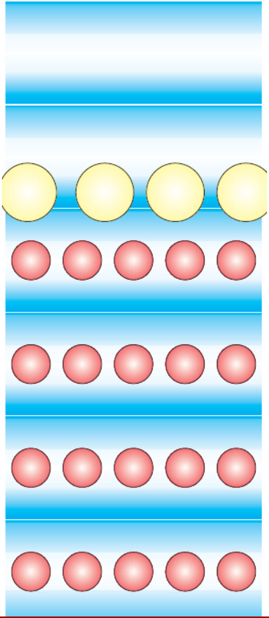




$\longleftarrow x = -1$

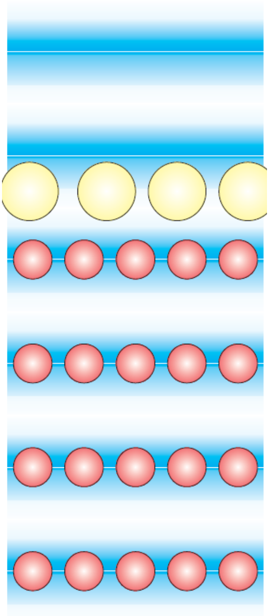
out of phase

Standing waves

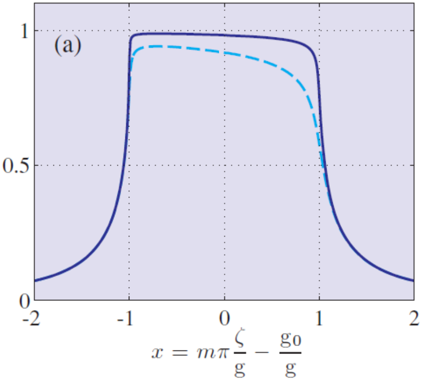


$\longleftarrow x = -1$
out of phase

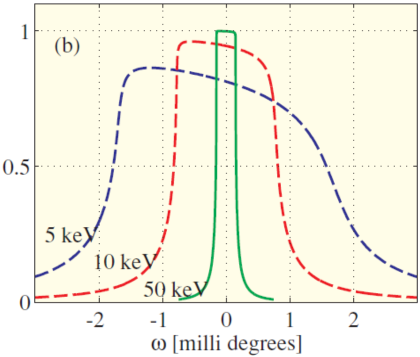
$x = +1 \longrightarrow$
in phase



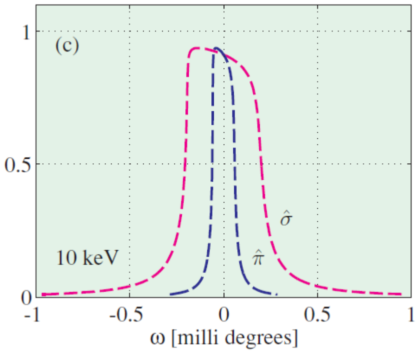
Absorption effects



Energy dependence

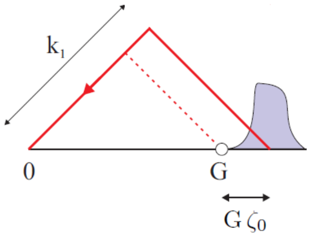


Polarization dependence



Harmonic suppression

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



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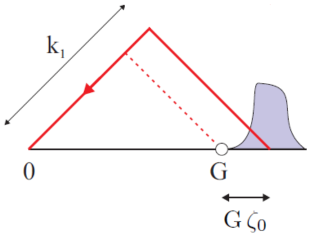

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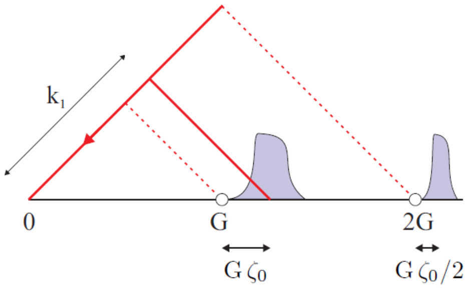

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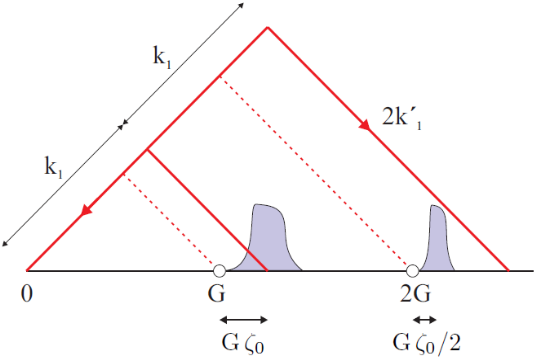

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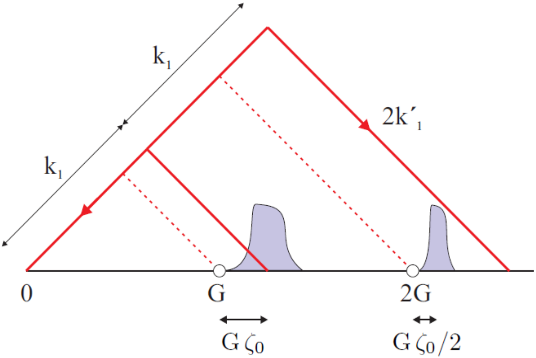

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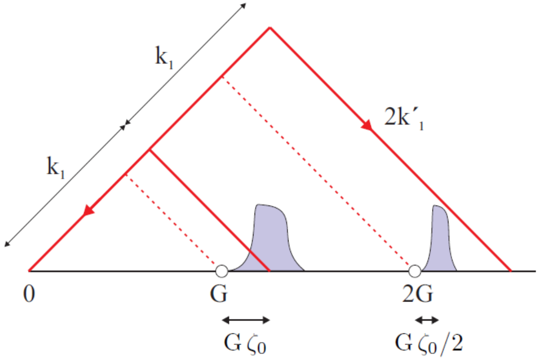
By tuning a bit off on the "high" side we get even more suppression. This is called "detuning".

Angular offset

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



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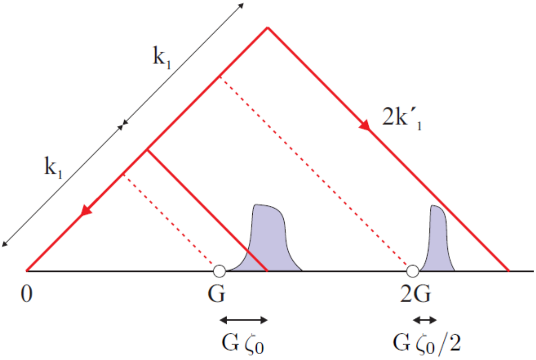

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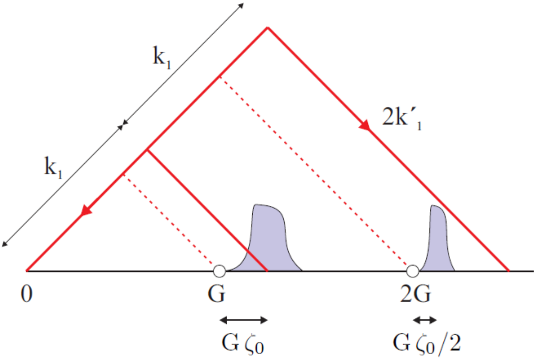
We can calculate the angular offset by noting that the offset and width have many common factors. Converting this to an angular offset.



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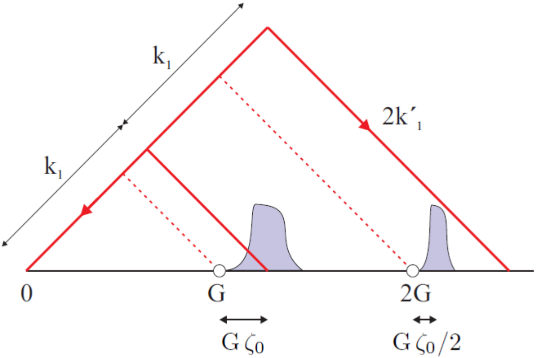

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For the Si(111) at $\lambda = 1.54056$Å

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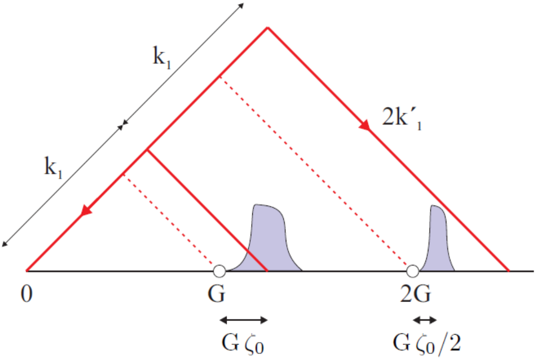

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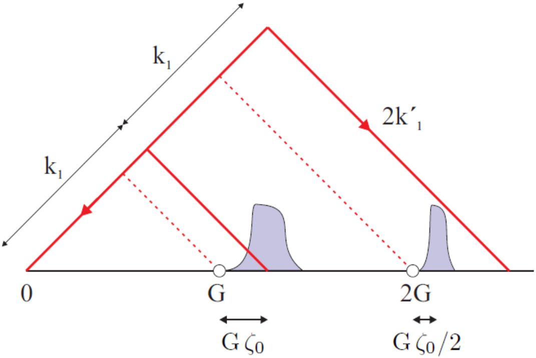
$$\omega_D^{total} = 0.0020^\circ$$

Angular offset

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



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

$$\zeta_D = \frac{4d^2|F|r_0}{\pi m^2 v_c}$$

$$\zeta^{off} = \frac{\zeta_0}{m} = \frac{\zeta_D}{2}\frac{|F|}{|F_0|}$$

$$\Delta\theta^{off} = \frac{\zeta_D}{2}\frac{|F|}{|F_0|}\tan\theta$$

For the Si(111) at $\lambda = 1.54056$Å

$$\omega_D^{total} = 0.0020^\circ \qquad \Delta\theta^{off} = 0.0018^\circ$$

Darwin widths

	$\zeta_D^{FWHM} \times 10^6$								
	(111)			(220)			(400)		
Diamond	61.0			20.9			8.5		
a= 3.5670 Å	3.03	0.018	-0.01	1.96	0.018	-0.01	1.59	0.018	-0.01
Silicon	139.8			61.1			26.3		
a= 5.4309 Å	10.54	0.25	-0.33	8.72	0.25	-0.33	7.51	0.25	-0.33
Germanium	347.2			160.0			68.8		
a= 5.6578 Å	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 $\cos(2\theta)$.