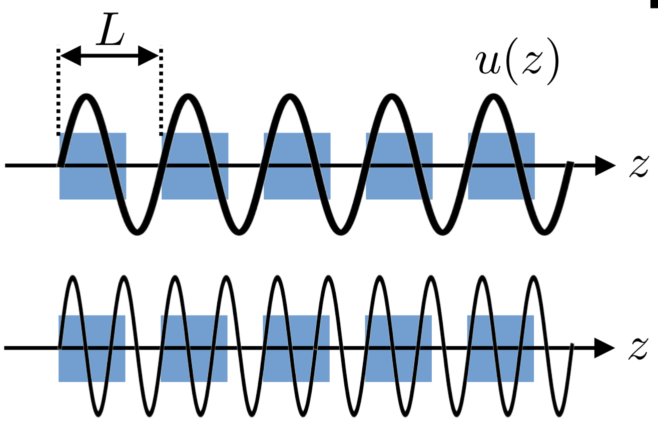
Lecture 11

Periodic Systems

Bloch-Floquet Theorem



This other wave also satisfies the periodicity but accumulates more phase

The wave is periodic. It must therefore satisfy

$$u(z+L) = Cu(z) \longrightarrow u(z) = e^{j\beta L}u(z+L)$$

C is the phase accumulated by the wave after a distance *L*

$$C = e^{-j\beta L}$$

β: propagation constant

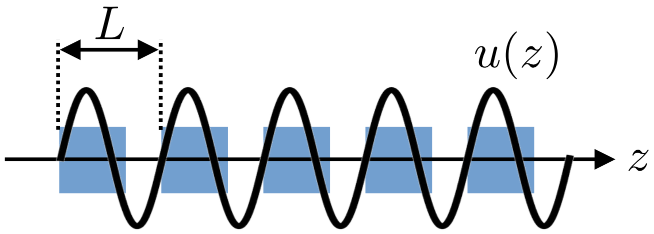
The amplitude of the wave at any *z* position

$$\boxed{u(z) = A(z)e^{-j\beta z}} \longrightarrow A(z) = e^{j\beta z}u(z)$$

Naturally *A(z)* is also a periodic function

$$A(z+L) = e^{j\beta(z+L)}u(z+L) = e^{j\beta z}e^{j\beta L}u(z+L) = e^{j\beta z}u(z) = A(z)$$

Bloch-Floquet Theorem



Since A(z) is a periodic function

$$A(z) = A(z + L)$$

A(z) exactly follows the periodicity of the system

We can express it as a Fourier series

$$A(z) = \sum_{n=-\infty}^{\infty} A_n e^{-j\frac{2n\pi}{L}z} \quad \text{where } A_n = \frac{1}{L}\int_{-L/2}^{L/2} A(z) e^{j\frac{2n\pi}{L}z}\, dz$$

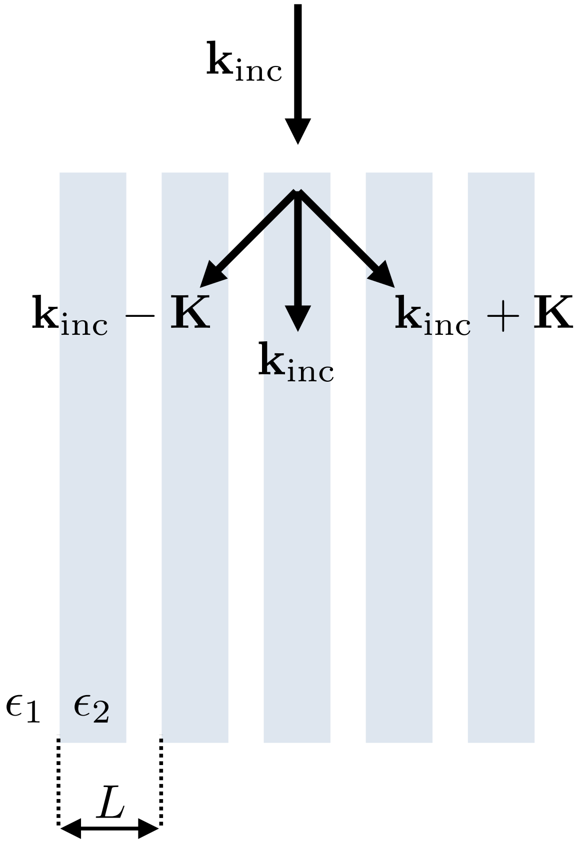
The wave does not exactly follow the periodicity of the system, only A(z) does

$$u(z) = A(z) e^{-j\beta z}$$

$$u(z) = \sum_{n=-\infty}^{\infty} A_n e^{-j\beta z - j\frac{2n\pi}{L}z} = \sum_{n=-\infty}^{\infty} A_n e^{-j\beta_n z}$$

$$u(z) = \sum_{n=-\infty}^{\infty} A_n e^{-j\beta_n z} \quad \text{where } \beta_n = \beta + \frac{2\pi n}{L}$$

Wave Interaction with a Periodic Structure



Consider a structure with spatially varying permittivity

$$\epsilon_{\mathrm{r}} = \epsilon_{\mathrm{r,av}} + \Delta\epsilon \cos\left(\mathbf{K} \cdot \mathbf{r}\right)$$

The electric field of a wave inside the structure is

$$E(\mathbf{r}) = A(\mathbf{r}) e^{-j\mathbf{k}_{\mathrm{inc}} \cdot \mathbf{r}}$$

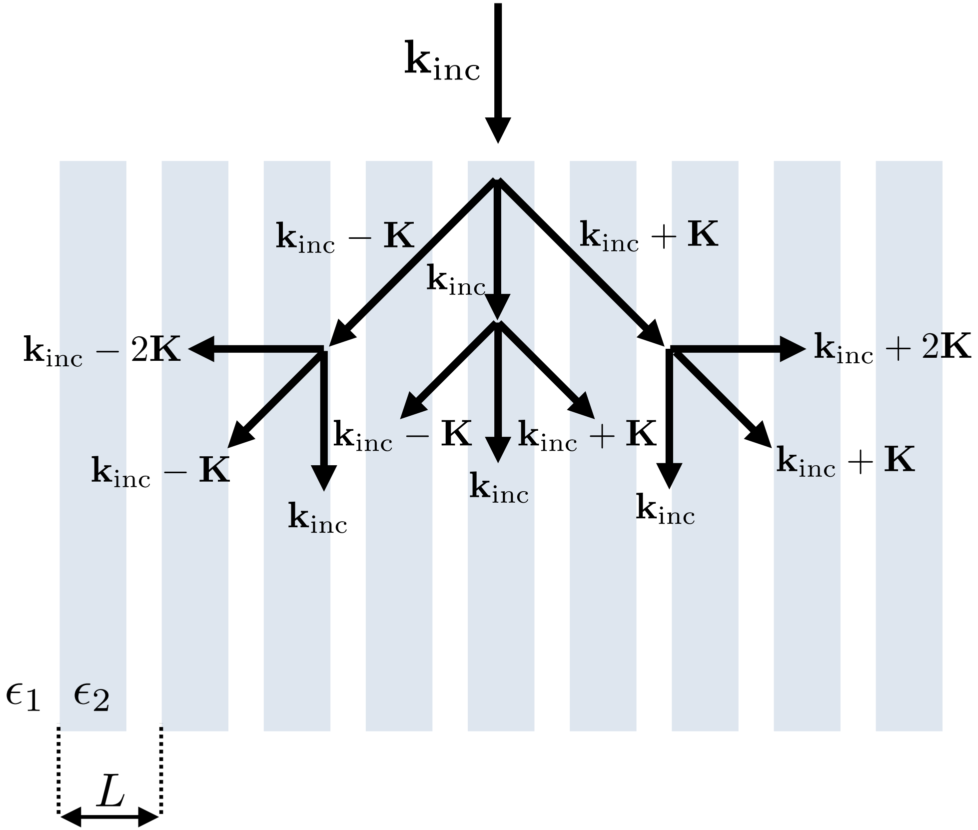
Since the amplitude $A(\mathbf{r})$ follows the periodicity of the system, we have

$$E(\mathbf{r}) = A\left[\epsilon_{\mathrm{r,av}} + \Delta\epsilon \cos\left(\mathbf{K} \cdot \mathbf{r}\right)\right] e^{-j\mathbf{k}_{\mathrm{inc}} \cdot \mathbf{r}}$$

Splitting the cosine function, we get

$$E(\mathbf{r}) = A\epsilon_{\mathrm{r,av}} e^{-j\mathbf{k}_{\mathrm{inc}} \cdot \mathbf{r}} + \frac{A\Delta\epsilon}{2} e^{-j(\mathbf{k}_{\mathrm{inc}} - \mathbf{K}) \cdot \mathbf{r}} + \frac{A\Delta\epsilon}{2} e^{-j(\mathbf{k}_{\mathrm{inc}} + \mathbf{K}) \cdot \mathbf{r}}$$

Wave Interaction with a Periodic Structure



Each wave splits into three waves with **k**-vector being modified by

$$\{-\mathbf{K}, 0, +\mathbf{K}\}$$

Several of these waves end up propagating in the same directions.

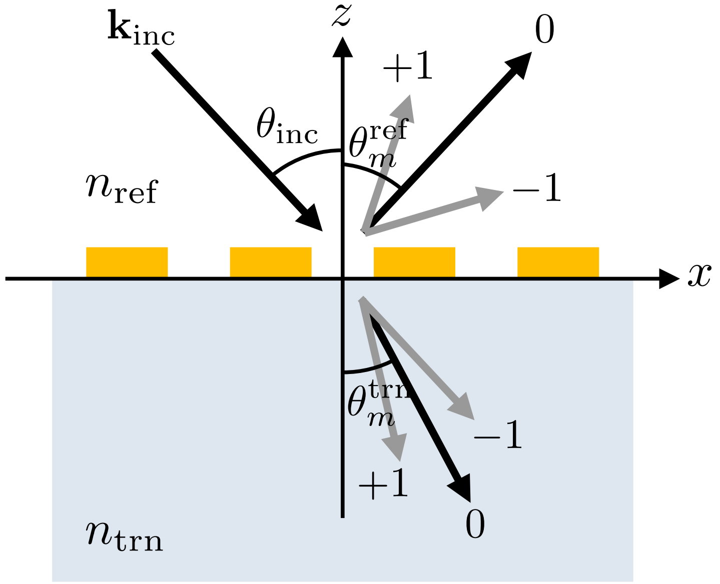
Overall, the scattered waves will have

$$\boxed{\mathbf{k}_m = \mathbf{k}_{\text{inc}} - m\mathbf{K}} \quad m \in \mathbb{N}$$

where $\quad |\mathbf{K}| = \dfrac{2\pi}{L}$

1D Diffraction Grating

1D Diffraction Grating Equation



$$k_{x,\text{inc}} = k_0 n_{\text{ref}} \sin\theta_{\text{inc}}$$

$$k_{x,\text{ref}} = k_0 n_{\text{ref}} \sin\theta_m^{\text{ref}}$$

$$k_{x,\text{trn}} = k_0 n_{\text{trn}} \sin\theta_m^{\text{trn}}$$

From Bloch-Floquet theorem, we have

$$\mathbf{k}_m = \mathbf{k}_{\text{inc}} - m\mathbf{K} \qquad m \in \mathbb{N}$$

For a grating in the x direction, we have

$$\mathbf{K} = \frac{2\pi}{L}\hat{\mathbf{x}}$$

The grating is only affecting the x-component of the wavevector

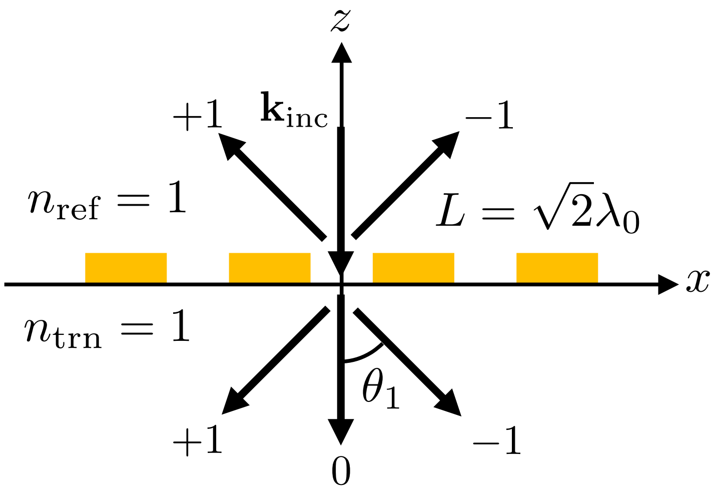
Applying this equation in the reflection region

$$n_{\text{ref}} \sin\theta_m^{\text{ref}} = n_{\text{inc}} \sin\theta_{\text{inc}} - m\frac{\lambda_0}{L}$$

Applying this equation in the transmission region

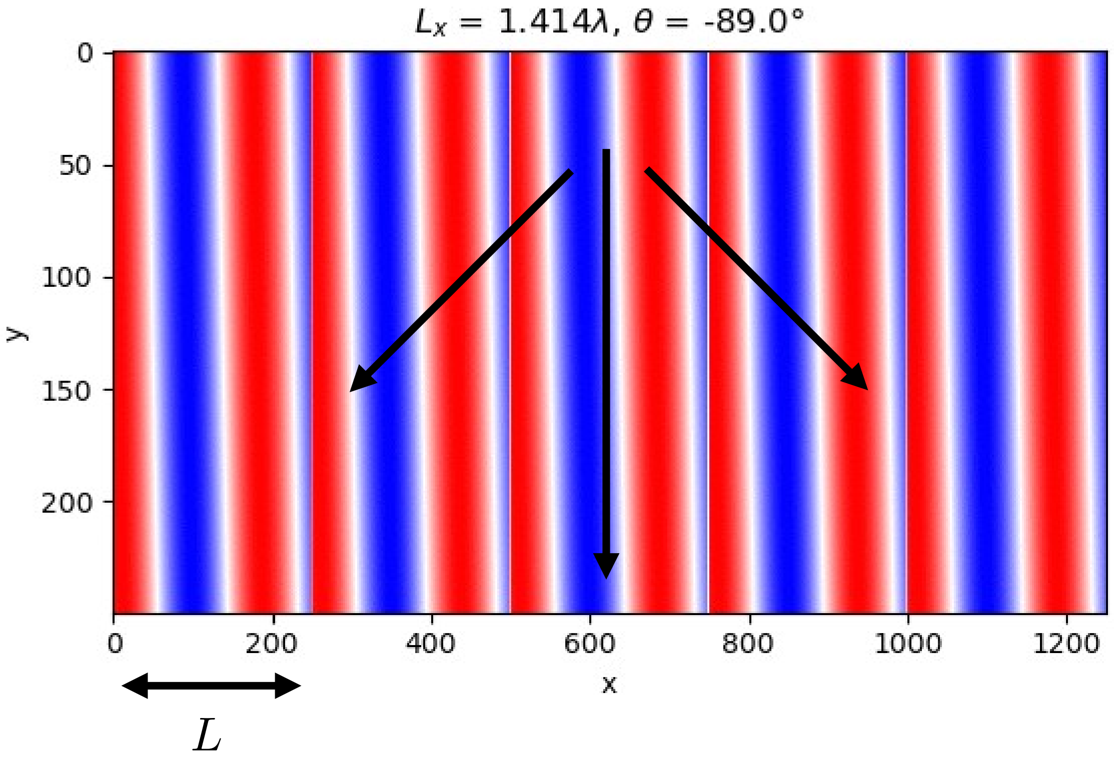
$$n_{\text{trn}} \sin\theta_m^{\text{trn}} = n_{\text{inc}} \sin\theta_{\text{inc}} - m\frac{\lambda_0}{L}$$

Visualizing Periodic Fields



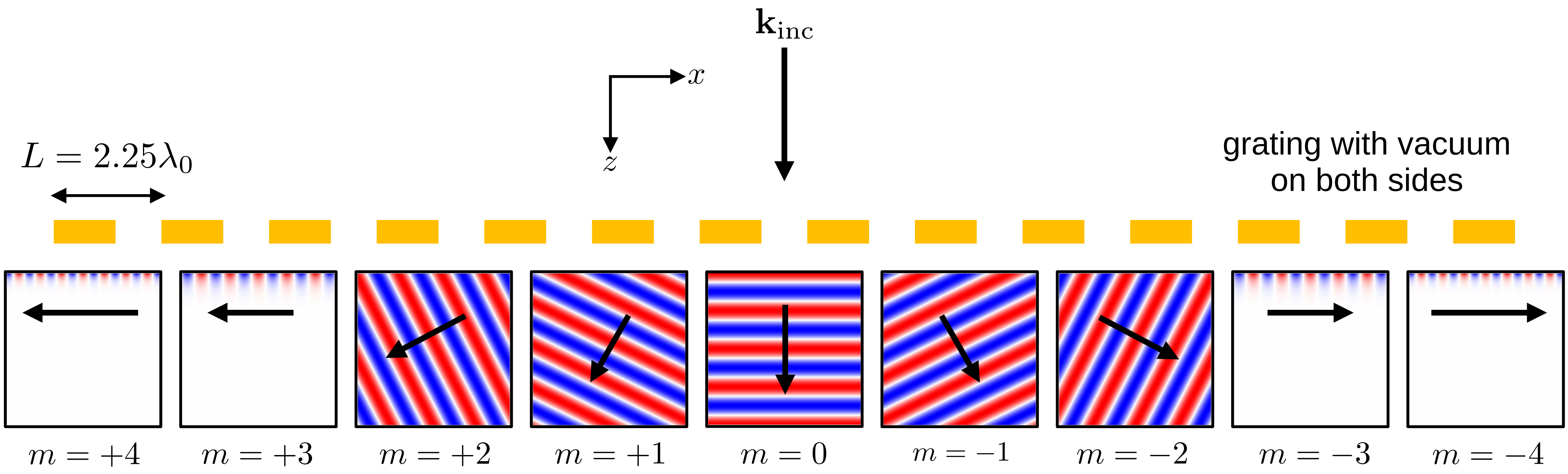
$$\theta_{\pm 1} = \pm 45^\circ$$

Plotting the real part of the scattered electric field assuming all possible angles



Diffraction orders exist when the periodicity of the system is satisfied. This happens only when the scattering angle matches that of the grating equation

1D Diffraction Grating

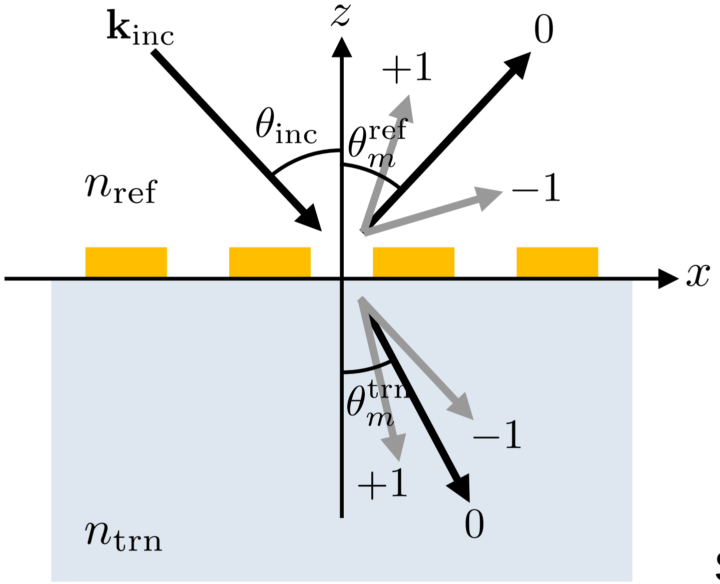


$$\mathbf{k}_m = \mathbf{k}_{\mathrm{inc}} - m\mathbf{K} \longrightarrow k_{x,\mathrm{trn}} = k_{x,\mathrm{inc}} - m\frac{2\pi}{L} \longrightarrow k_{z,\mathrm{trn}} = \sqrt{k_{\mathrm{trn}}^2 - k_{x,\mathrm{trn}}^2}$$

$\longrightarrow k_{z,\mathrm{trn}} = k_0\sqrt{1 - \left(\frac{m}{2.25}\right)^2}$ for all $|m| \geq 3$ we have that $k_{z,\mathrm{trn}} \in \mathbb{I}$

Infinite number of evanescent waves !

Total Number of Diffraction Orders



Grating equation

$$n_{\text{s}} \sin \theta_m^{\text{s}} = n_{\text{inc}} \sin \theta_{\text{inc}} - m \frac{\lambda_0}{L}$$

where $\text{s} = \{\text{ref}, \text{trn}\}$

Diffraction orders (DO) exist as long as $-1 < \sin \theta_m^{\text{s}} < 1$

$$-n_{\text{s}} < n_{\text{inc}} \sin \theta_{\text{inc}} - m_{\text{tot}} \frac{\lambda_0}{L} < n_{\text{s}}$$

Solving this equations for m_{tot} gives two solutions

floor(2.25) = 2

Total number of positive DO

$$U_{\text{s}} = \left\lfloor \left(n_{\text{inc}} \sin \theta_{\text{inc}} + n_{\text{s}} \right) \frac{L}{\lambda_0} \right\rfloor$$

Total number of negative DO

$$L_{\text{s}} = \left\lceil \left(n_{\text{inc}} \sin \theta_{\text{inc}} - n_{\text{s}} \right) \frac{L}{\lambda_0} \right\rceil$$

Total number of DO (including 0^{th})

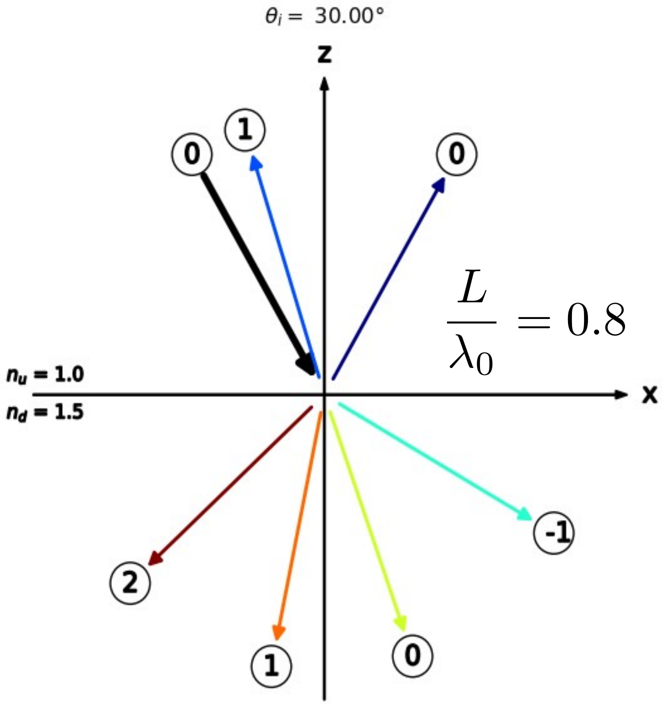
$$N_{\text{s}} = U_{\text{s}} - L_{\text{s}} + 1$$

ceil(2.25) = 3

At normal incidence

$$N_{\text{s}} = 1 + 2 \left\lfloor n_{\text{s}} \frac{L}{\lambda_0} \right\rfloor$$

Example of Application



$$\frac{L}{\lambda_0} = 0.8$$

Number of diffraction orders

$$U_s = \left\lfloor (n_{\text{inc}} \sin\theta_{\text{inc}} + n_s) \frac{L}{\lambda_0} \right\rfloor$$

$$L_s = \left\lceil (n_{\text{inc}} \sin\theta_{\text{inc}} - n_s) \frac{L}{\lambda_0} \right\rceil$$

$$N_s = U_s - L_s + 1$$

$$U_{\text{ref}} = \left\lfloor (\sin(30°) + 1) \frac{1}{0.8} \right\rfloor = 1 \qquad L_{\text{ref}} = \left\lceil (\sin(30°) - 1) \frac{1}{0.8} \right\rceil = 0 \qquad N_{\text{ref}} = U_{\text{ref}} - L_{\text{ref}} + 1 = 2$$

$$U_{\text{trn}} = \left\lfloor (\sin(30°) + 1.5) \frac{1}{0.8} \right\rfloor = 2 \qquad L_{\text{trn}} = \left\lceil (\sin(30°) - 1.5) \frac{1}{0.8} \right\rceil = -1 \qquad N_{\text{trn}} = U_{\text{trn}} - L_{\text{trn}} + 1 = 4$$

Condition for No Diffraction Orders

What is the condition so that only the 0th diffraction orders exist in the reflection and transmission regions?

$$k_{x,\mathrm{s}} = k_{x,\mathrm{inc}} - m\frac{2\pi}{L} \longrightarrow k_{z,\mathrm{s}} = \sqrt{k_{\mathrm{s}}^2 - k_{x,\mathrm{s}}^2}$$

where $\mathrm{s} = \{\mathrm{ref}, \mathrm{trn}\}$

We want $k_{z,s}$ to be imaginary for

$$|m| \geq 1$$

$$k_{\mathrm{s}}^2 < \left(k_{x,\mathrm{inc}} - \frac{2\pi}{L}\right)^2$$

$$n_{\mathrm{s}}^2 < \left(n_{\mathrm{ref}} \sin\theta_{\mathrm{inc}} - \frac{\lambda_0}{L}\right)^2$$

Solving the inequality for *L*

At normal incidence ($\theta_{\mathrm{inc}} = 0°$)

$$L < \frac{\lambda_0}{n_{\mathrm{s}}}$$

General condition

$$L < \frac{\lambda_0}{n_{\mathrm{ref}}|\sin\theta_{\mathrm{inc}}| + n_{\mathrm{s}}}$$

At grazing angle ($\theta_{\mathrm{inc}} = 90°$)

$$L < \frac{\lambda_0}{n_{\mathrm{ref}} + n_{\mathrm{s}}}$$

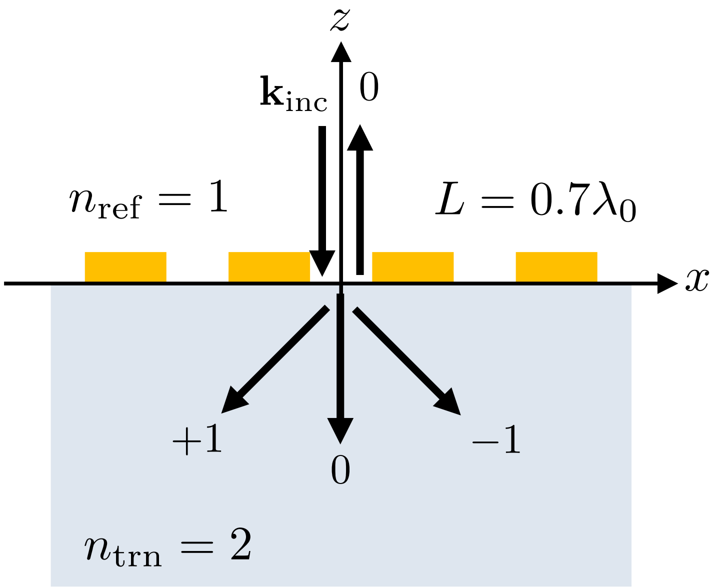
For the reflection region: $L < \frac{\lambda_0}{2n_{\mathrm{ref}}}$

Condition for No Diffraction Orders

Keep in mind that the numbers of DO in the reflection and transmission regions may be different

At normal incidence ($\theta_{\text{inc}} = 0°$)

$$L < \frac{\lambda_0}{n_s}$$



Condition for no DO

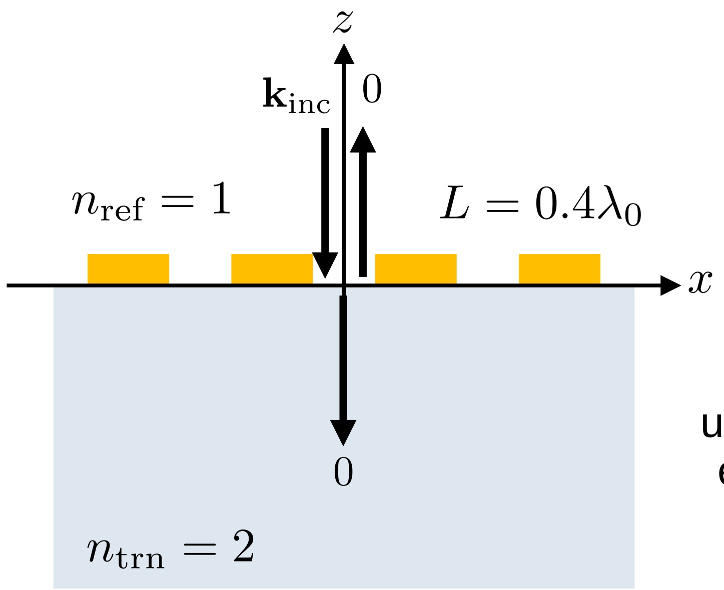
$L < \lambda_0$ Satisfied

$L < \frac{\lambda_0}{2}$ Not satisfied !

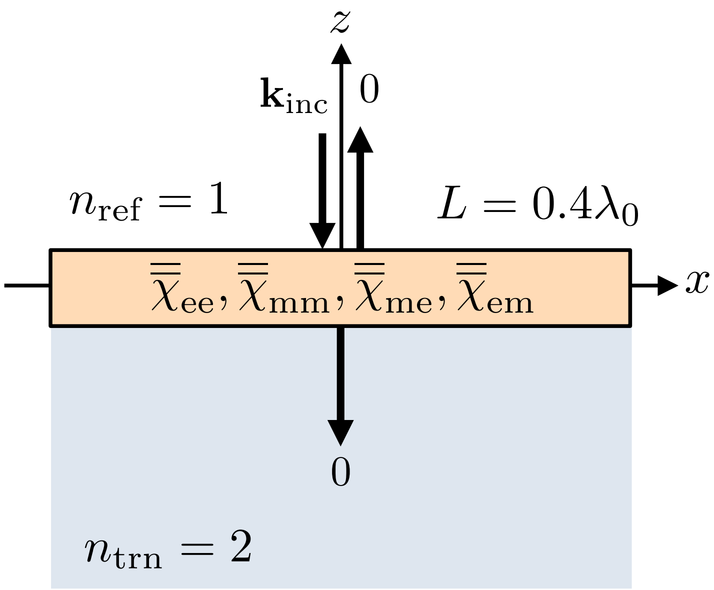
What is a Metasurface ?

A metasurface is typically a resonant subwavelength grating

$$L < \frac{\lambda_0}{n_s}$$



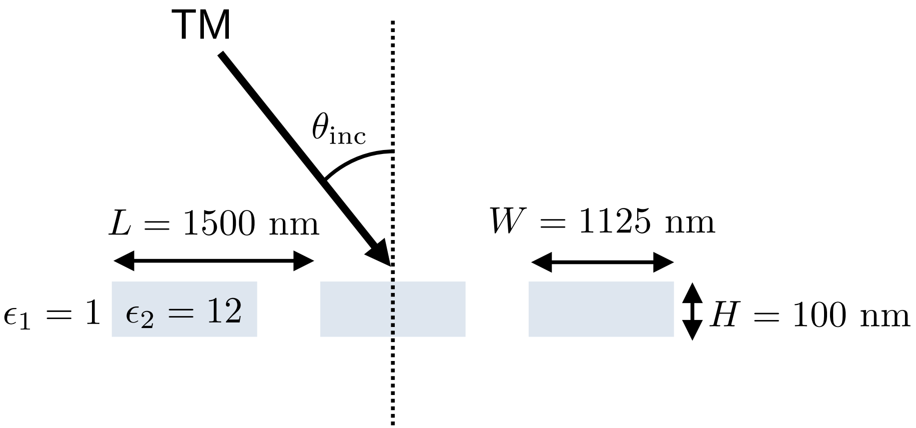
Homogenization



Homogenization consists in replacing the grating by a uniform and continuous layer of effective material parameters.

Homogenization only works if no DO are produced.

Visualizing Diffraction Orders



Grating equation

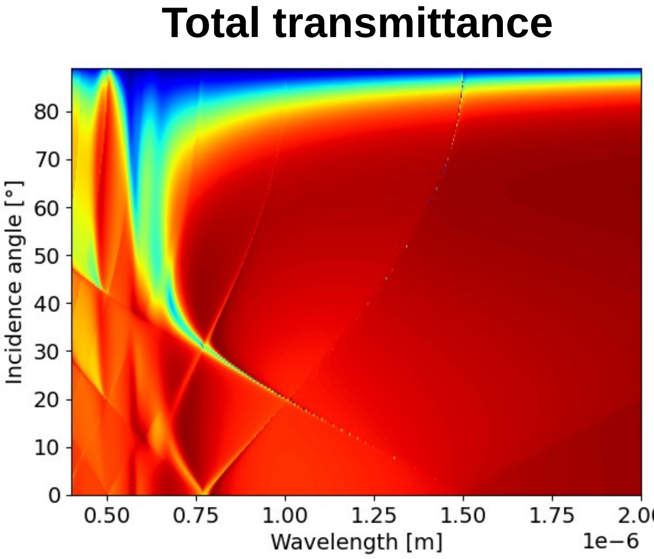
$$n_{\rm s} \sin\theta_m^{\rm s} = n_{\rm inc}\sin\theta_{\rm inc} - m\frac{\lambda_0}{L}$$

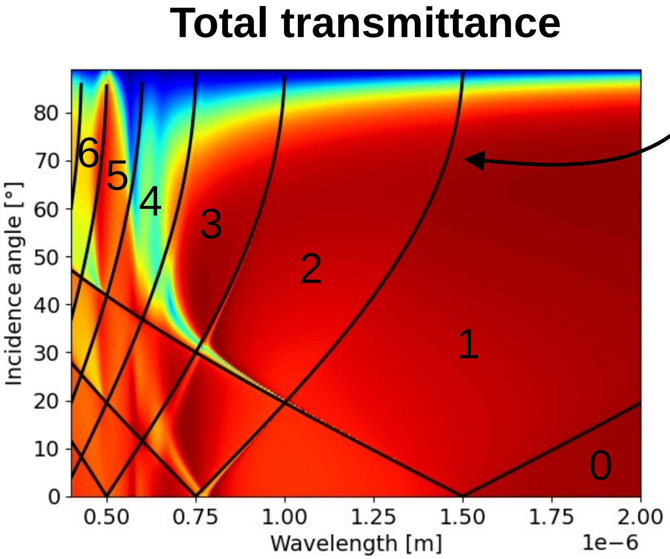
when $\theta_m^{\rm s} = \pm 90°$

$$\pm n_{\rm s} = n_{\rm inc}\sin\theta_{\rm inc} - m\frac{\lambda_0}{L}$$

$$\theta_{\rm inc} = \arcsin\left[\frac{1}{n_{\rm inc}}\left(m\frac{\lambda_0}{L} \pm n_{\rm s}\right)\right]$$

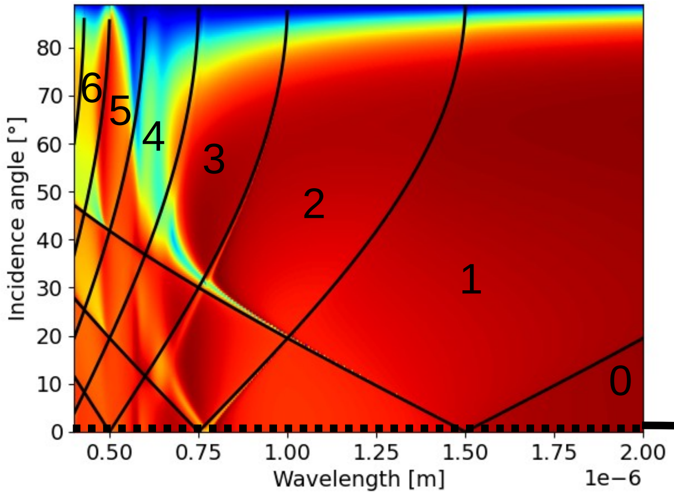
Diffraction orders cut-off angle





Rayleigh Anomalies

Total transmittance



Grating equation

$$n_{\mathrm{s}} \sin \theta_m^{\mathrm{s}} = n_{\mathrm{inc}} \sin \theta_{\mathrm{inc}} - m \frac{\lambda_0}{L}$$

when $\theta_m^{\mathrm{s}} = \pm 90^\circ$

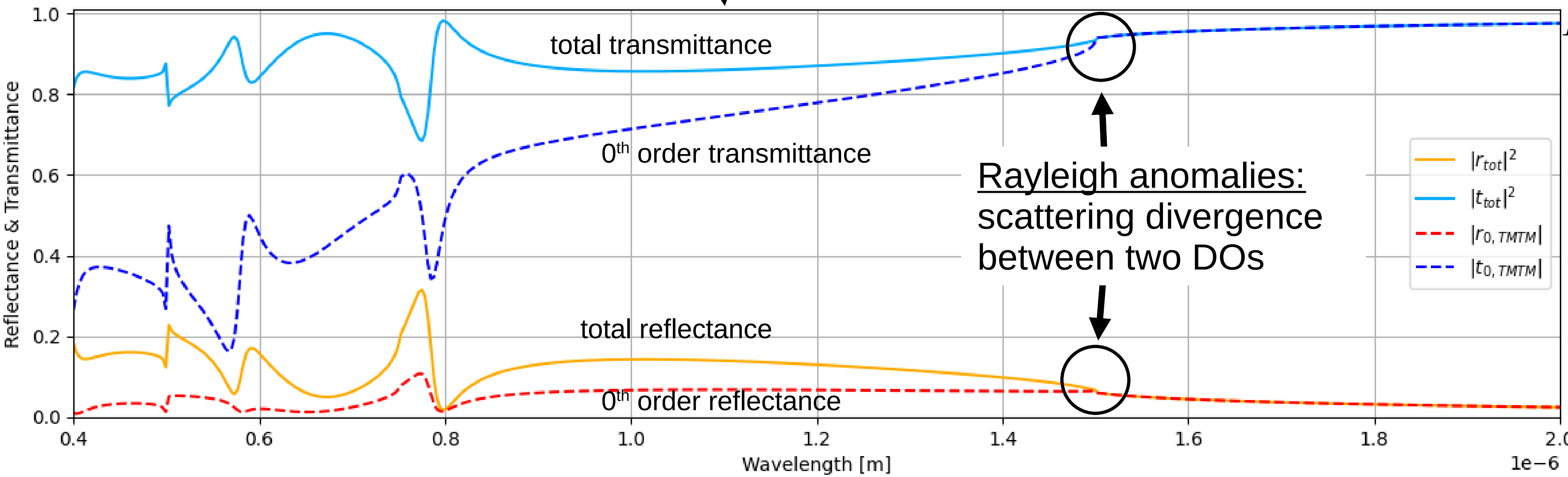
$$\pm n_{\mathrm{s}} = n_{\mathrm{inc}} \sin \theta_{\mathrm{inc}} - m \frac{\lambda_0}{L}$$

$$\lambda_{\mathrm{RA}} = \frac{L}{m} \left(n_{\mathrm{inc}} \sin \theta_{\mathrm{inc}} \pm n_{\mathrm{s}} \right)$$

At normal incidence

$$\lambda_{\mathrm{RA}} = n_{\mathrm{s}} \frac{L}{|m|}$$

$\theta_{\mathrm{inc}} = 0^\circ$

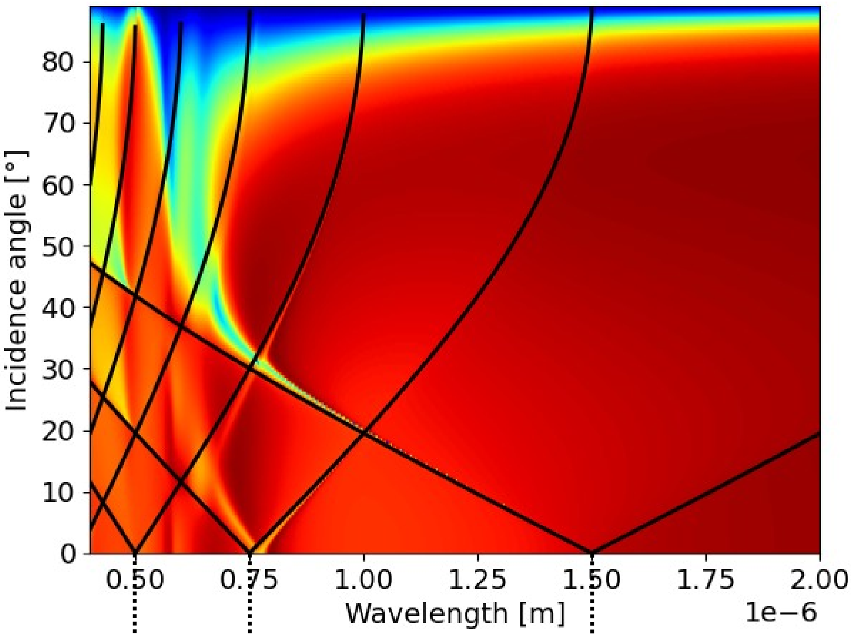


$L = 1500$ nm

$n_{\mathrm{s}} = 1$

Diffraction Orders Transitions at Normal Incidence

Total transmittance



Array period

$L = 1500 \text{ nm}$

Refractive index

$n_{\mathrm{s}} = 1$

At normal incidence

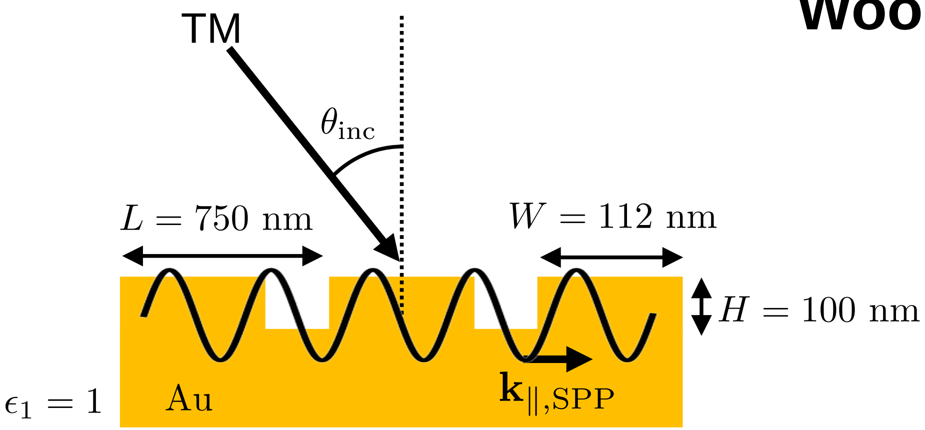
$$\lambda_{\mathrm{RA}} = n_{\mathrm{s}} \frac{L}{|m|}$$

The Rayleigh anomaly wavelength tells us when a new diffraction order appears

The order.. $|m| = 3$ $|m| = 2$ $|m| = 1$

..appears when.. $\lambda = \frac{L}{3}$ $\lambda = \frac{L}{2}$ $\lambda = L$

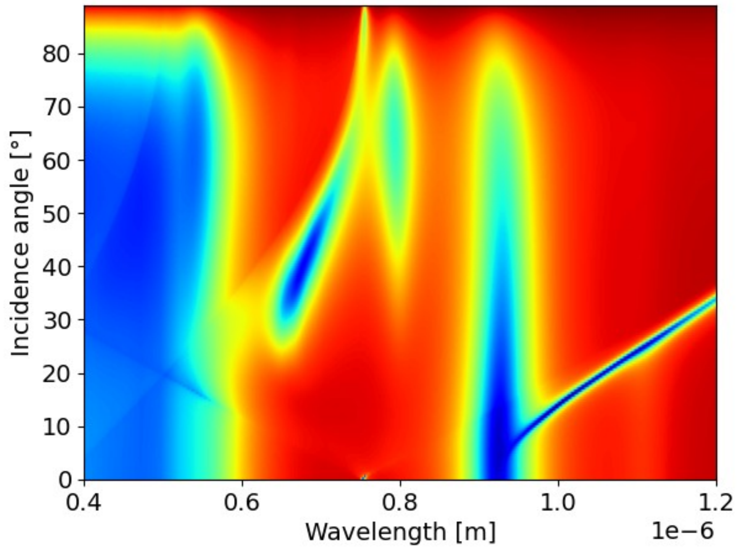
Wood Anomalies

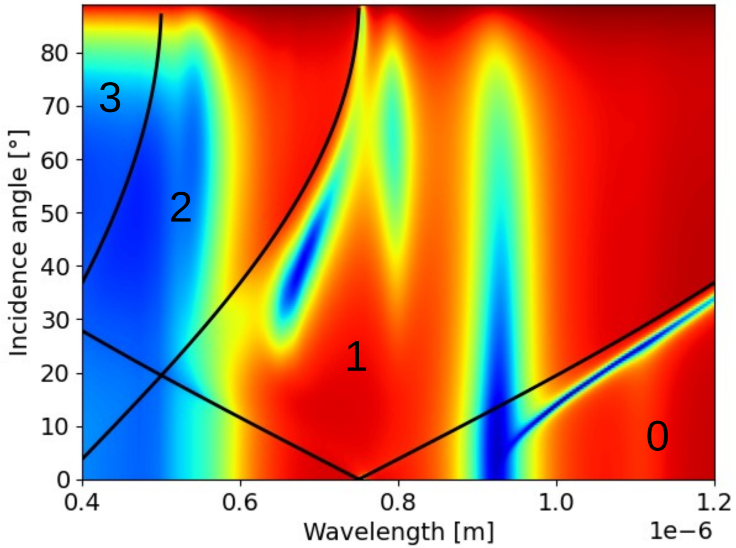


Wood anomalies:
coupling between incident wave and surface plasmon via a grating

$$\mathbf{k}_{\parallel,\text{SPP}} = \mathbf{k}_{\parallel,\text{inc}} + \mathbf{K}$$

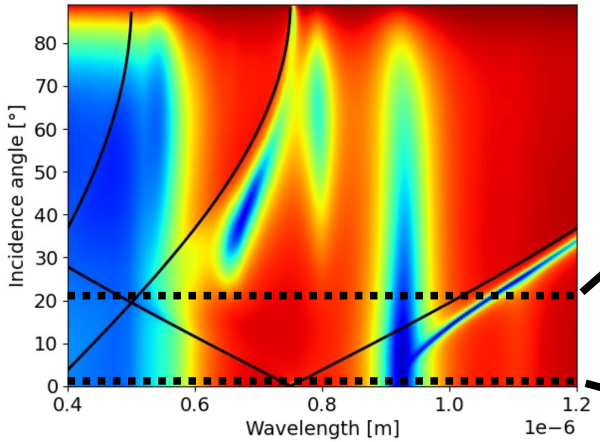
where $|\mathbf{K}| = \frac{2\pi}{L}$





Rayleigh and Wood Anomalies

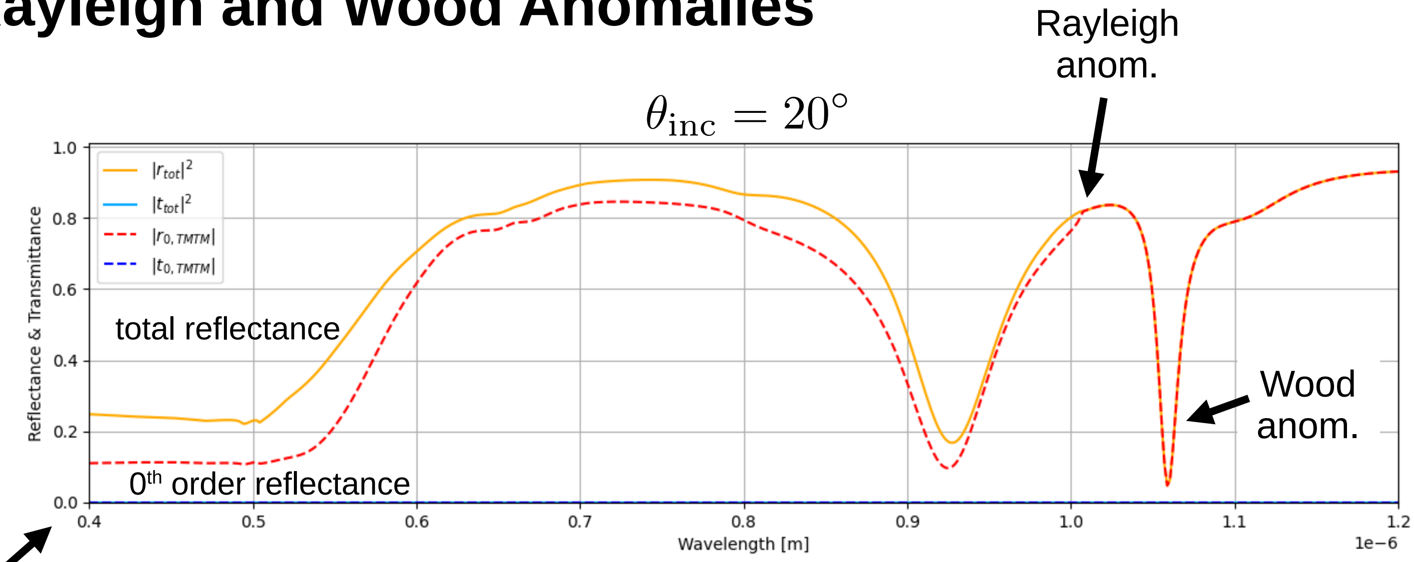
Total reflectance

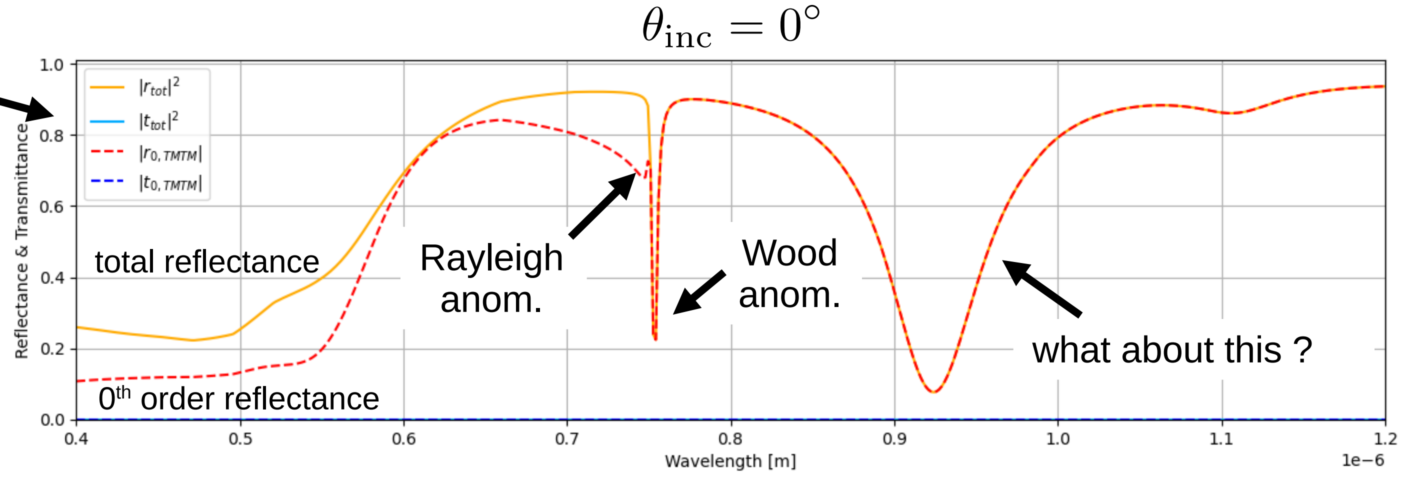


Wood anomalies

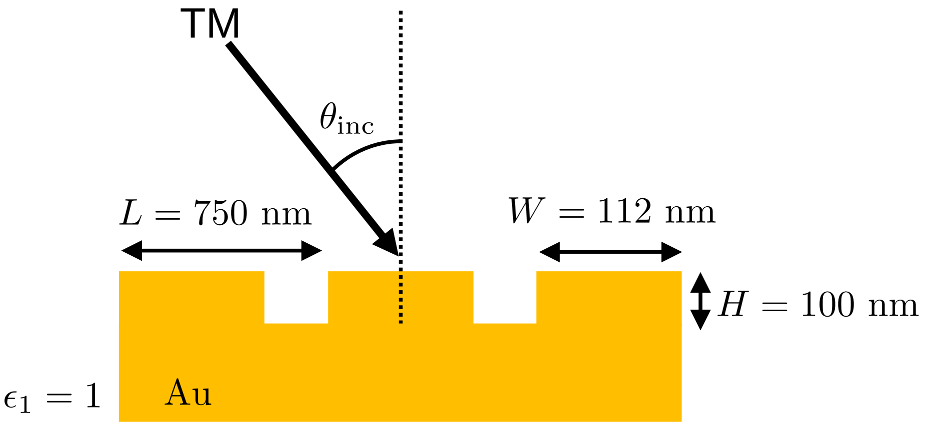
$$\mathbf{k}_{\text{SPP}} = \mathbf{k}_{\parallel,\text{inc}} + \mathbf{K}$$

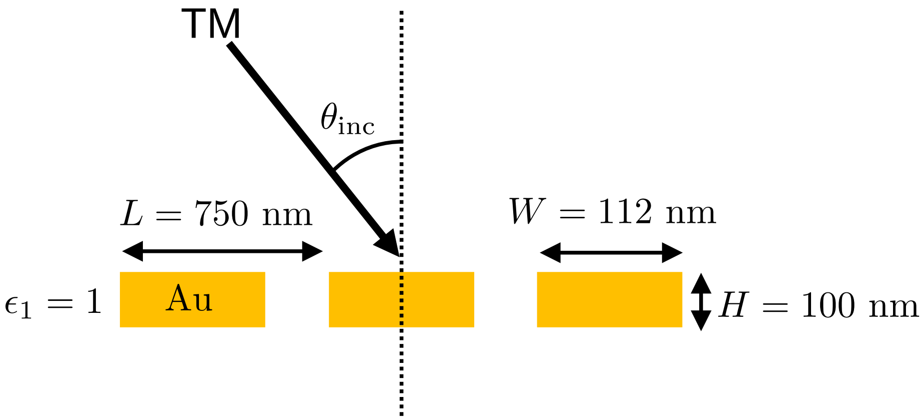
Rayleigh anomalies
scattering divergence
between two DOs



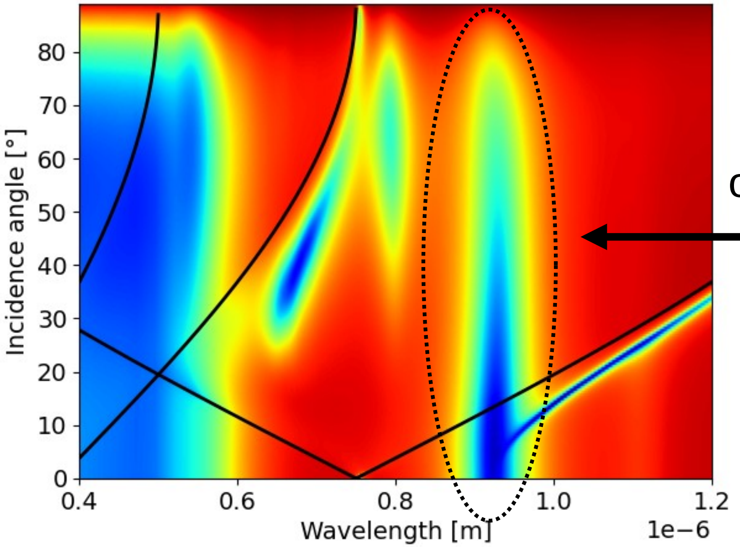


Localized Resonance



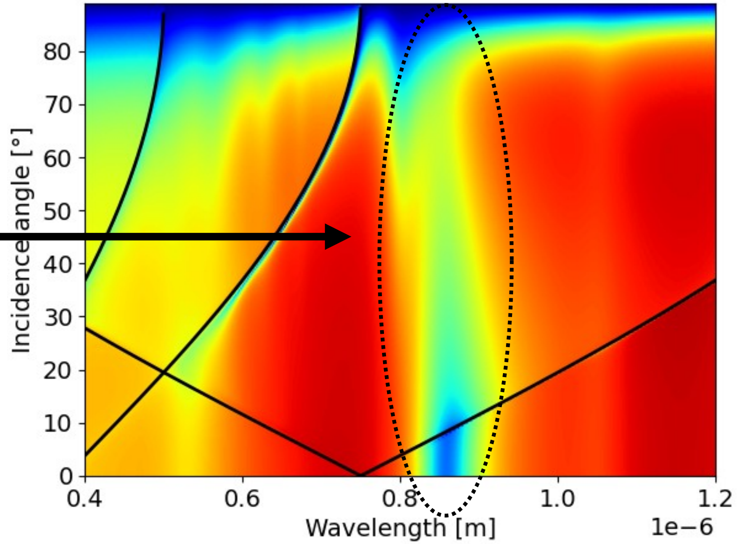


Total reflectance

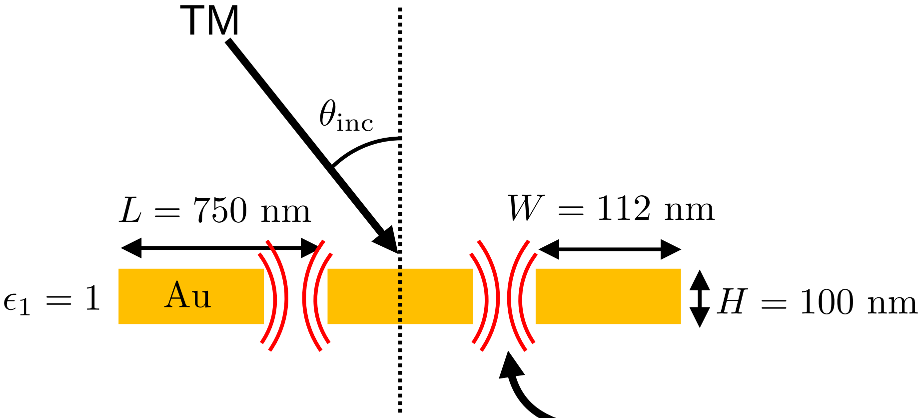


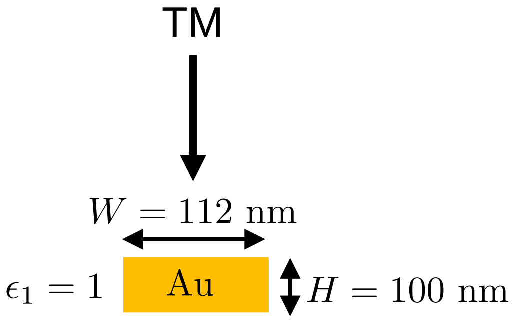
Exists in both systems.
Corresponds to resonance
of the individual gold blocks

Total transmittance



Localized Resonance



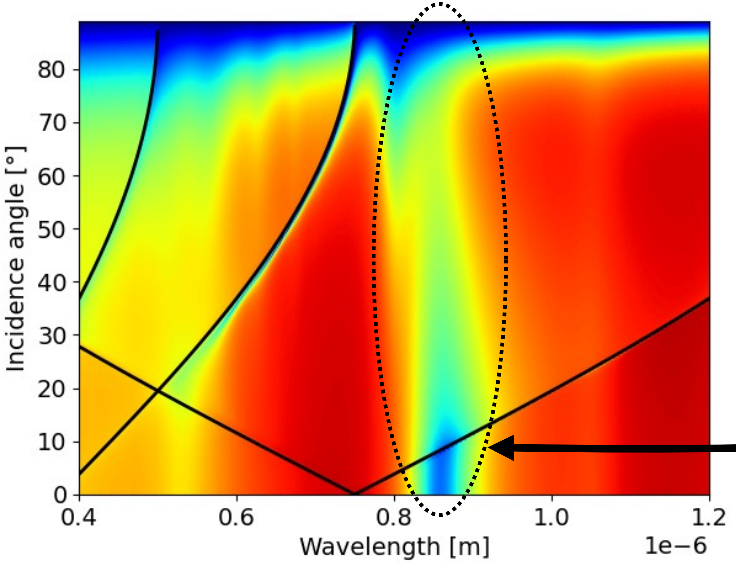


particle interactions
increase capacitance

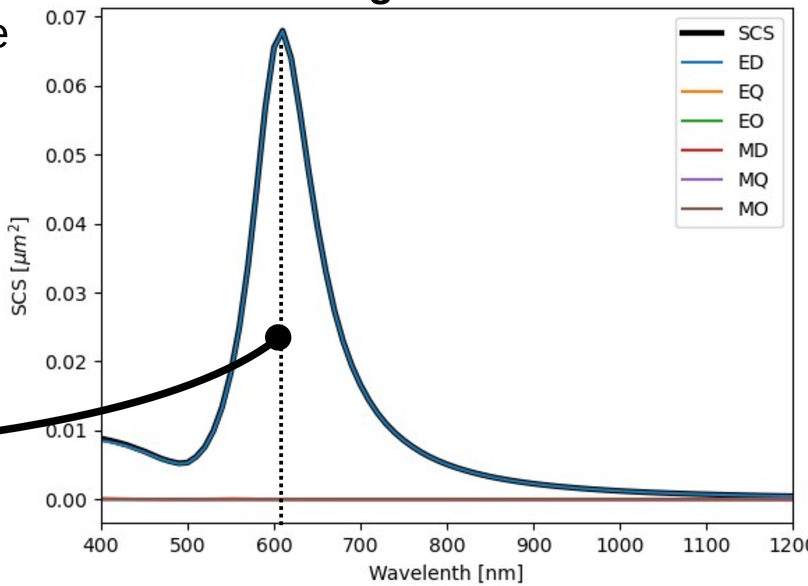
$$\lambda = \frac{2\pi}{c}\sqrt{LC}$$

resonance “redshift”

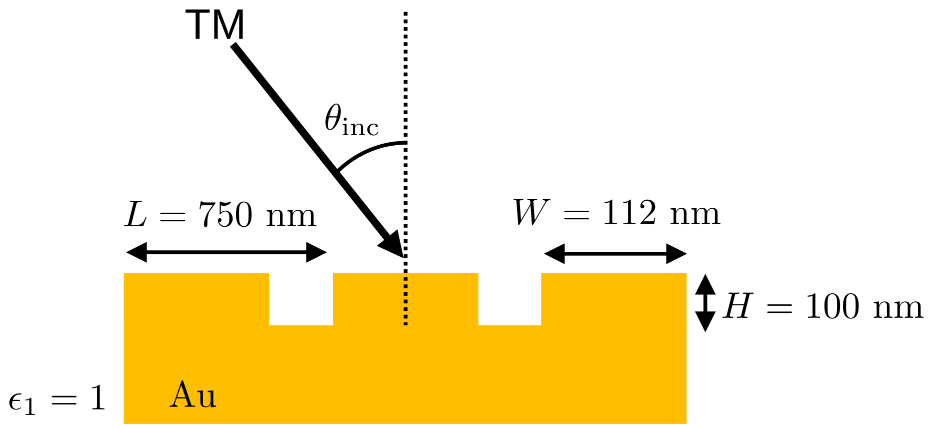
Total transmittance



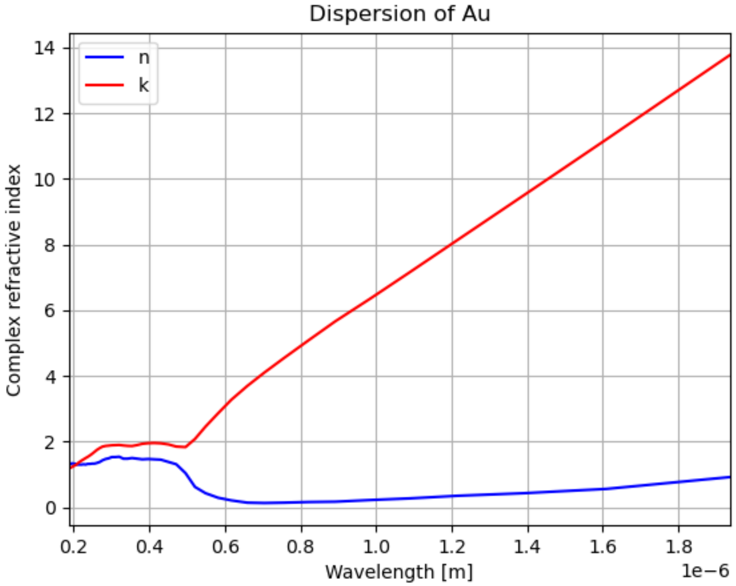
Scattering cross section



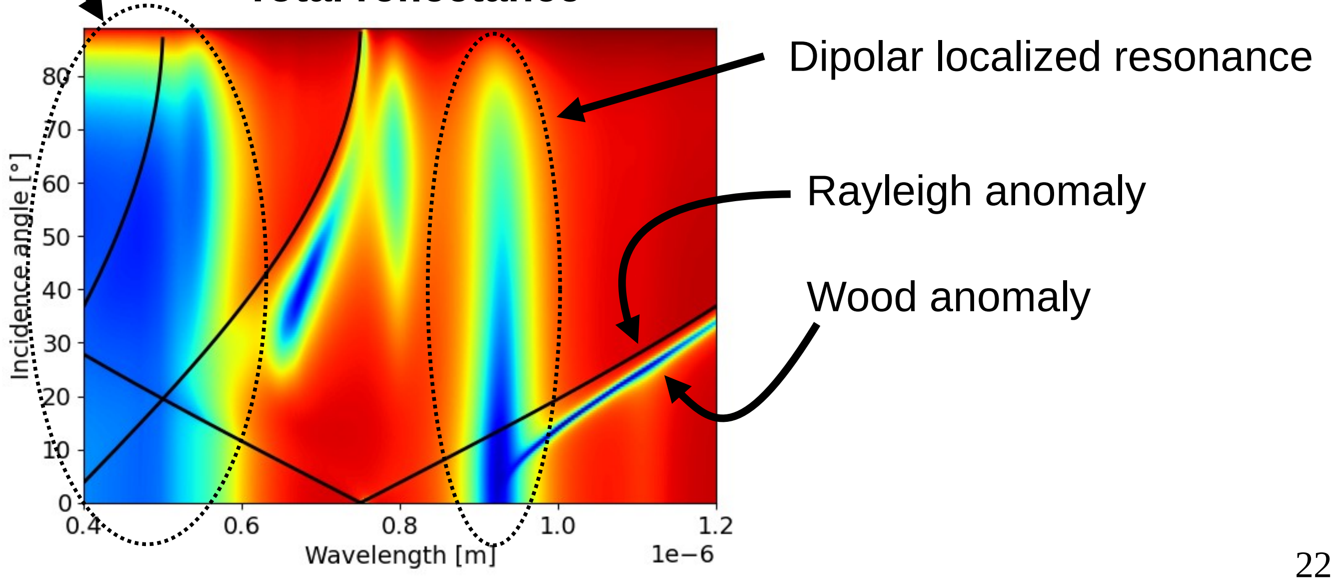
Simple Structure, Complex Response



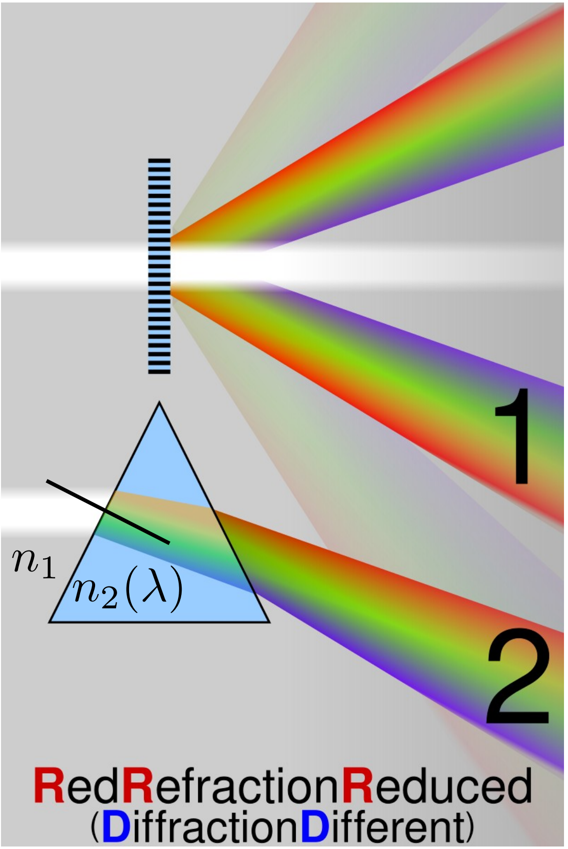
Gold behaves as a lossy dielectric



Total reflectance



Diffraction vs Refraction



https://commons.wikimedia.org/wiki/File:Comparison_refraction_diffraction_spectra.svg#/media/File:Comparison_refraction_diffraction_spectra.svg

Diffraction

$$n_s \sin\theta_m^s = n_{inc} \sin\theta_{inc} - m\frac{\lambda_0}{L}$$

at normal incidence in air

$$\theta_m^s = -\arcsin\left(m\frac{\lambda_0}{L}\right)$$

Larger wavelengths are <u>more diffracted</u> than smaller ones

Refraction

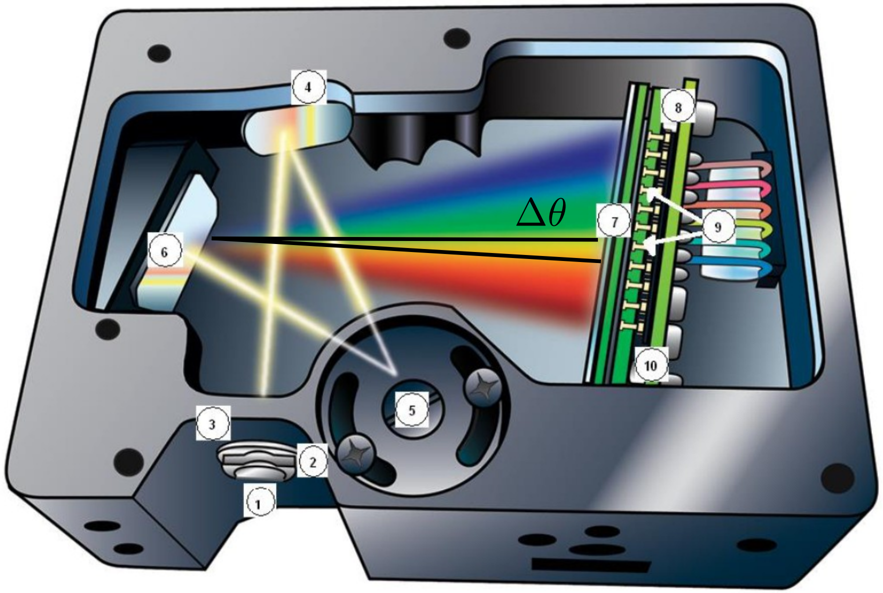
$$n_1 \sin\theta_1 = n_2 \sin\theta_2$$

$$\theta_2 = \arcsin\left(\frac{n_1}{n_2(\lambda)}\sin\theta_1\right) \approx \frac{n_1}{n_2(\lambda)}\theta_1$$

$n_2(\lambda)$ smaller for larger wavelengths

Larger wavelengths are <u>less refracted</u> than smaller ones

Spectral Sensitivity of a Diffraction Grating



USB2000+ OceanOptics spectrometer
1) SMA Connector
2) Slit
3) Filter
4) Collimating Mirror
5) Grating
6) Focusing Mirror
7) Collection Lens
8) Detector

Diffraction

$$n_s \sin\theta_m^s = n_{inc} \sin\theta_{inc} - m\frac{\lambda_0}{L}$$

At normal incidence and in air, the spectral sensitivity is

$$\frac{\partial \lambda_0}{\partial \theta} = \frac{L}{m}\cos\theta_m$$

$$\Delta\lambda_0 = \frac{L}{m}\cos\theta_m \Delta\theta$$

where $\Delta\theta$ is a pixel detection cone angle

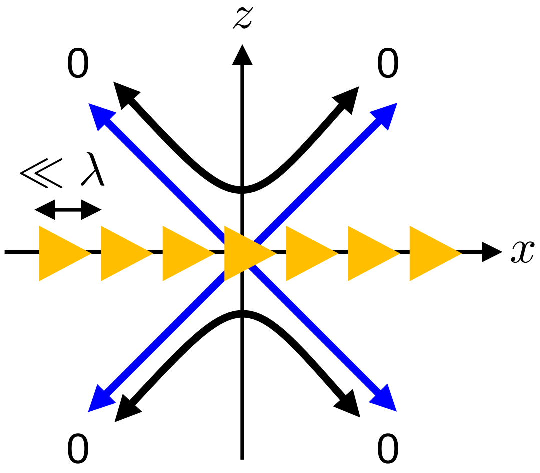
What Have We Learned So Far….

- When a wave interacts with a periodic structure, its amplitude follows the periodicity of the structure while its phase is composed of an infinite number of plane wave components.
- This means that, upon interaction with a grating, an infinite number of waves are produced. Most of them being evanescent.
- To only have the 0th DO at normal incidence, the array period should be lower than λ/n_s. At a grazing angle, it should be lower than $\lambda/(n_{ref} + n_s)$.
- Rayleigh anomalies are sharp redistribution of energy between the diffraction orders at the cut-offs. At normal incidence, the cut-offs are defined in terms of the wavelength as: $n_s L/|m|$
- Wood anomalies correspond to wave coupling to surface wave modes on metallic gratings. They typically appear close to Rayleigh anomalies.
- Localized dipolar resonances typically exhibit low angular dispersion and tend to be redshifted by the coupling in the array.
- The spectral sensitivity of a diffraction grating is improved by reducing the grating period

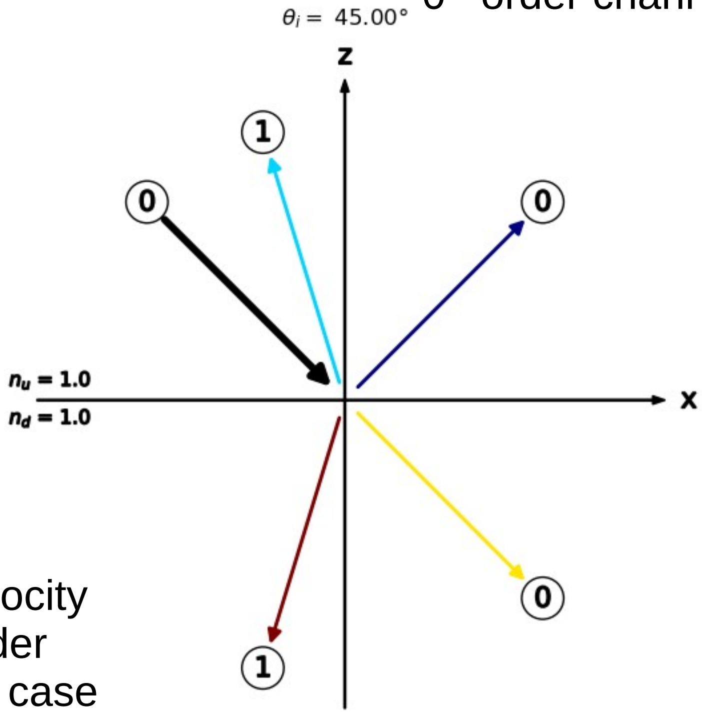
Grating and Spatial Symmetries

Grating with Broken Symmetry

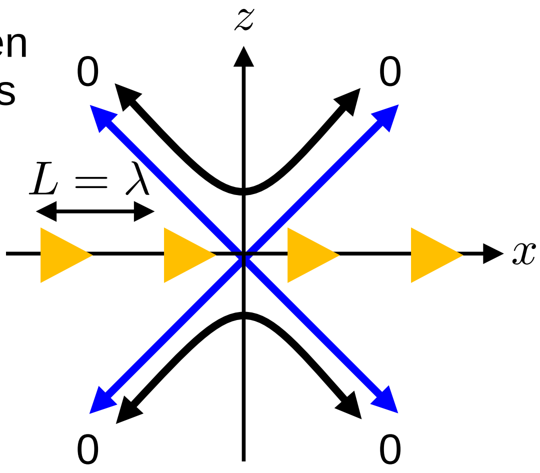
Subwavelength metasurface with broken σ_x symmetry

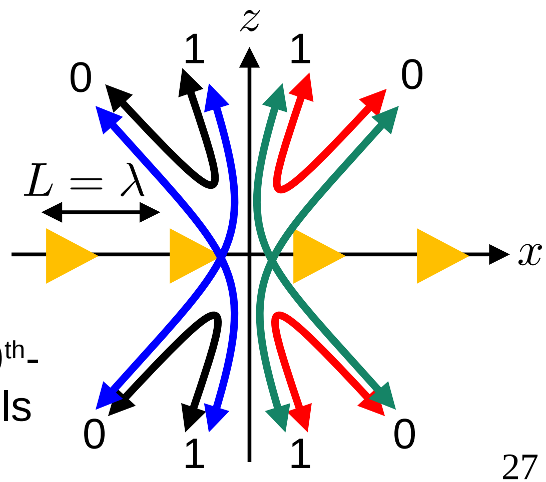


Diffraction grating with broken σ_x symmetry



Scattering between 0^{th}-order channels



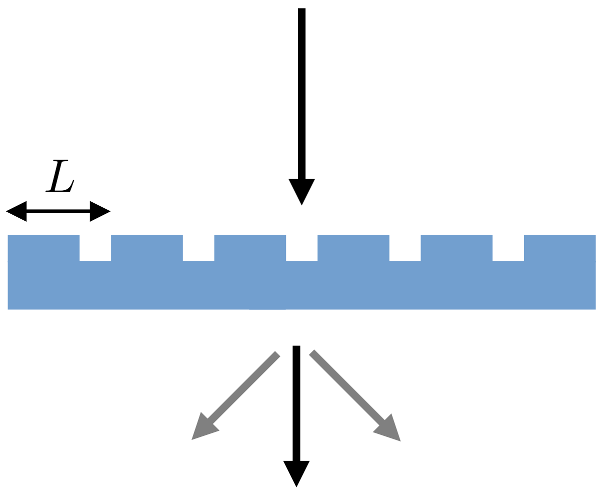


Scattering between 0^{th}- and 1^{st}-order channels

Despite the broken symmetry, reciprocity forces the scattering between 0^{th}-order channels to be identical. It is not the case anymore when higher-order diffraction orders are considered.

Diffraction Channels and Broken Symmetry

Symmetric grating

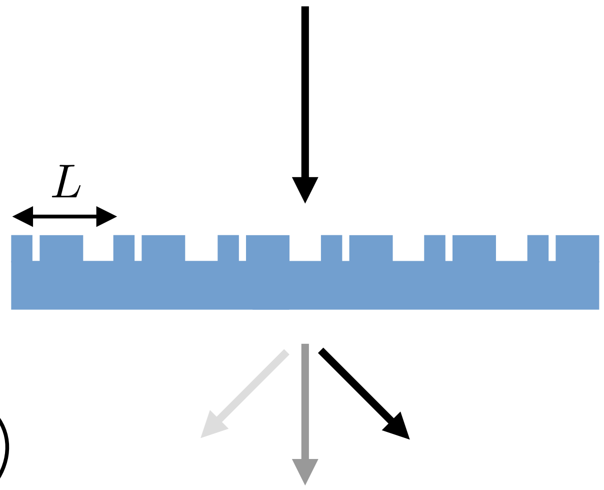


Total number of DO at normal incidence

$$N_{\mathrm{s}} = 1 + 2\left\lfloor n_{\mathrm{s}} \frac{L}{\lambda_0} \right\rfloor$$

The only thing that determines the number of DO is this ratio

Asymmetric grating



Diffraction orders should be seen as “channels” in which the energy can flow. The ratio above determines how many of these channels are open regardless of the material, shape and spatial symmetries. Changing the material composition, the shape and breaking symmetries allows controlling how much energy goes into each opened channel.

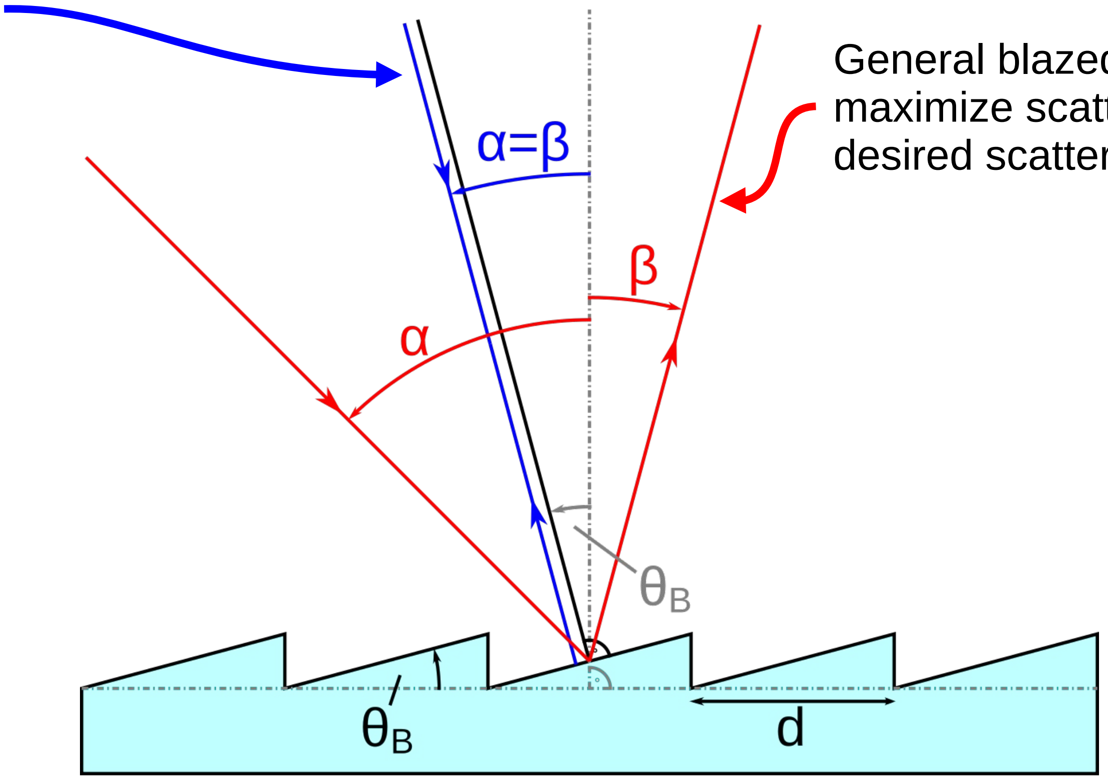
Blazed Gratings

Littrow configuration (retro-reflection)

$$\sin\theta_m = \sin\theta_{\text{inc}} - m\frac{\lambda_0}{L}$$

$$-\sin\theta_{\text{inc}} = \sin\theta_{\text{inc}} - m\frac{\lambda_0}{L}$$

$$2\sin\theta_{\text{inc}} = m\frac{\lambda_0}{L}$$



General blazed grating operation: maximize scattering into the desired scattering angle β

spectral sensitivity

$$\frac{\partial\lambda_0}{\partial\theta} = 2\frac{L}{m}\cos\theta$$

$$\Delta\lambda_0 = 2\frac{L}{m}\cos\theta\Delta\theta$$

https://commons.wikimedia.org/wiki/File:Blazed_grating.svg#/media/File:Blazed_grating.svg

What Have We Learned So Far….

- Diffraction gratings provide more degrees of freedom for controlling light compared to subwavelength metasurfaces since they scatter light in several diffraction channels.
- Breaking the σ_x symmetry of a metasurface does not affect its angular scattering response. However, it breaks the angular scattering between 0^{th} and 1^{st} DO of a diffraction grating.
- At normal incidence, the ratio ($n_s L/\lambda_0$) is the only thing that determines the number of opened diffraction channels. How the incident wave energy spreads into these channels is determined by the material, the geometry and the symmetries of the diffraction grating.
- Blazed gratings are diffraction gratings optimized to redirect the incident energy into only one DO.

Subwavelength Gratings

Effective Permittivity of Subwavelength Gratings

Parallel polarization

At the boundaries, we have

$$\begin{cases} E_{\parallel,1} = E_{\parallel,2} = E_{\parallel} \\ D_{\parallel,1} \neq D_{\parallel,2} \end{cases}$$

$$D_{\parallel,\mathrm{av}} = f D_{\parallel,1} + (1-f) D_{\parallel,2}$$

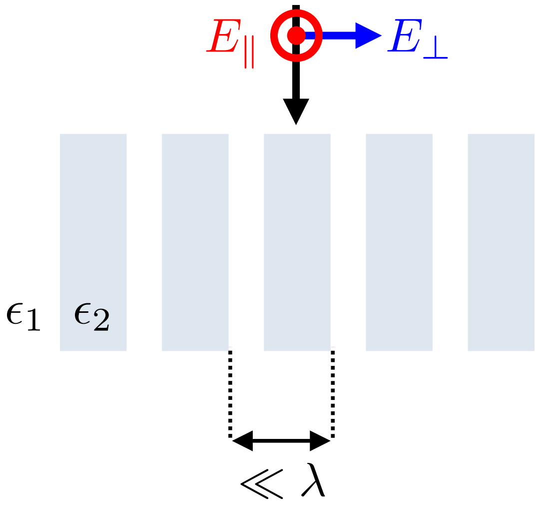
$$D_{\parallel} = \epsilon E_{\parallel}$$

$$\epsilon_{\parallel,\mathrm{av}} E_{\parallel} = f\epsilon_1 E_{\parallel,1} + (1-f)\epsilon_2 E_{\parallel,2}$$

$$\epsilon_{\parallel,\mathrm{av}} = f\epsilon_1 + (1-f)\epsilon_2$$

Design equation

$$f = \frac{\epsilon_2 - \epsilon_{\parallel,\mathrm{av}}}{\epsilon_2 - \epsilon_1}$$



f: filling fraction

Perpendicular polarization

At the boundaries, we have

$$\begin{cases} D_{\perp,1} = D_{\perp,2} = D_{\perp} \\ E_{\perp,1} \neq E_{\perp,2} \end{cases}$$

$$E_{\perp,\mathrm{av}} = f E_{\perp,1} + (1-f) E_{\perp,2}$$

$$E_{\perp} = \epsilon^{-1} D_{\perp}$$

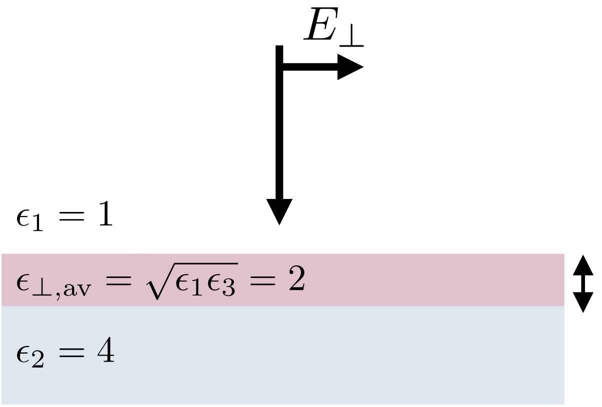
$$\epsilon_{\perp,\mathrm{av}}^{-1} D_{\perp} = f\epsilon_1^{-1} D_{\perp,1} + (1-f)\epsilon_2^{-1} D_{\perp,2}$$

$$\frac{1}{\epsilon_{\perp,\mathrm{av}}} = \frac{f}{\epsilon_1} + \frac{(1-f)}{\epsilon_2}$$

Design equation

$$f = \frac{\epsilon_1\left(\epsilon_{\perp,\mathrm{av}} - \epsilon_2\right)}{\epsilon_{\perp,\mathrm{av}}\left(\epsilon_1 - \epsilon_2\right)}$$

Anti-Reflection Coating Using a Subwavelength Grating

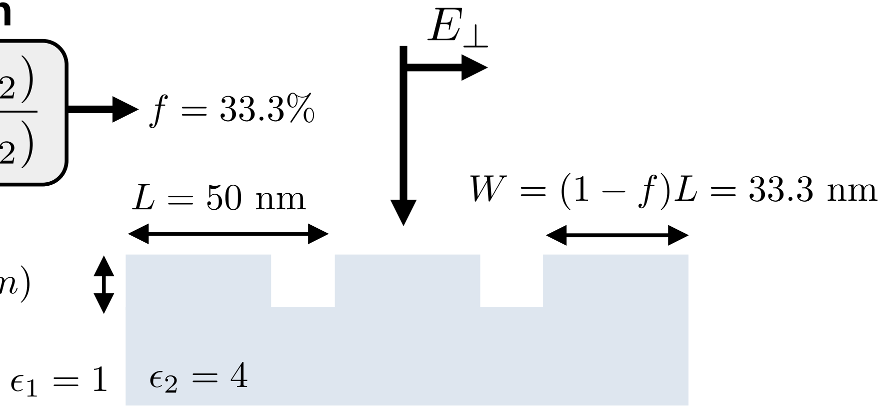


Design equation

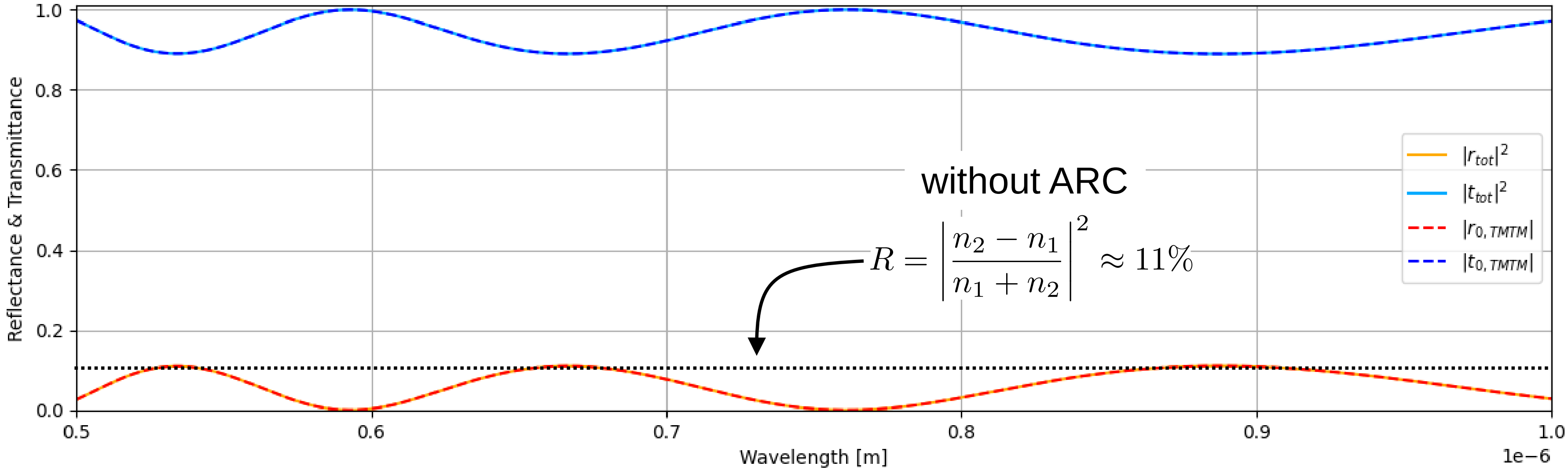
$$f = \frac{\epsilon_1 \left(\epsilon_{\perp,\mathrm{av}} - \epsilon_2\right)}{\epsilon_{\perp,\mathrm{av}} \left(\epsilon_1 - \epsilon_2\right)}$$

$\rightarrow f = 33.3\%$

$$H = \frac{\lambda_0}{4\sqrt{\epsilon_{\perp,\mathrm{av}}}}(1 + 2m)$$



Design for *m* = 3 at λ_0 = 750 nm



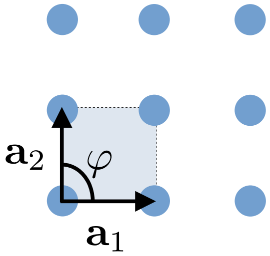
What Have We Learned So Far….

- Deeply subwavelength gratings maybe used to implement effective refractive indices. This is achieved by controlling the grating period and filling fraction.
- Note that such structures are inherently birefringent and thus lead to different effective refractive indices for TE and TM waves
- The design equations of subwavelength gratings are only indicative. They bring you close to the desired response but further optimization is often required.

2D Periodic Systems

2D Bravais Lattices

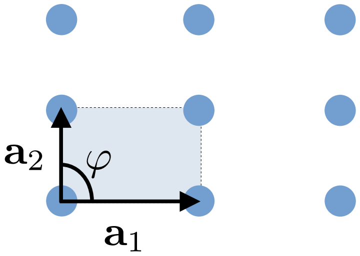
Square



$|\mathbf{a}_1| = |\mathbf{a}_2|$

$\varphi = 90^\circ$

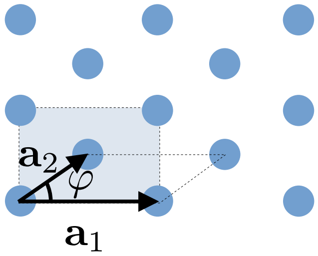
Rectangular



$|\mathbf{a}_1| \neq |\mathbf{a}_2|$

$\varphi = 90^\circ$

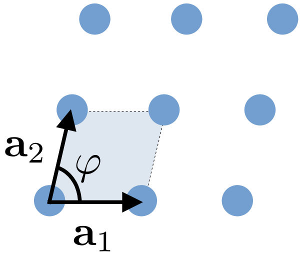
Rhombic
(centered rectangular)



$|\mathbf{a}_1| \neq |\mathbf{a}_2|$

$\varphi \neq 90^\circ$

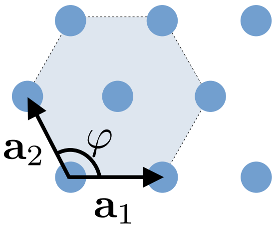
Oblique



$|\mathbf{a}_1| \neq |\mathbf{a}_2|$

$\varphi \neq 90^\circ$

Hexagonal

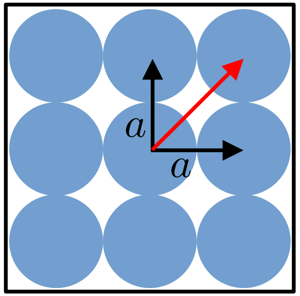


$|\mathbf{a}_1| = |\mathbf{a}_2|$

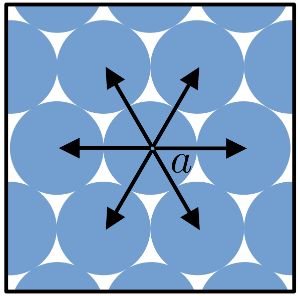
$\varphi = 120^\circ$

Packing Density: Square vs Hexagonal Array

Square



Hexagonal



$$f_{\text{square}} = \pi \left(\frac{r}{a}\right)^2$$

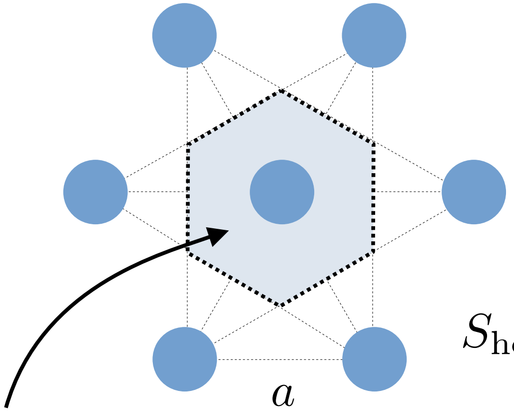
$$\frac{f_{\text{hexagonal}}}{f_{\text{square}}} = \frac{\sqrt{3}}{2\pi} \approx 1.155$$

$$f_{\text{hexagonal}} = \frac{2\pi}{\sqrt{3}} \left(\frac{r}{a}\right)^2$$

The hexagonal lattice not only has a higher (~15%) filling fraction than the square lattice but its inter-element spacing is identical meaning that they all couple to each other in the same way. Additionally, the hexagonal lattice leads to lower resonance frequency than the square lattice.

Hexagonal Lattice Unit Cell

Hexagonal unit cell



Wigner-Seitz primitive unit cell

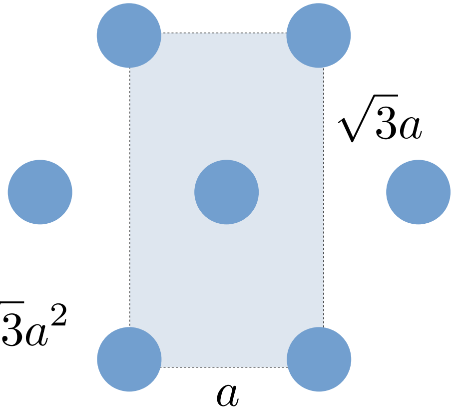
Unit cell surface area

$$S_{\text{hex}} = \frac{3\sqrt{3}}{8}a^2$$

$$S_{\text{rec}} = \sqrt{3}a^2$$

$$\frac{S_{\text{rec}}}{S_{\text{hex}}} = \frac{8}{3} \approx 2.66$$

Hexagonal structure with rectangular unit cell



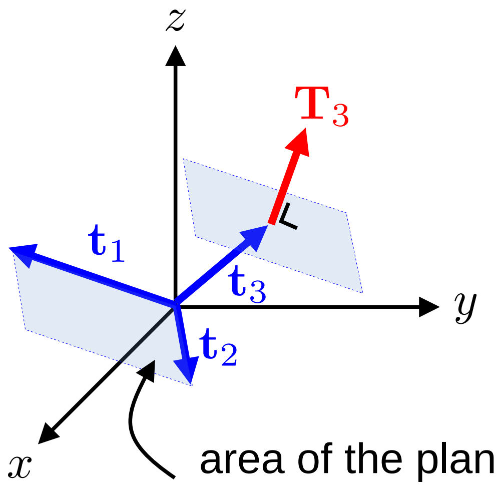
A rectangular unit cell may be used to simulate a hexagonal lattice but would require more computational power as it is bigger than the Wigner-Seitz cell.

<u>Construction:</u>
1) Draw lines between one element and all its neighbors
2) In the middle of these lines, draw a perpendicular
3) The intersections of the perpendicular lines form the unit cell

Primitive and Reciprocal Lattice Vectors

The primitive lattice vectors are the smallest vectors that can be used to describe a unit cell.

The reciprocal lattice vectors represent the wavevectors of the lattice in Fourier space.



area of the plane

$$A = |\mathbf{t}_1 \times \mathbf{t}_2|$$

Volume defined by the two planes

$$V = \mathbf{t}_3 \cdot (\mathbf{t}_1 \times \mathbf{t}_2)$$

We define $|\mathbf{T}_3| = \dfrac{2\pi}{L_3}$ where $\dfrac{\mathbf{T}_3}{|\mathbf{T}_3|} = \dfrac{\mathbf{t}_1 \times \mathbf{t}_2}{|\mathbf{t}_1 \times \mathbf{t}_2|}$

where L_3 is the distance between the repeated planes defined by

$$L_3 = \frac{V}{A} = \frac{\mathbf{t}_3 \cdot (\mathbf{t}_1 \times \mathbf{t}_2)}{|\mathbf{t}_1 \times \mathbf{t}_2|}$$

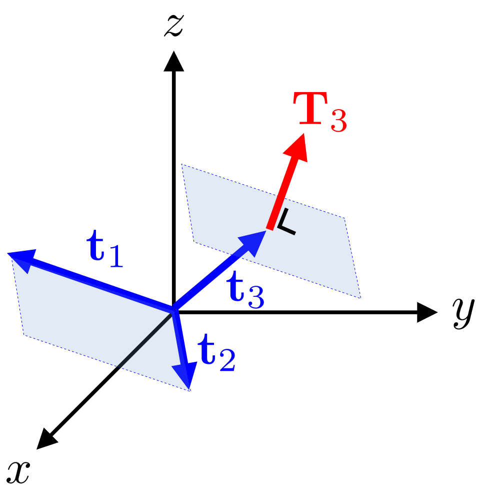
Combining these different results, we have

$$\mathbf{T}_3 = |\mathbf{T}_3| \frac{\mathbf{t}_1 \times \mathbf{t}_2}{|\mathbf{t}_1 \times \mathbf{t}_2|} = \frac{2\pi}{L_3} \frac{\mathbf{t}_1 \times \mathbf{t}_2}{|\mathbf{t}_1 \times \mathbf{t}_2|} = \frac{2\pi}{\frac{\mathbf{t}_3 \cdot (\mathbf{t}_1 \times \mathbf{t}_2)}{|\mathbf{t}_1 \times \mathbf{t}_2|}} \frac{\mathbf{t}_1 \times \mathbf{t}_2}{|\mathbf{t}_1 \times \mathbf{t}_2|}$$

↓

$$\mathbf{T}_3 = 2\pi \frac{\mathbf{t}_1 \times \mathbf{t}_2}{\mathbf{t}_3 \cdot (\mathbf{t}_1 \times \mathbf{t}_2)}$$

Primitive and Reciprocal Lattice Vectors



In three dimensions

$$\mathbf{T}_1 = 2\pi \frac{\mathbf{t}_2 \times \mathbf{t}_3}{\mathbf{t}_1 \cdot (\mathbf{t}_2 \times \mathbf{t}_3)} \qquad \mathbf{t}_1 = 2\pi \frac{\mathbf{T}_2 \times \mathbf{T}_3}{\mathbf{T}_1 \cdot (\mathbf{T}_2 \times \mathbf{T}_3)}$$

$$\mathbf{T}_2 = 2\pi \frac{\mathbf{t}_3 \times \mathbf{t}_1}{\mathbf{t}_1 \cdot (\mathbf{t}_2 \times \mathbf{t}_3)} \qquad \mathbf{t}_2 = 2\pi \frac{\mathbf{T}_3 \times \mathbf{T}_1}{\mathbf{T}_1 \cdot (\mathbf{T}_2 \times \mathbf{T}_3)}$$

$$\mathbf{T}_3 = 2\pi \frac{\mathbf{t}_1 \times \mathbf{t}_2}{\mathbf{t}_3 \cdot (\mathbf{t}_1 \times \mathbf{t}_2)} \qquad \mathbf{t}_3 = 2\pi \frac{\mathbf{T}_1 \times \mathbf{T}_2}{\mathbf{T}_1 \cdot (\mathbf{T}_2 \times \mathbf{T}_3)}$$

In two dimensions

By setting

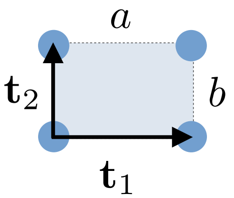
$$\mathbf{t}_3 = \hat{\mathbf{z}}$$

$$\mathbf{T}_1 = \frac{2\pi}{|\mathbf{t}_1 \times \mathbf{t}_2|} \begin{bmatrix} t_{2,y} \\ -t_{2,x} \end{bmatrix} \qquad \mathbf{t}_1 = \frac{2\pi}{|\mathbf{T}_1 \times \mathbf{T}_2|} \begin{bmatrix} T_{2,y} \\ -T_{2,x} \end{bmatrix}$$

$$\mathbf{T}_2 = \frac{2\pi}{|\mathbf{t}_1 \times \mathbf{t}_2|} \begin{bmatrix} -t_{1,y} \\ t_{1,x} \end{bmatrix} \qquad \mathbf{t}_2 = \frac{2\pi}{|\mathbf{T}_1 \times \mathbf{T}_2|} \begin{bmatrix} -T_{1,y} \\ T_{1,x} \end{bmatrix}$$

Primitive Lattice Vectors of Rectangular and Hexagonal Array

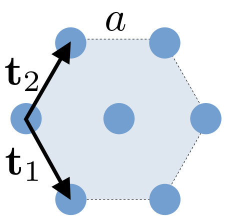
Rectangular



$$\begin{bmatrix} \mathbf{t}_1 \\ \mathbf{t}_2 \end{bmatrix} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \cdot \begin{bmatrix} \hat{\mathbf{x}} \\ \hat{\mathbf{y}} \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{T}_1 \\ \mathbf{T}_2 \end{bmatrix} = \begin{bmatrix} \frac{2\pi}{a} & 0 \\ 0 & \frac{2\pi}{b} \end{bmatrix} \cdot \begin{bmatrix} \hat{\mathbf{x}} \\ \hat{\mathbf{y}} \end{bmatrix}$$

Hexagonal



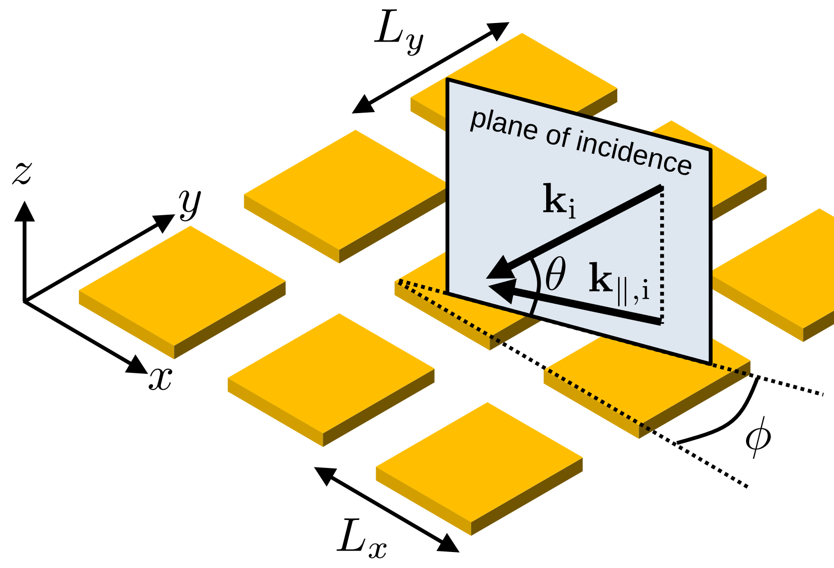
$$\begin{bmatrix} \mathbf{t}_1 \\ \mathbf{t}_2 \end{bmatrix} = \frac{a}{2} \begin{bmatrix} 1 & -\sqrt{3} \\ 1 & \sqrt{3} \end{bmatrix} \cdot \begin{bmatrix} \hat{\mathbf{x}} \\ \hat{\mathbf{y}} \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{T}_1 \\ \mathbf{T}_2 \end{bmatrix} = \frac{2\pi}{a} \begin{bmatrix} 1 & -\frac{1}{\sqrt{3}} \\ 1 & \frac{1}{\sqrt{3}} \end{bmatrix} \cdot \begin{bmatrix} \hat{\mathbf{x}} \\ \hat{\mathbf{y}} \end{bmatrix}$$

The reciprocal lattice vectors are obtained using

$$\mathbf{T}_1 = \frac{2\pi}{|\mathbf{t}_1 \times \mathbf{t}_2|} \begin{bmatrix} t_{2,y} \\ -t_{2,x} \end{bmatrix} \qquad \mathbf{T}_2 = \frac{2\pi}{|\mathbf{t}_1 \times \mathbf{t}_2|} \begin{bmatrix} -t_{1,y} \\ t_{1,x} \end{bmatrix}$$

2D Diffraction Gratings



Reciprocal lattice vectors

$$\begin{bmatrix} \mathbf{T}_1 \\ \mathbf{T}_2 \end{bmatrix} = \begin{bmatrix} \frac{2\pi}{L_x} & 0 \\ 0 & \frac{2\pi}{L_y} \end{bmatrix} \cdot \begin{bmatrix} \hat{\mathbf{x}} \\ \hat{\mathbf{y}} \end{bmatrix}$$

The tangential k-vector components of the waves diffracted by the grating are functions of the reciprocal lattice vectors

$$\mathbf{k}_{\|}(p,q) = \mathbf{k}_{\|,\mathrm{i}} - p\mathbf{T}_1 - q\mathbf{T}_2$$

The normal wavevector component for the reflected and transmitted DO are given by

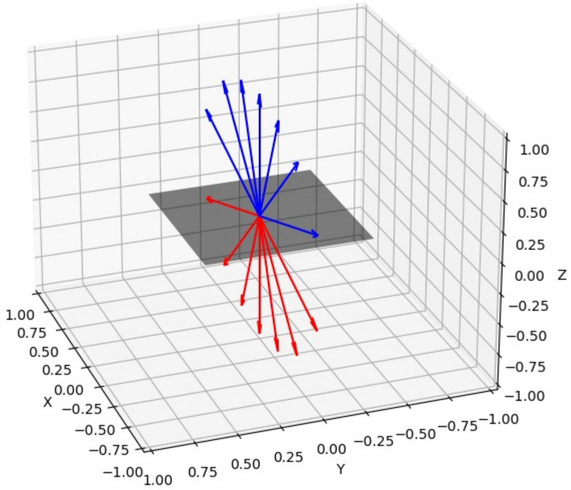
$$\mathbf{k}_{\perp,\mathrm{r}}(p,q) = -\hat{\mathbf{z}}\sqrt{k_r^2 - |\mathbf{k}_{\|}(p,q)|^2}$$

$$\mathbf{k}_{\perp,\mathrm{t}}(p,q) = +\hat{\mathbf{z}}\sqrt{k_t^2 - |\mathbf{k}_{\|}(p,q)|^2}$$

Illustration of Diffraction by 2D Gratings

$$\theta_\mathrm{i} = 0^\circ,\ \phi_\mathrm{i} = 0^\circ$$

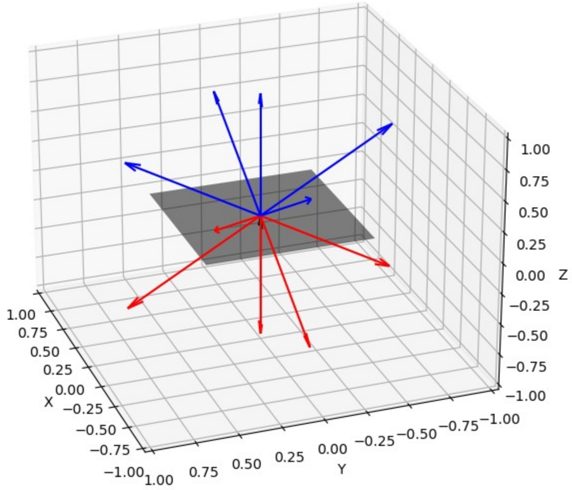
$$L_x = 3.25\lambda,\ L_y = 0.5\lambda$$



Subwavelength along y.
All DO are in the xz-plane.

$$\theta_\mathrm{i} = 0^\circ,\ \phi_\mathrm{i} = 0^\circ$$

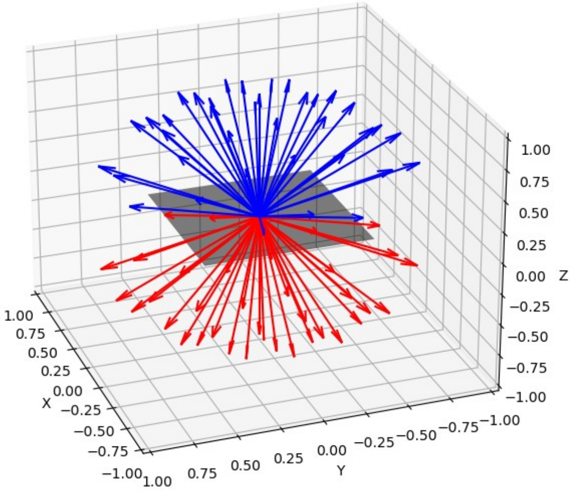
$$L_x = 1.25\lambda,\ L_y = 1.25\lambda$$



Square lattice barely larger than the wavelength. All DO are in the xz- and yz-planes.

$$\theta_\mathrm{i} = 0^\circ,\ \phi_\mathrm{i} = 0^\circ$$

$$L_x = 3.5\lambda,\ L_y = 3.5\lambda$$



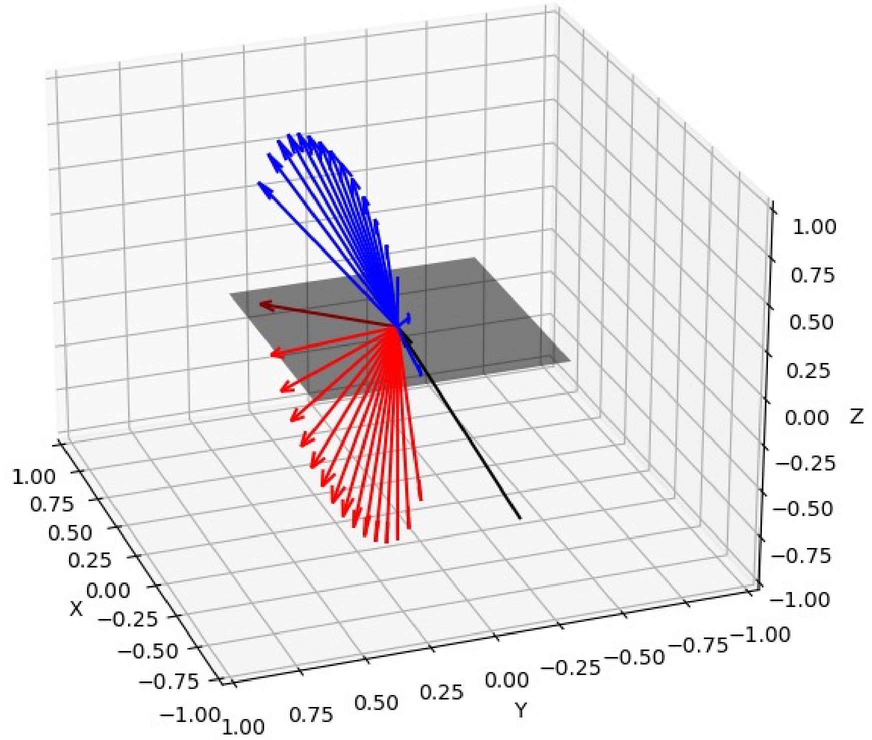
Square lattice larger than the wavelength. The DO spread everywhere.

Conical Diffraction

$$\theta_{\mathrm{i}} = 45^\circ,\ \phi_{\mathrm{i}} = 20^\circ$$

$$L_x = 8.25\lambda,\ L_y = 0.5\lambda$$

Subwavelength along y. The oblique incidence makes the DO spread over a cone.

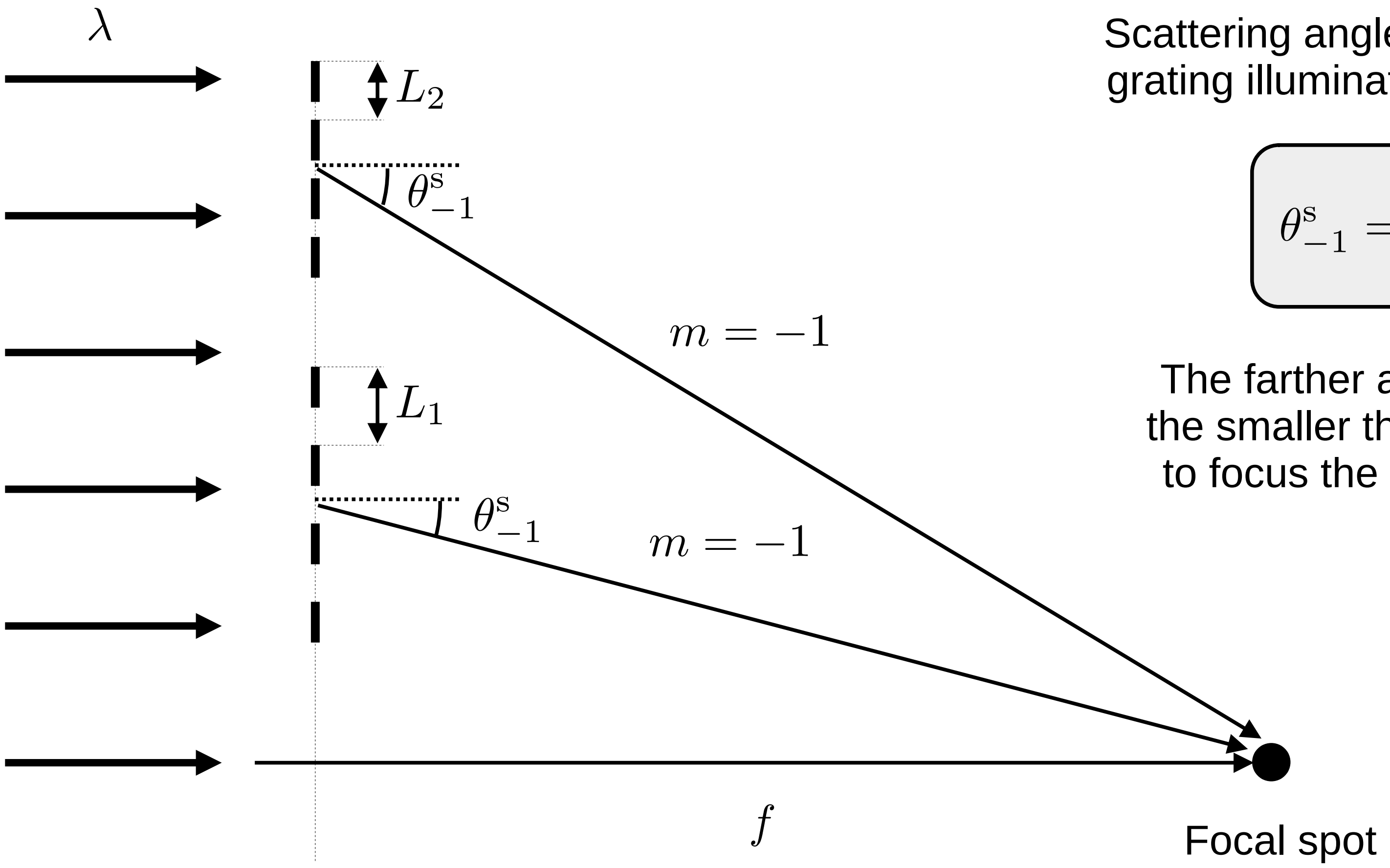


What Have We Learned So Far….

- For 2D periodic structures, there exists 5 types of (Bravais) lattices. The most used ones are the square, rectangular and hexagonal lattices.
- Hexagonal lattices have the advantage of having a ~15% higher filling ratio than square lattices and exhibit equal coupling between neighboring elements. They also typically lead to lower resonance frequencies.
- If one does not possess a Maxwell solver able to simulate hexagonal lattices, it is still possible to simulate them using rectangular lattices at the cost of larger simulation domains and thus higher computational cost.
- The primitive lattice vectors are used to represent the geometry of a lattice in direct space. From these primitive lattice vectors, one can compute the corresponding reciprocal lattice vectors that correspond to wavevectors in Fourier space.
- The reciprocal lattice vectors are very useful to determine the direction of propagation of the DO of 2D diffraction gratings.
- Under oblique illumination, a 2D diffraction grating may see its DO spread over a conical region.

Fresnel Zone Plate

Focusing Light Using Diffraction

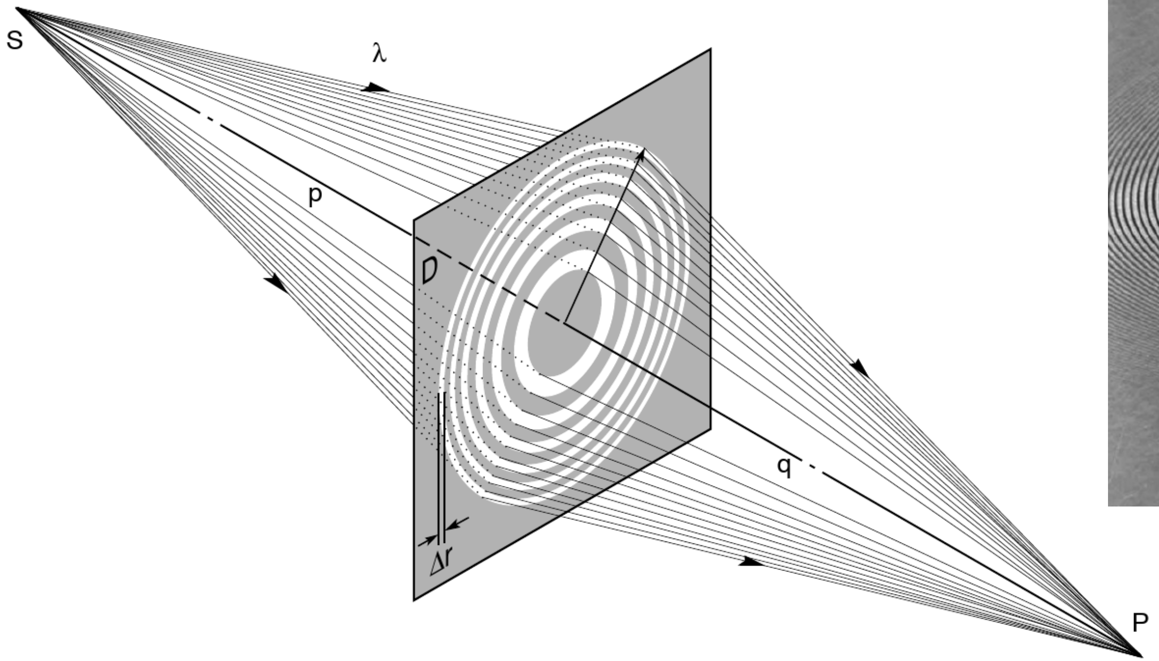


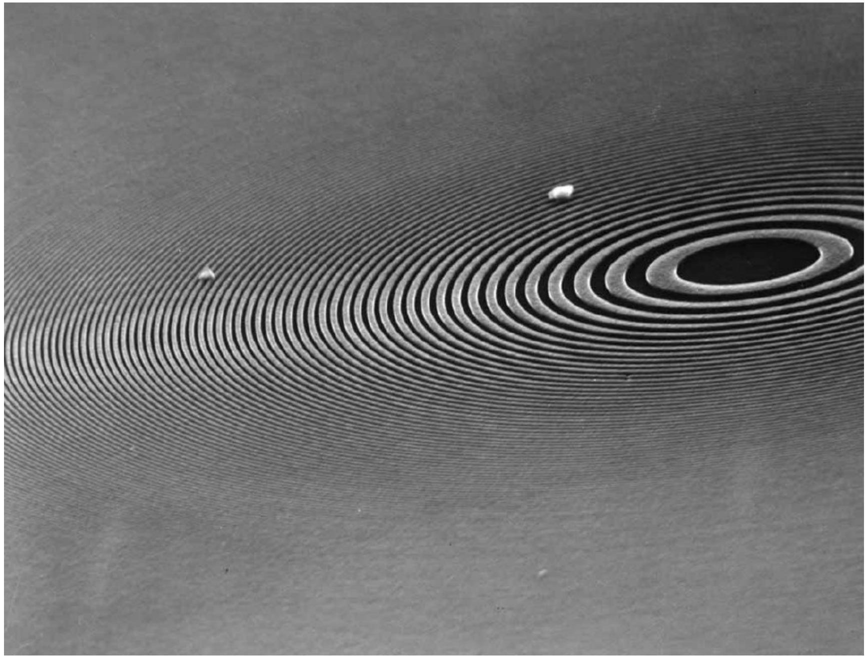
Scattering angle for the m = -1 DO of a grating illuminated at normal incidence

$$\theta^{s}_{-1} = \arcsin\left(\frac{\lambda_0}{L}\right)$$

The farther away from the center, the smaller the grating period must to focus the light at the focal spot

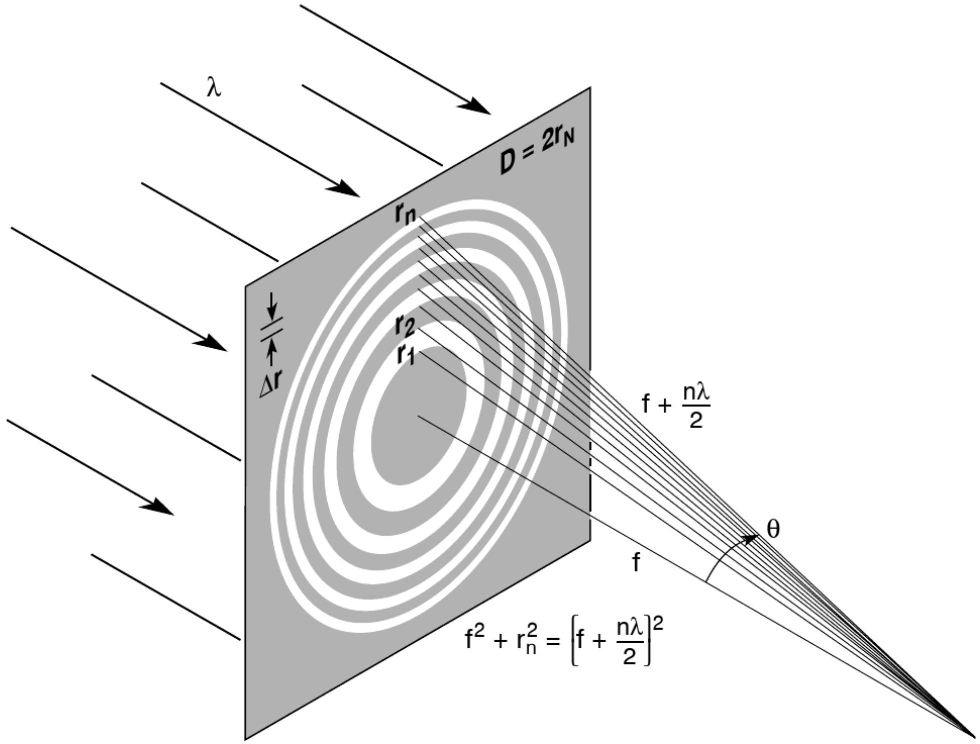
Fresnel Zone Plate





Attwood, “Soft x-rays and extreme ultraviolet radiation: principles and applications”, 2000.

2D Diffraction Gratings



Design equation

$$r_n = \sqrt{nf\lambda + \frac{1}{4}n^2\lambda^2}$$

For long focal distance compared to the wavelength

$$r_n \approx \sqrt{nf\lambda}$$

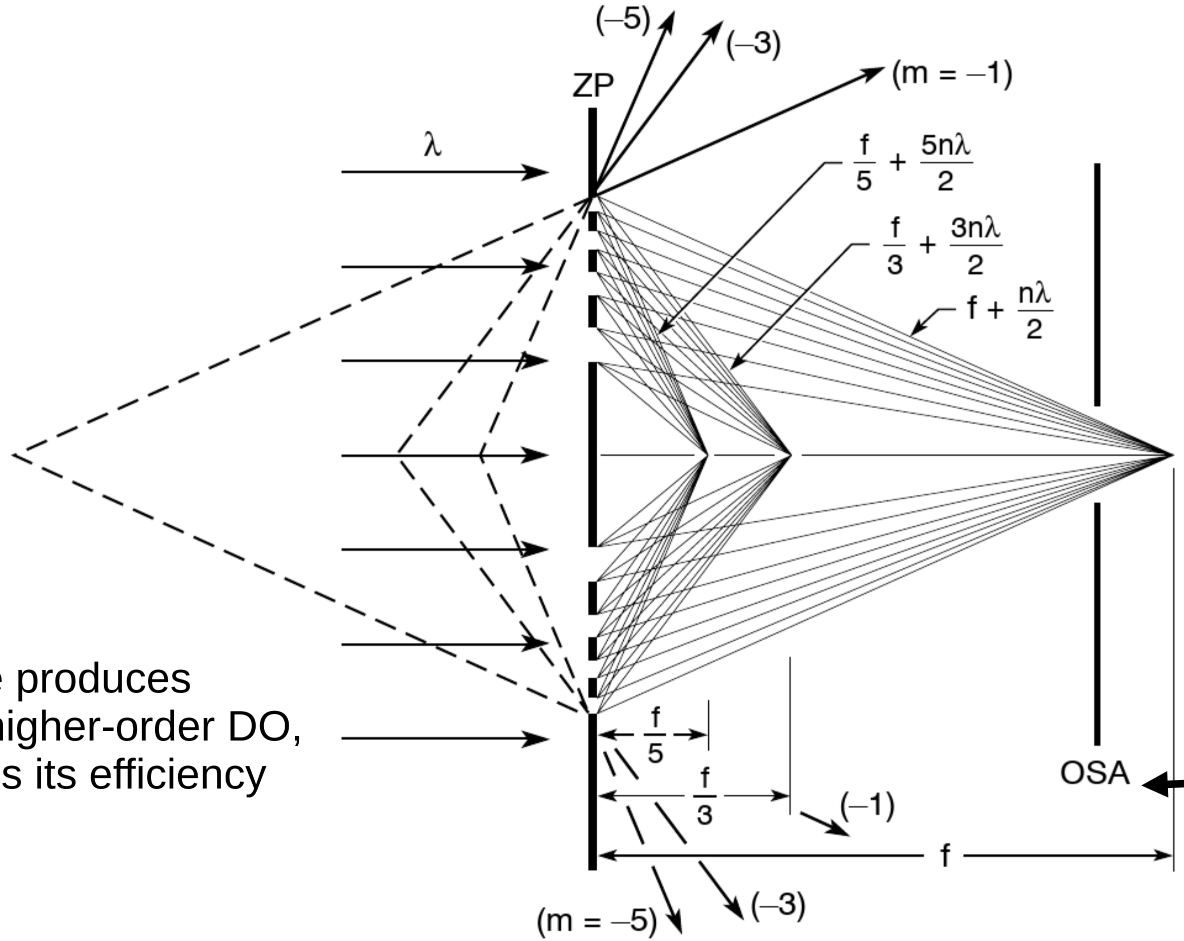
Note that the surface area of each ring is identical

$$\pi\left(r_{n+1}^2 - r_n^2\right) = \pi\left(f\lambda + \frac{1}{4}\lambda^2\right)$$

meaning that only 50% of the light goes through

Attwood, "Soft x-rays and extreme ultraviolet radiation: principles and applications", 2000.

Diffraction Orders Produce Multiple Foci



A Fresnel zone plate produces multiple foci due to higher-order DO, which further reduces its efficiency

Order sorting aperture

Attwood, “Soft x-rays and extreme ultraviolet radiation: principles and applications”, 2000.

What Have We Learned So Far….

- Fresnel zone plates are non-uniform gratings tuned to create a focal spot via diffraction effects.
- Although the efficiency of such “lenses” is not very high, they are useful in frequency regime where it is difficult to create conventional lenses (for instance in the X-ray regime).