Chapter 3

Modeling and Numerical Analysis Approaches

2024年3月12日

Why do we need computational numerical methods?

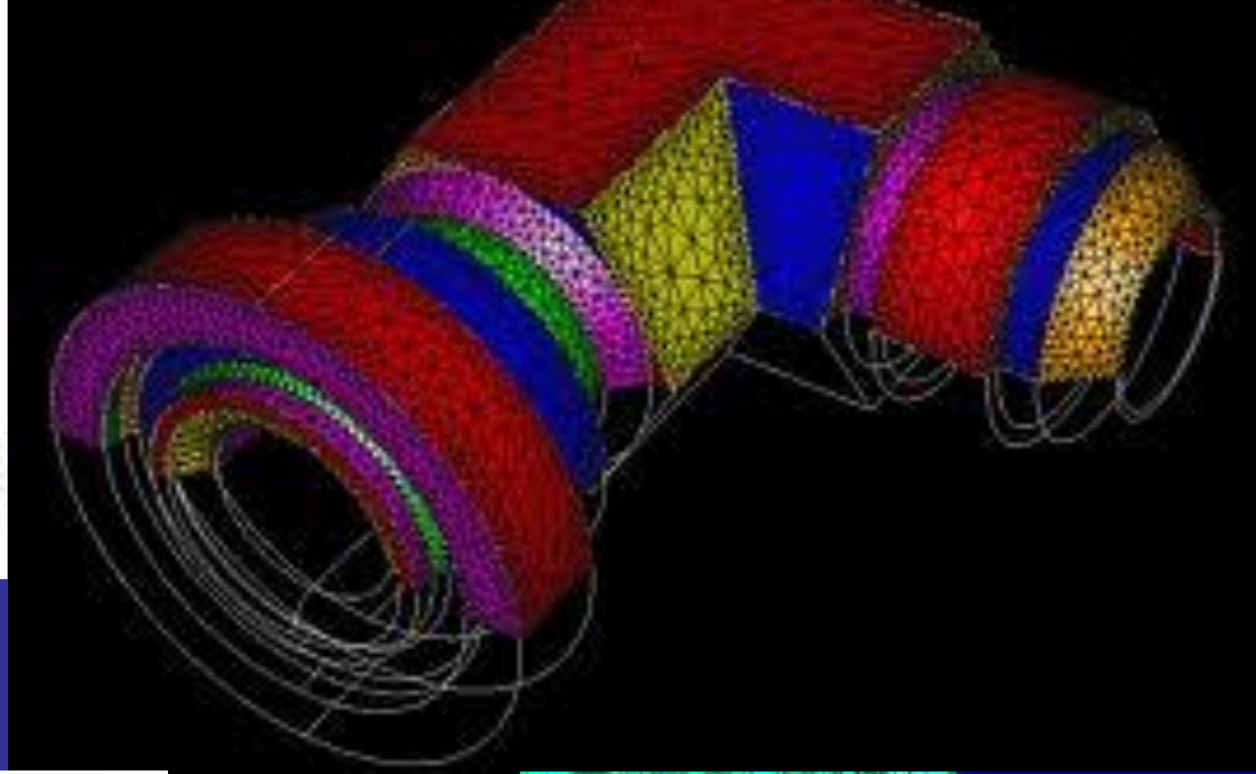
Answer:

It is difficult to calculate **EM** fields of structures with complicated shapes by means of pure theoretical analyses.

目前几乎所有的电磁场分析软件都是基于有限元和FDTD算法设计的

什么是有限元法？

有限元法



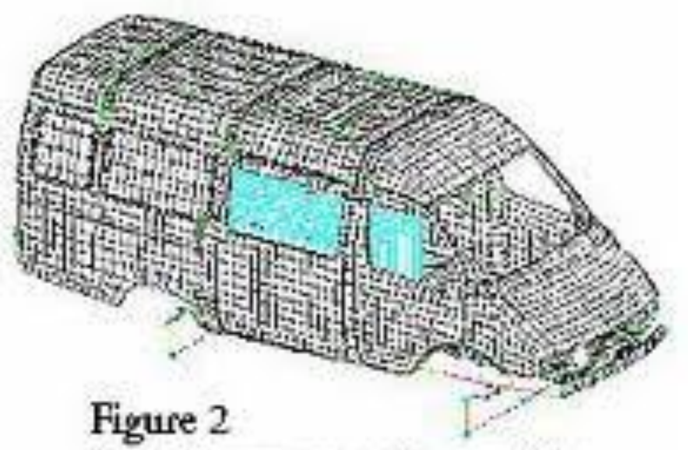
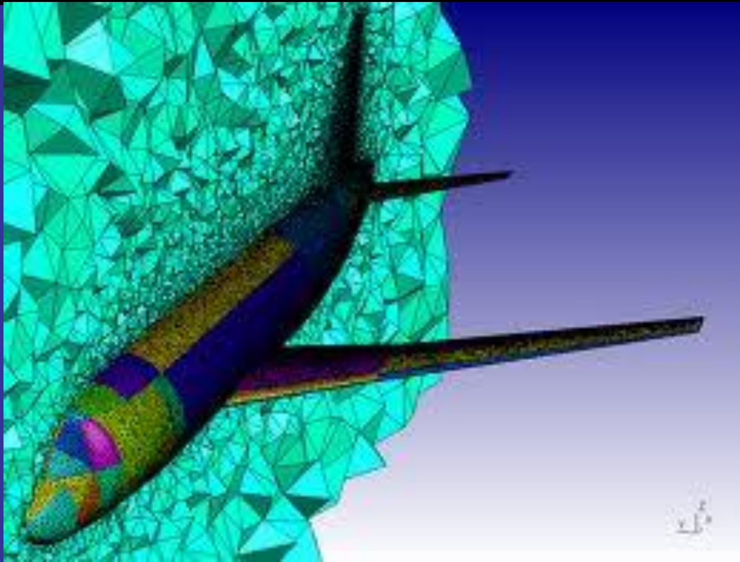
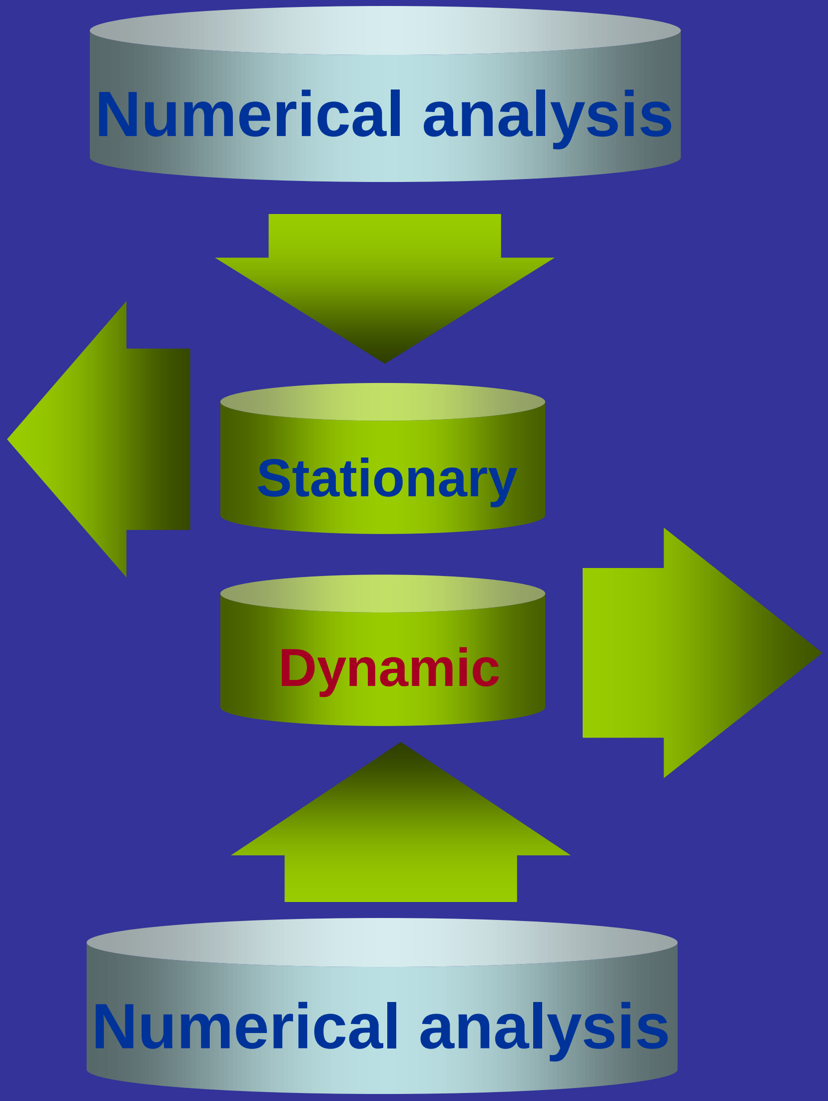


Figure 2
http://www.macsch.com:80
/tech/mscworld/van.html



Numerical Analysis Approaches

- ✓RCWA/FMM
- ✓MMP
- ✓Mie theory
- ✓DDA



- ✓FDTD
- ✓BPM

Introduced in this course

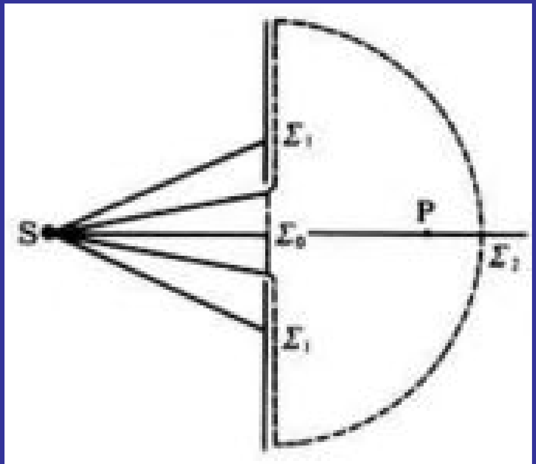
- Rigorous coupling wave analysis (RCWA/FMM)
- Finite difference and time domain (FDTD)
- Discrete dipole approximation (DDA)
- Mutiple multipole program (MMP)
- Mie theory
- Beam propagation method

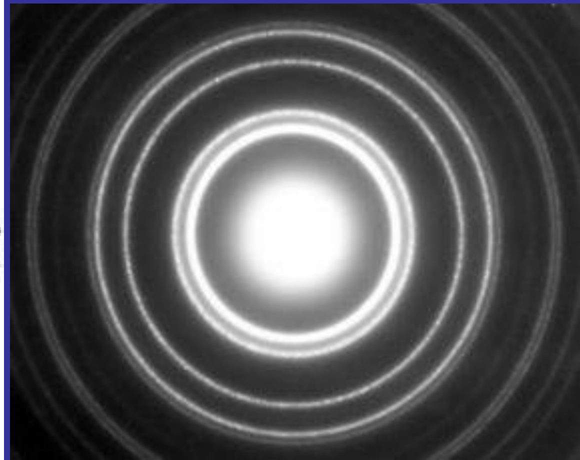
光波的衍射

J.C. Maxwell and H.R. Hertz

电磁波的衍射

当电磁波在传播过程中遇到障碍物或者透过屏幕上的小孔时，会导致偏离原来入射方向的出射电磁波，这种现象称为衍射(**diffraction phenomenon**)。衍射现象的研究对于光学和无线电波的传播都是很重要的。





Optical diffraction theory

- **Scalar diffraction theory** ← $a>5\lambda$

Feature size

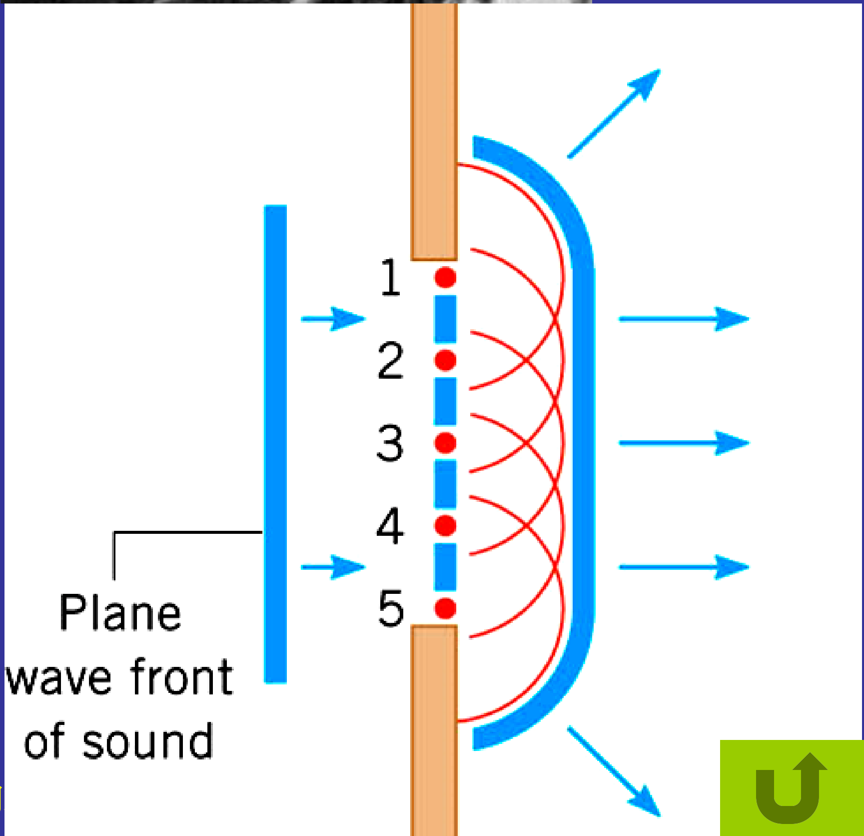
$\lambda \le a \le 5\lambda$

- **Vector diffraction theory** ← $a<\lambda$

Huygen's principle

- Huygen's principle offers an explanation for why and how waves bend (or *diffract*) when passing an obstruction
  - every point on a wave front acts as a source of tiny spherical *wavelets* that travel forward with the same speed as the wave
  - the wave front at a later time is then the ***linear superposition*** of all the wavelets

Christian Huygens (1629-1695)



Vector diffraction theory

$$\nabla \times \boldsymbol{H} = \boldsymbol{J} + j\omega\epsilon\boldsymbol{E}$$

$$\nabla \cdot \boldsymbol{E} = \frac{1}{\epsilon}\rho$$

$$\nabla \times \boldsymbol{E} = -\boldsymbol{J}_m - j\omega\mu\boldsymbol{H}$$

$$\nabla \cdot \boldsymbol{H} = \frac{1}{\mu}\rho_m$$

无任何近似条件地求解
Maxwell Equations

$$\boldsymbol{E} = \frac{1}{j\omega\mu\epsilon}[\nabla \times (\nabla \times \boldsymbol{A}) - \mu\boldsymbol{J}] - \frac{1}{\epsilon}\nabla \times \boldsymbol{A}_m$$

$$\boldsymbol{H} = \frac{1}{j\omega\mu\epsilon}[\nabla \times (\nabla \times \boldsymbol{A}_m) - \epsilon\boldsymbol{J}_m] + \frac{1}{\mu}\nabla \times \boldsymbol{A}$$

Scalar diffraction theory

光波作为标量的条件：

1. 衍射孔径较光波波长大得多，d>>λ；

2. 在远离孔径外观察衍射场, z>>d。

<u>旁轴近似</u>：近轴光学是所有光学基本公式的设定条件，满足sinθ≈θ、cosθ≈1，当然这是为基本计算方便而设定的，由此带来了计算的不精确性，产生球差、象散、畸变等所谓的象差，1 º夹角显然太极端，一般以小于10 º都认为是近轴或称旁轴。

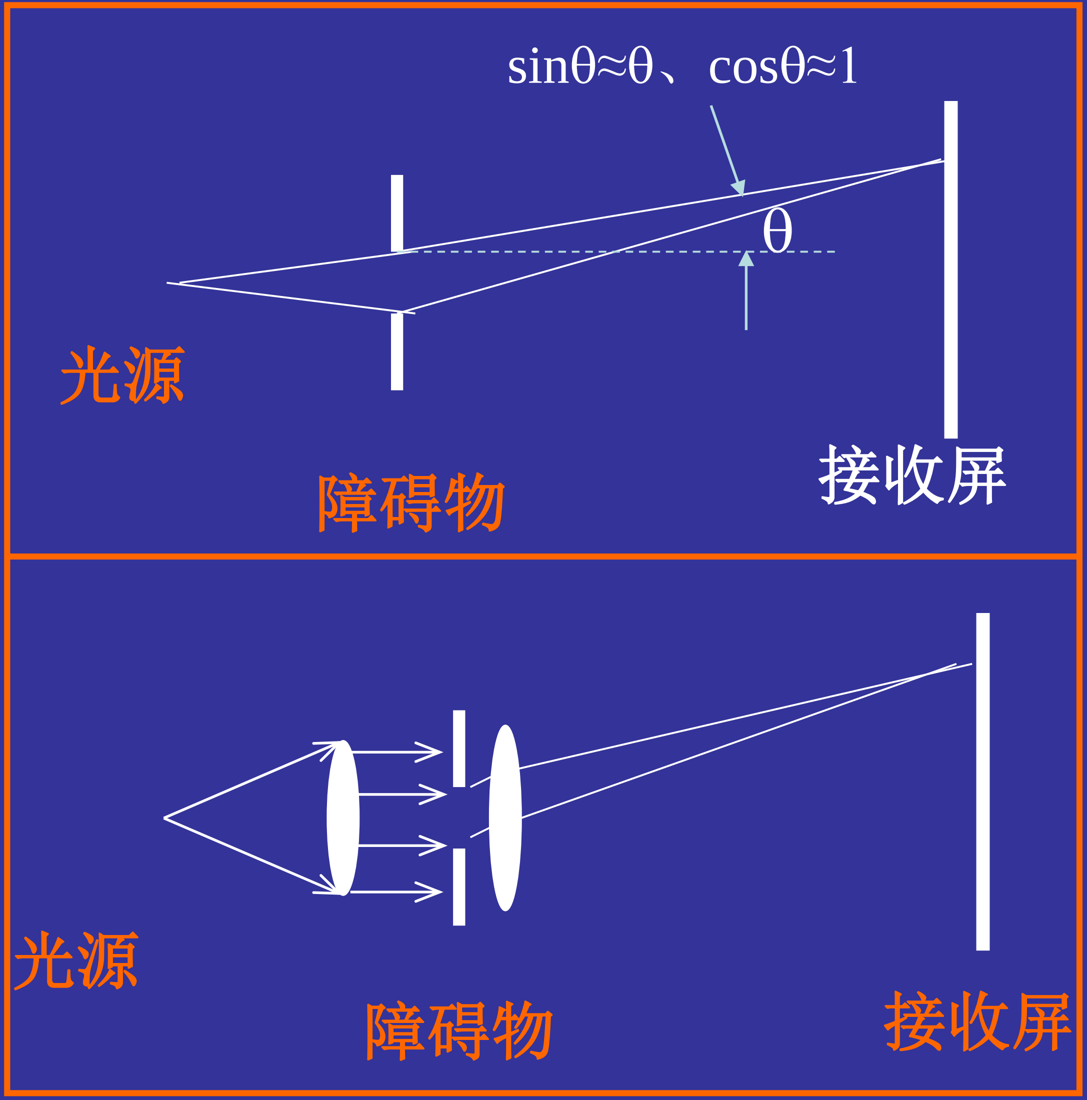
<u>远场近似</u>：单缝距光源和接收屏均为无限远或者相当于无限远，即：入射波和衍射波都可看作是平面波。

School of Physics 物理学院

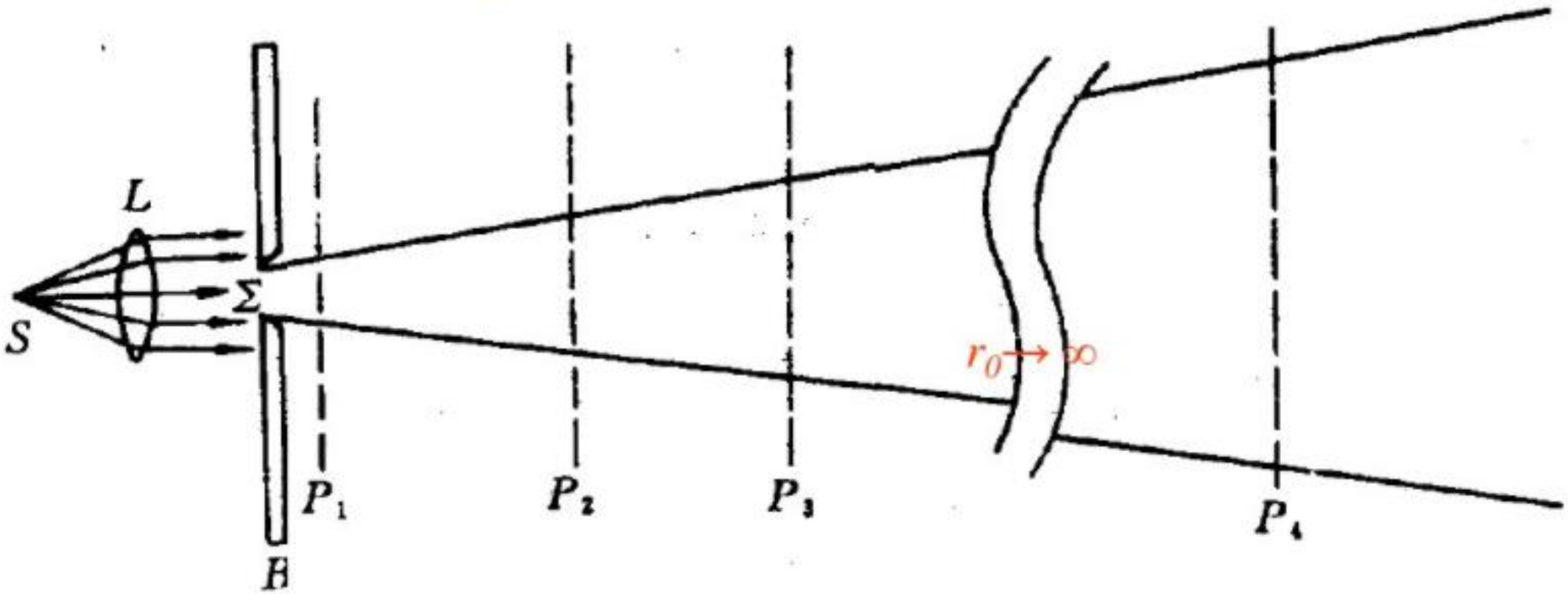
三. 菲涅耳近场衍射和夫琅禾费远场衍射

光源或接收屏距离衍射屏为有限远--菲涅耳衍射 均 满 足 傍 轴 近 似

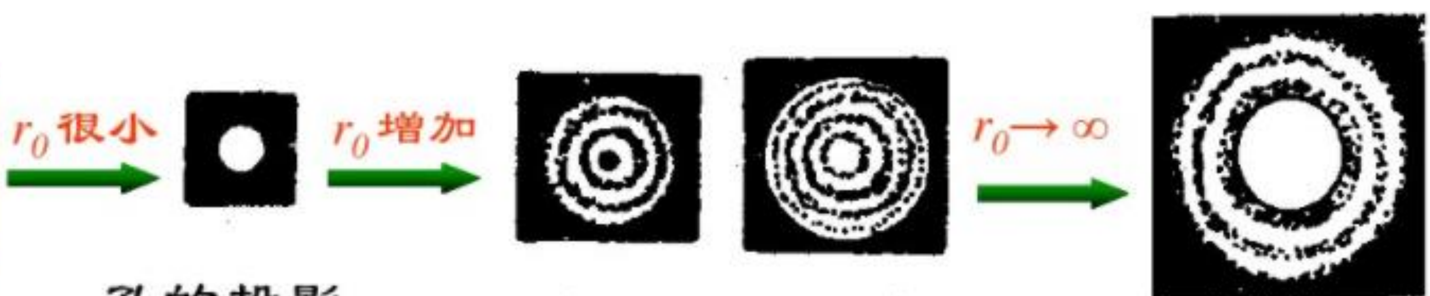
光源或接收屏距离衍射屏都相当于无限远—衍射物上的入射波和衍射波都可看成平面波→夫琅禾费衍射均满足远场近似



圆孔的衍射图样随 r_0 的变化 $(R=\infty)$ ：



屏上图形：



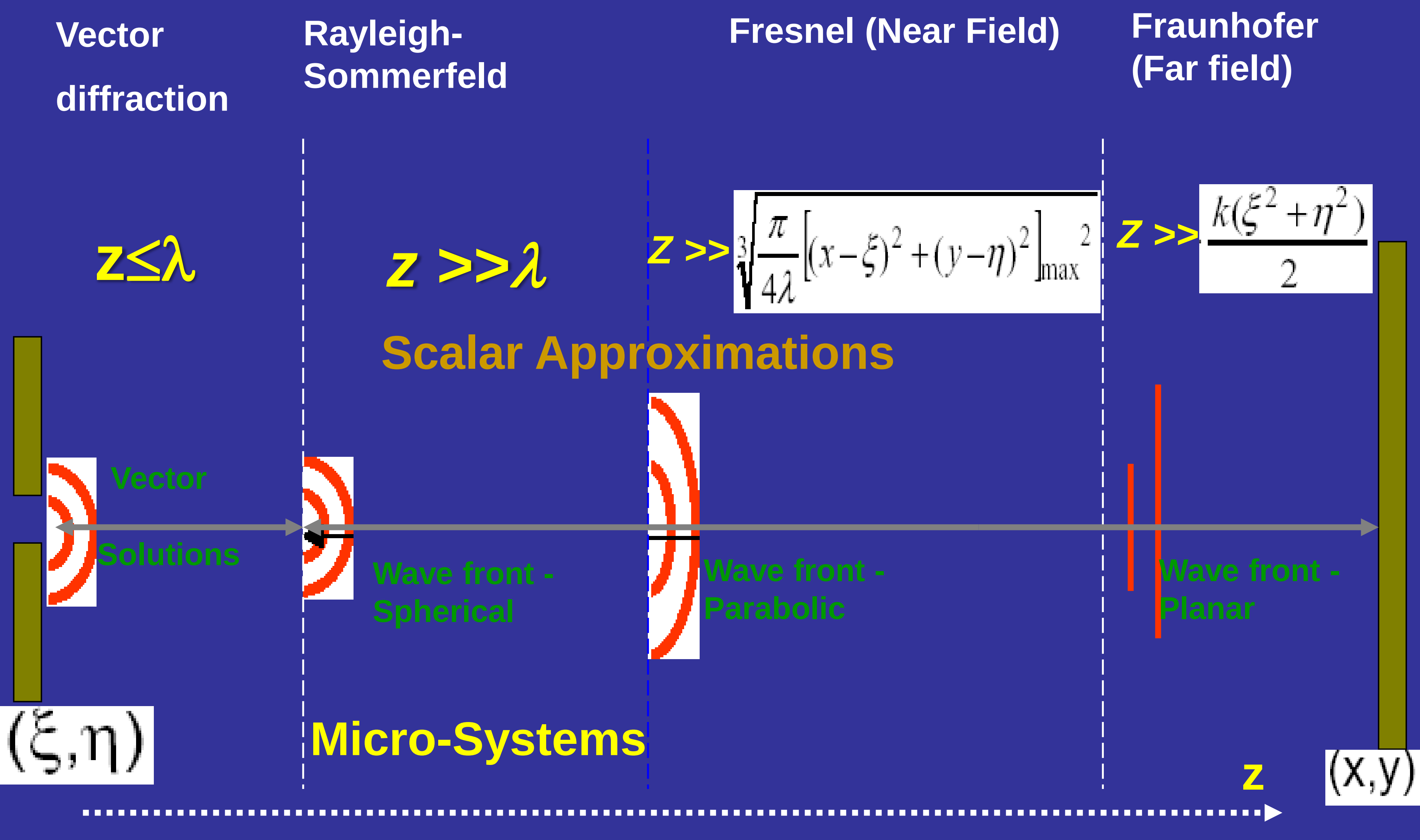
孔的投影

（光直线传播）

菲涅耳衍射

夫琅禾费衍射

标量场的有效性


Vector diffraction
Rayleigh-Sommerfeld
Fresnel (Near Field)
Fraunhofer (Far field)
$z \le \lambda$
$z >> \lambda$
$z >> \sqrt[3]{\frac{\pi}{4\lambda}\left[(x-\xi)^2+(y-\eta)^2\right]^2_{max}}$
$z >> \frac{k(\xi^2+\eta^2)}{2}$
Scalar Approximations
Vector Solutions
Wave front - Spherical
Wave front - Parabolic
Wave front - Planar
(ξ,η)
Micro-Systems
z
(x,y)

衍射分类的几种表述

		菲涅耳衍射	夫琅禾费衍射
特点	1	源和场点均满足傍轴近似，但不满足远场近似。	源点和场点均满足远场近似
	2	源和场点或者之一在有限远	源和场点均在无限远
	3	非平行光衍射	平行光衍射
	4	光源和接收平面是非物像共轭面	光源和接收平面为物像共轭面

标量衍射中的四个经典方程/函数/公式概述

a) 亥姆霍兹方程 (Helmholtz’s equation)

b) 格林函数（Green’s function)

c) 格林公式 (Green’s formula)

d) 基尔霍夫公式 (Kirchhoff’s formula)

严格耦合波分析法(RCWA)/傅里叶模型法(FMM)

RCWA算法通过将Maxwell方程转化成求解特征函数的问题，然后利用边界条件和传输矩阵将每一层联系起来，最后求解出整个结构的场分布。

RCWA与标量衍射处理方法的不同点在于：它考虑到了光波的偏振特性，认为光波的各个电磁分量在衍射光学结构介质都有各自不同的行为，并且衍射光学结构会作为其媒质使各个场分量相互作用。使用RCWA需要用到严格的电磁场理论，在没有任何近似条件下，严格求解MAXWELL方程组。是一种针对**薄层**光栅进行计算的方法。

严格耦合波分析法(RCWA)/傅里叶模型法(FMM)

分析和设计衍射结构的自由程序，它是被光栅结构衍射的电磁波的麦克斯韦方程的严格解。

主要应用：

1.平面电介质或吸收全息光栅的透射和反射；

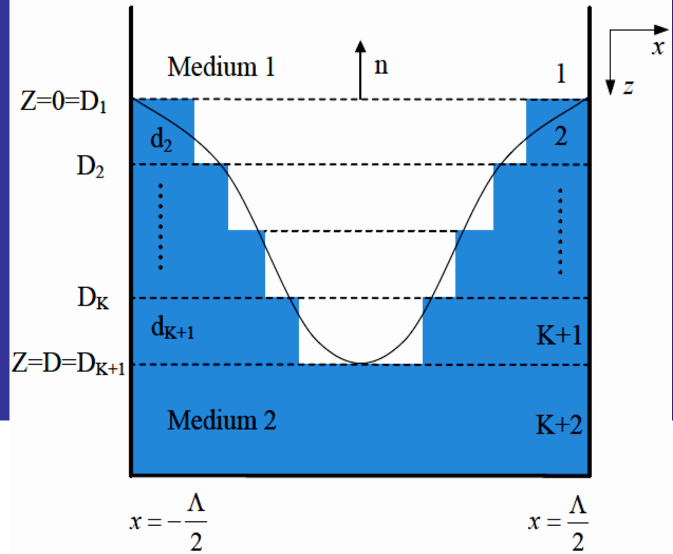
2.任意形貌的电介质或金属的表面浮雕结构光栅；

3.多路复用全息光栅；

4.二维表面浮雕结构光栅；

5.各向异性光栅。

RCWA



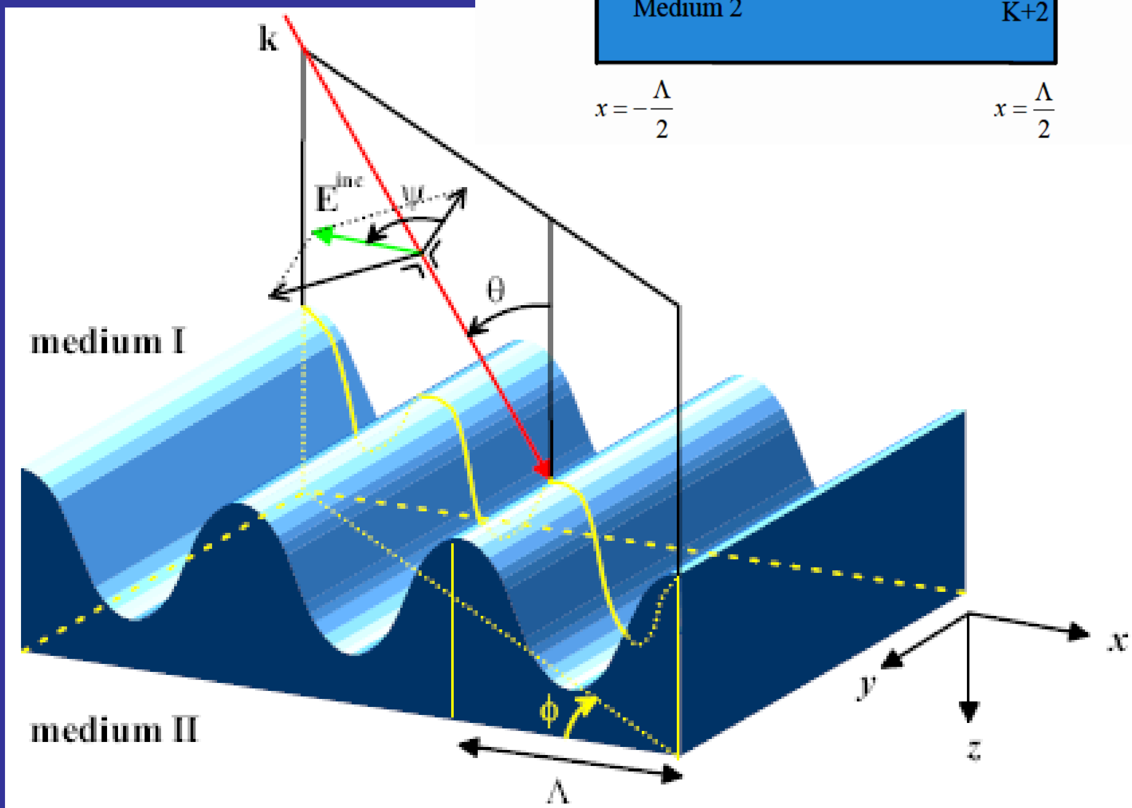


Fig. 3-1 Schematic diagram of one dimensional periodic grating.

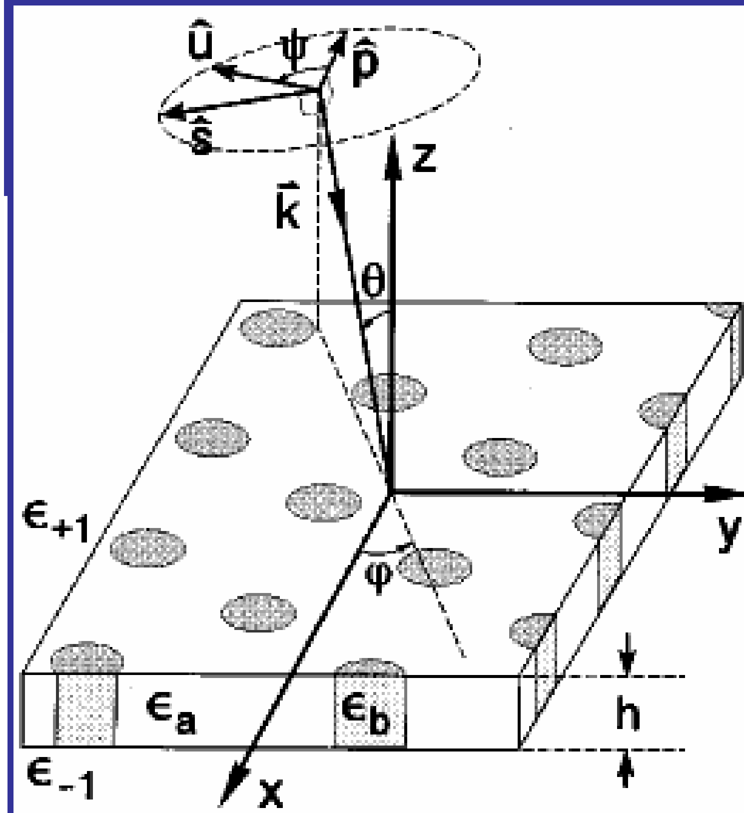


Fig.3-3 2D grating illuminated by a plane wave.

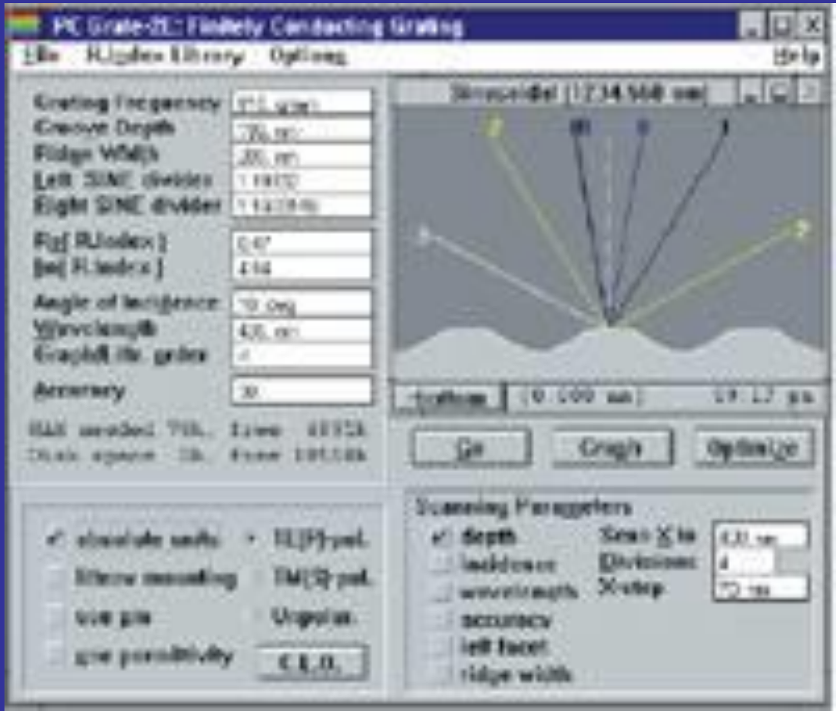
主要参考文献

- ✓ Lifeng Li, J. Opt. Soc. Am. A 14 (10), 2758-2767 (1997)

- ✓ M.G.M.M.v.Kraaij. A more Rigorous Coupled-Wave Analysis (MSolver). Master's thesis, Technische Universiteit Eindhoven, 2004.

- ✓ Software: The PCGrate-S(X) Series

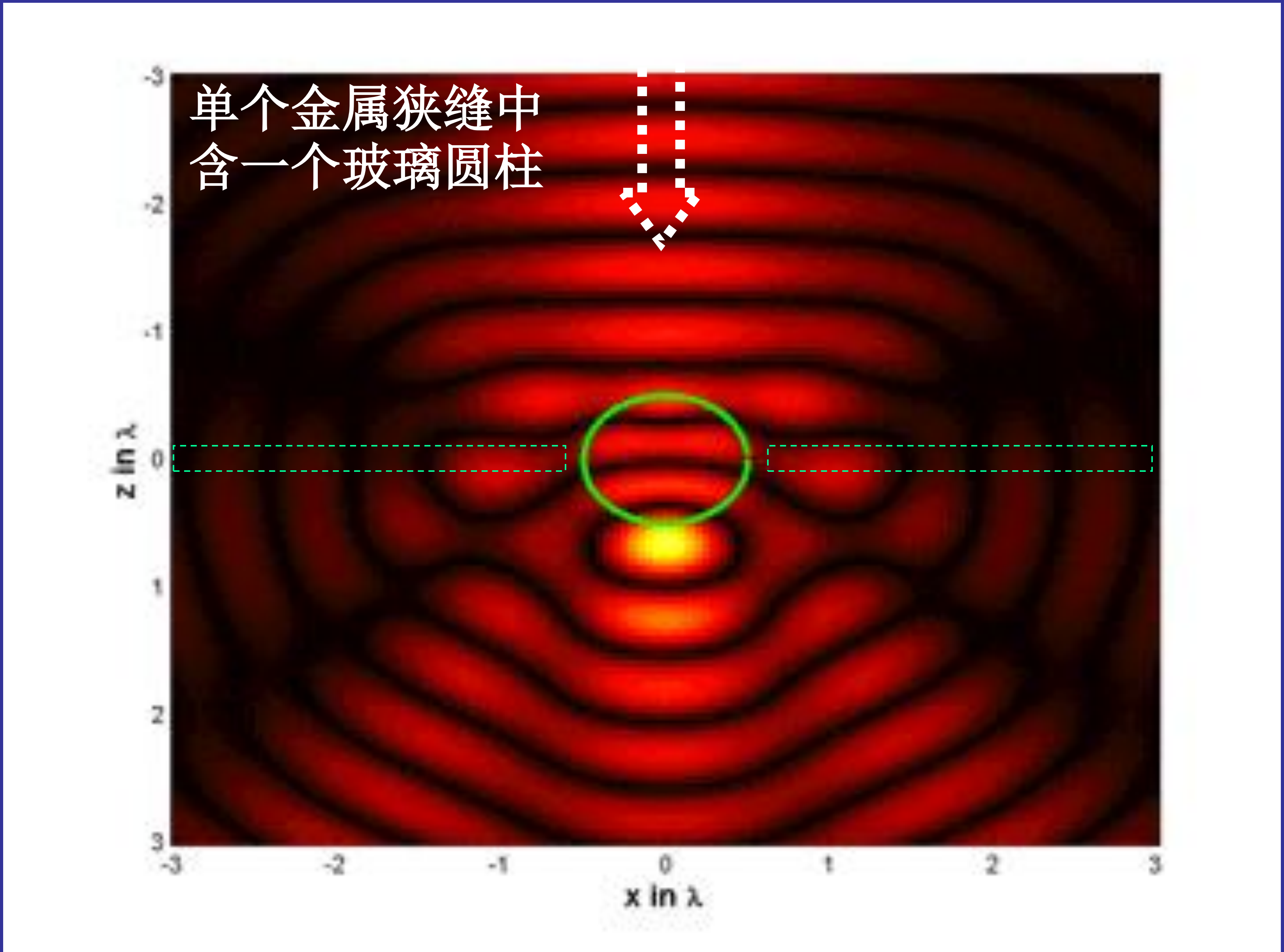
  http://www.pcgrate.com/loadpurc/download



计算实例

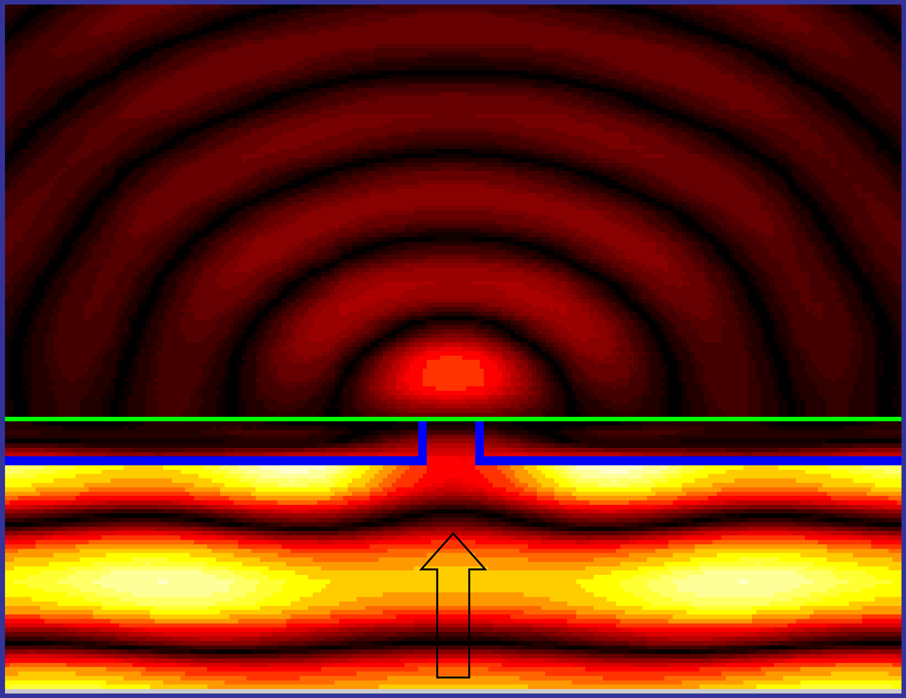
- ✓ 单个金属狭缝
- ✓双缝衍射时的线宽调制
- ✓带有周期耦合沟槽结构的金属狭缝
- ✓ 微型菲涅尔透镜
- ✓ 纳光子结构

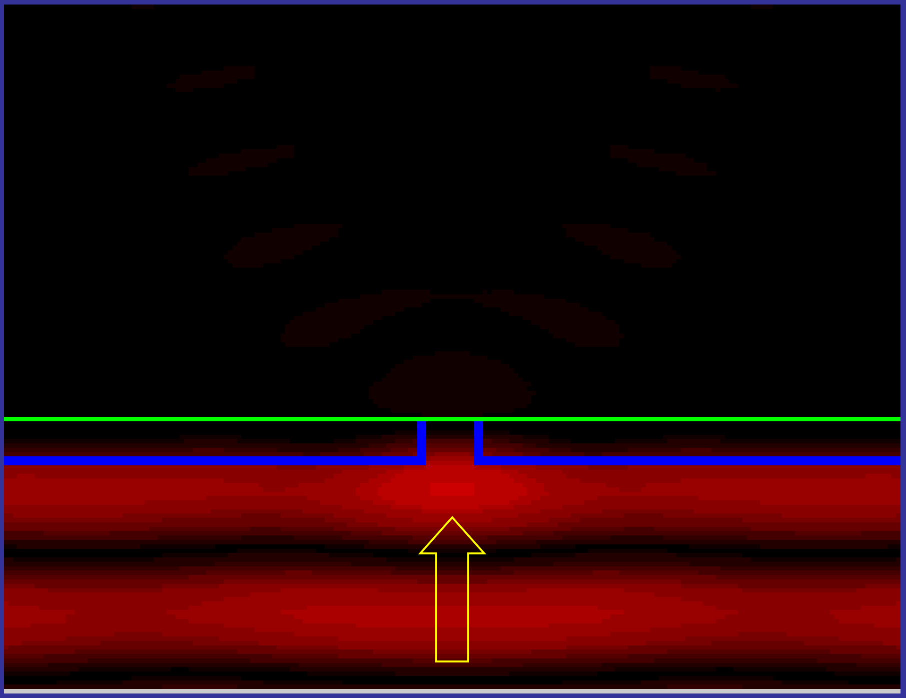
RCWA is also called Fourier Modal Method



Diffraction of a Gaussian beam by a single metal slit

Interaction of a **plan wave** with a slit-on-glass aperture. The plane wave is incident from the bottom and has a wavelength of 549 nm. The slit is 100 nm wide, the Cr layer is 100 nm thick. The left image is TM polarization and the right image TE polarization.





TM **TE**

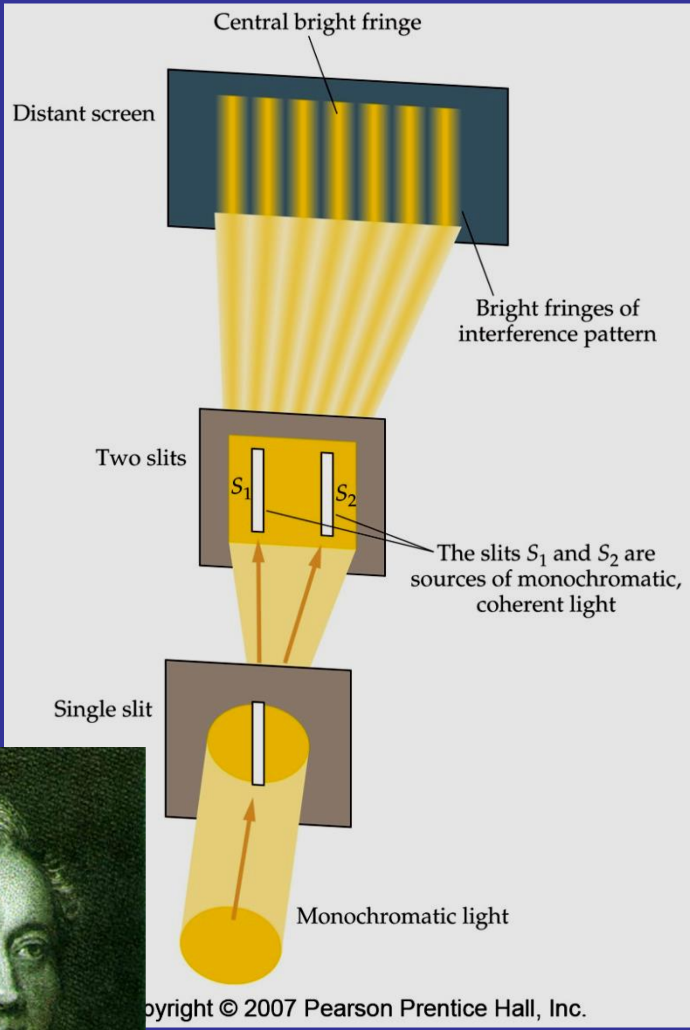
Figure 3: Passage of light through a slit using the FMM

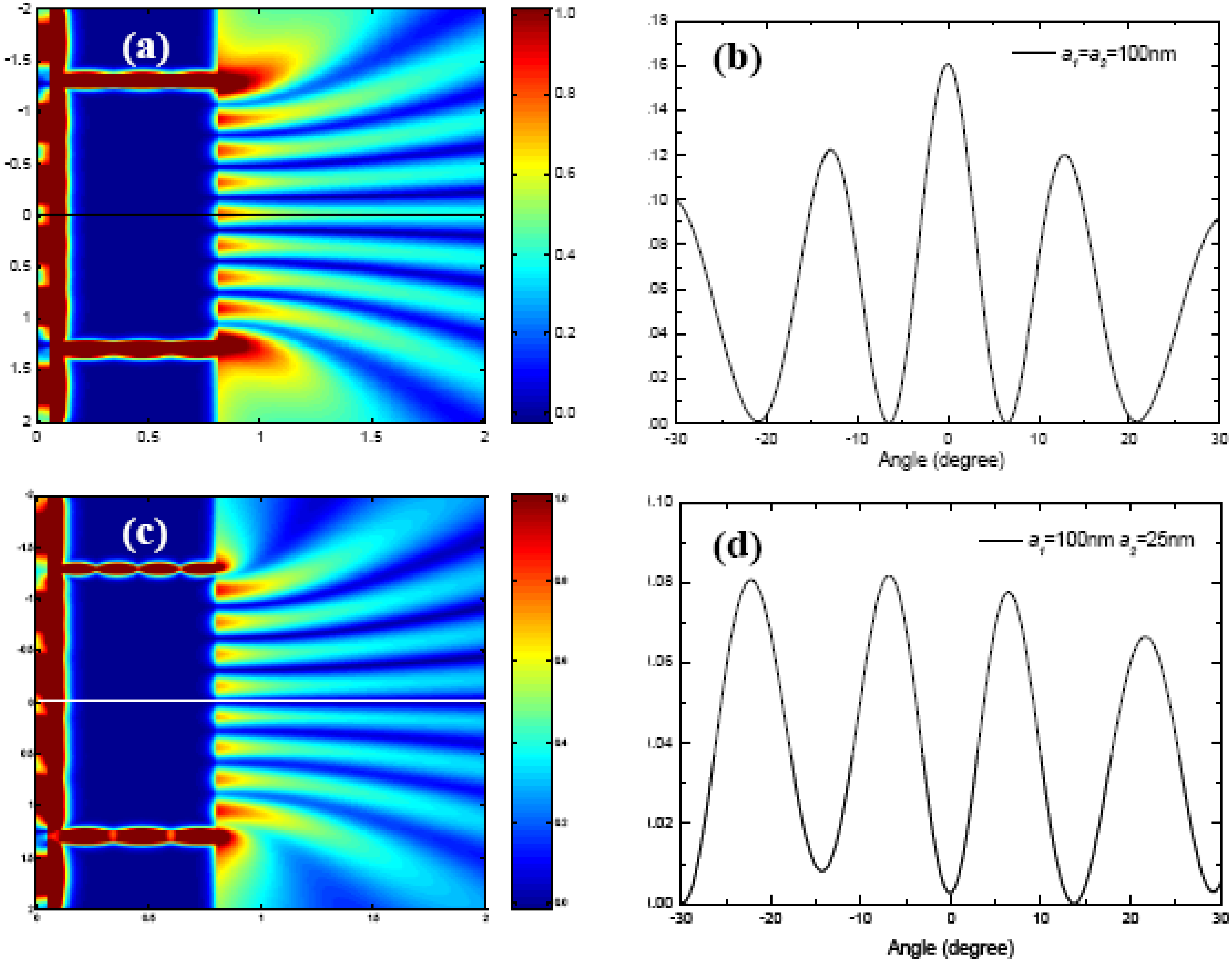
Young's double slit experiment

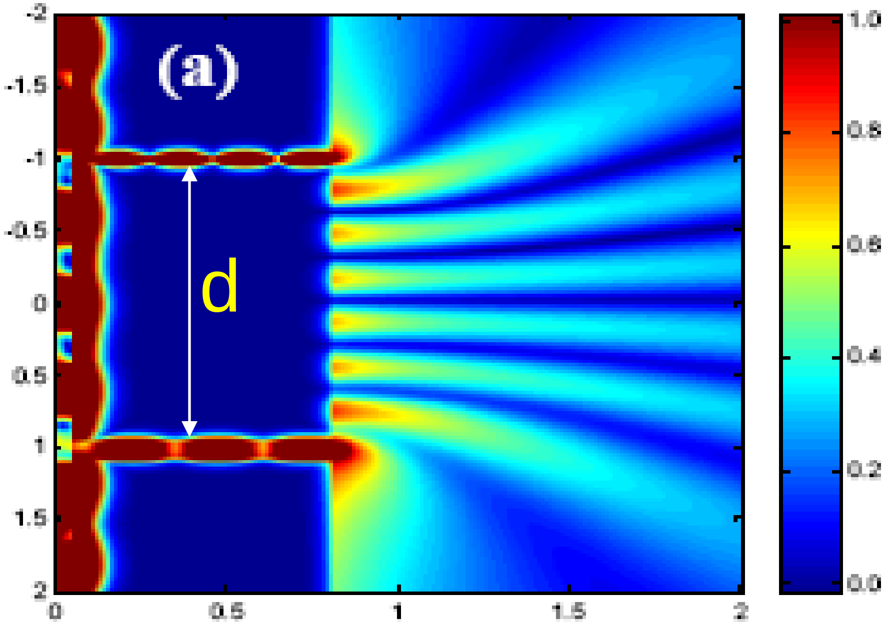
光通过双缝时的双缝干涉条件：

a)同一光源发出的光。
b)它们的频率必须相同。
c)两列波的光程差不能太大。
d)两列波的振幅不能悬殊太大。

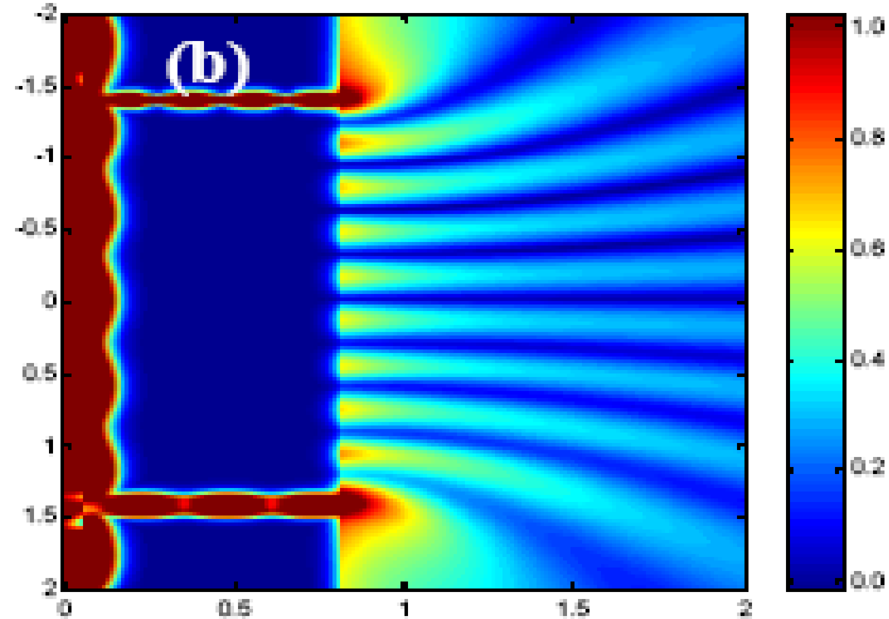
上述四个干涉条件，在物理光学中叫做相干条件(Condition of coherence)。



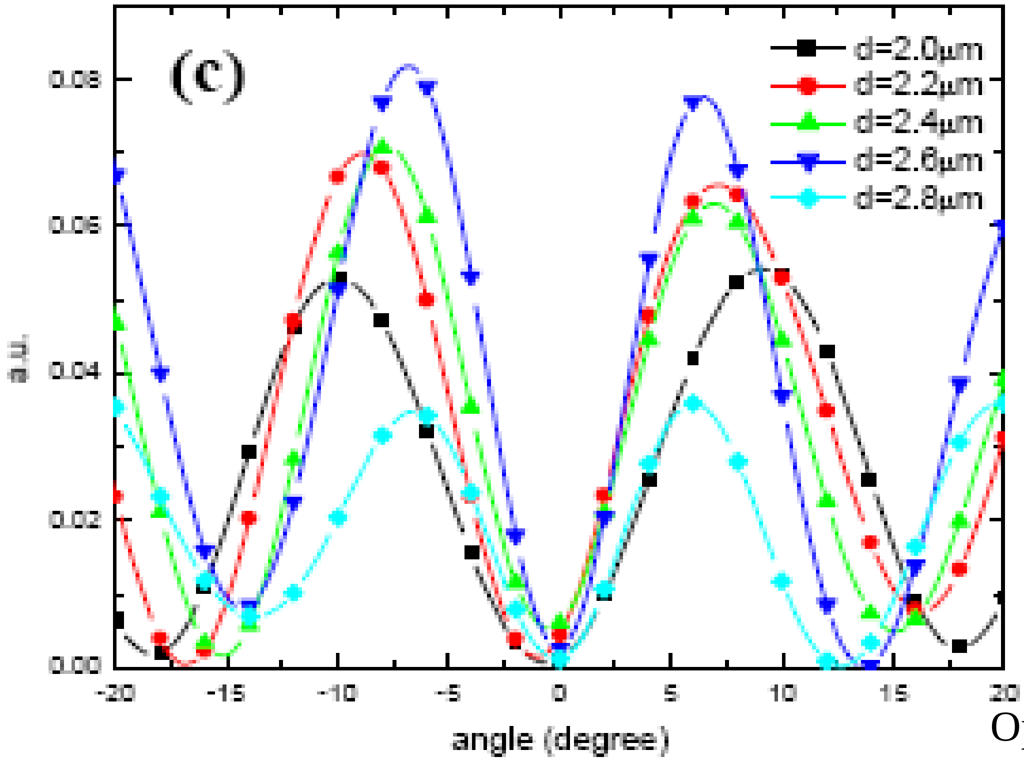

(a)
(b)
(c)
(d)
a1=a2=100nm
a1=100nm a2=25nm
Angle (degree)
Angle (degree)



d=2.0μm

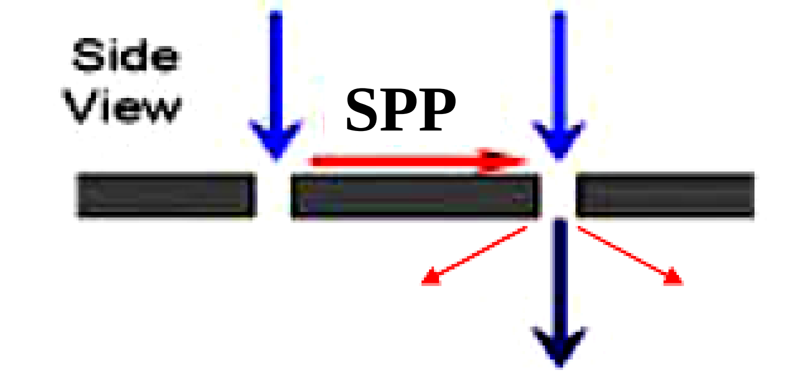


d=2.8μm



Opt. Express 15, 11321 (2007).

Diffraction of nano-sized structures



Lalanne et al. Nature Phy. (2006)
Gay et al. Nature Phy. (2006)

Constructive interference among the beams from slits;

Each slit is at F-P resonance

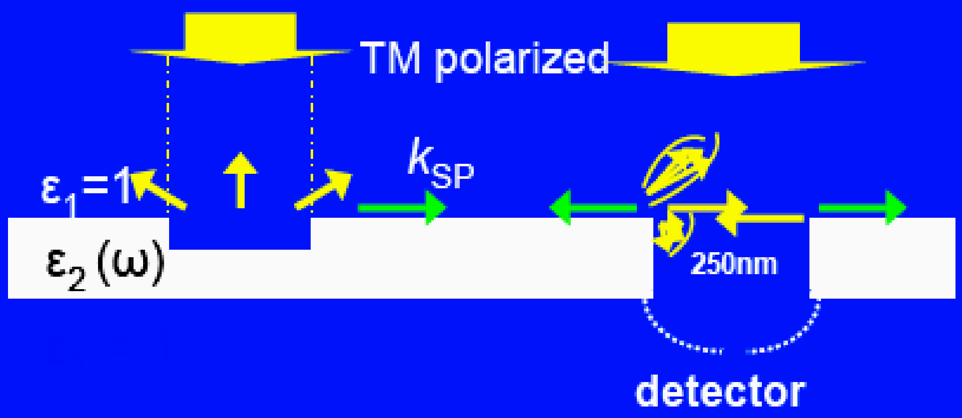
Interference of SW/SPP with incident wave

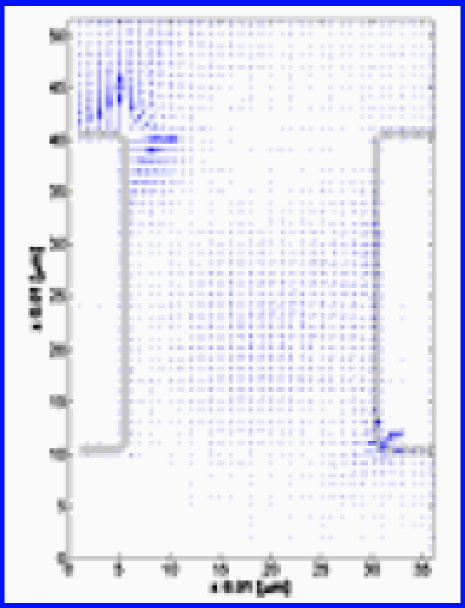
Remarks : Before arriving the slit, the two waves are of
Orthogonal polarizations
Orthogonal wave vectors ?

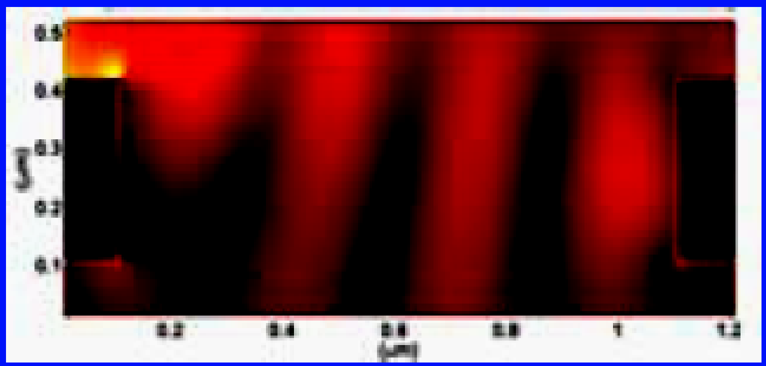
Their interference is done by mediation of SPP

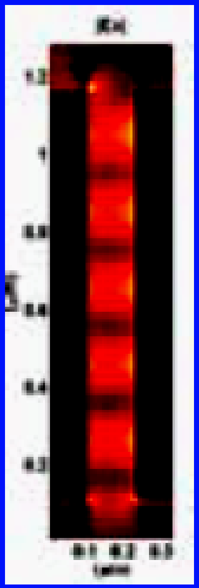
How Conversion SPP/Light, and Interference occur ?

SPP coupling & Interference at nano-slit







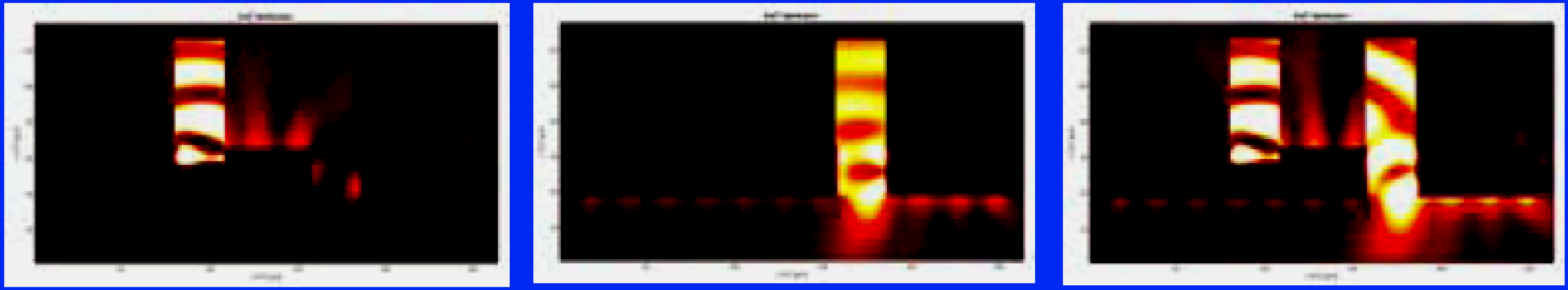


Coupling mechanism:
the incident SPP induces oblique dipole that reradiates Bulk waves and SPPs
Interference occurs at the slit.

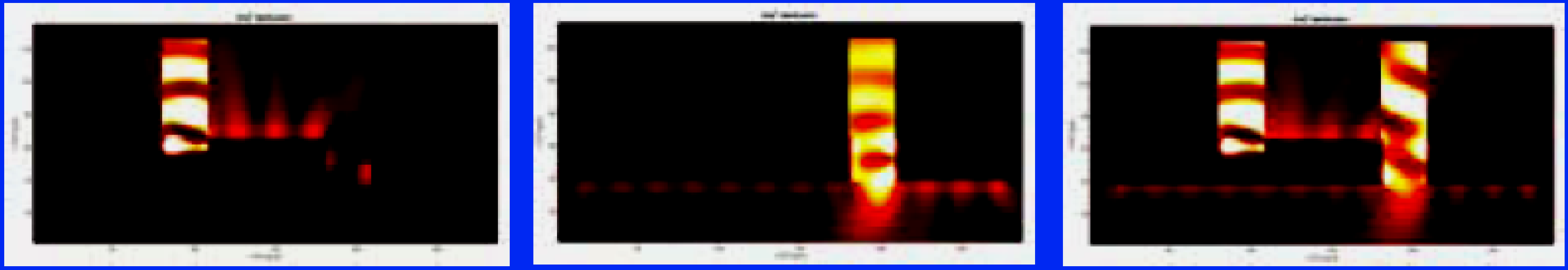
Ung, Sheng, Opt. express (2007)
Invited Paper OSA Nanophotonic (2007)

Demonstration of the Interference of SPP with incident beam (H$_z$ field)

Constructive interference: *L* = 520nm

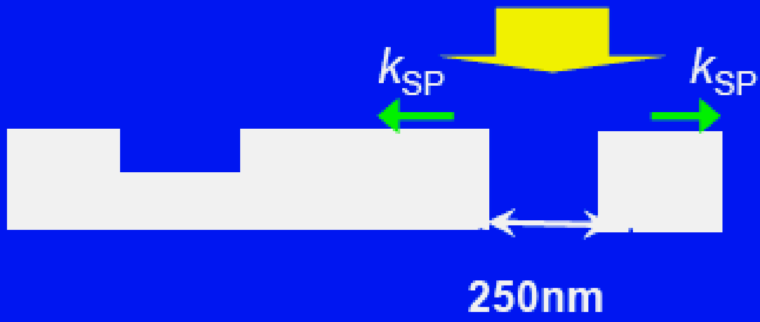


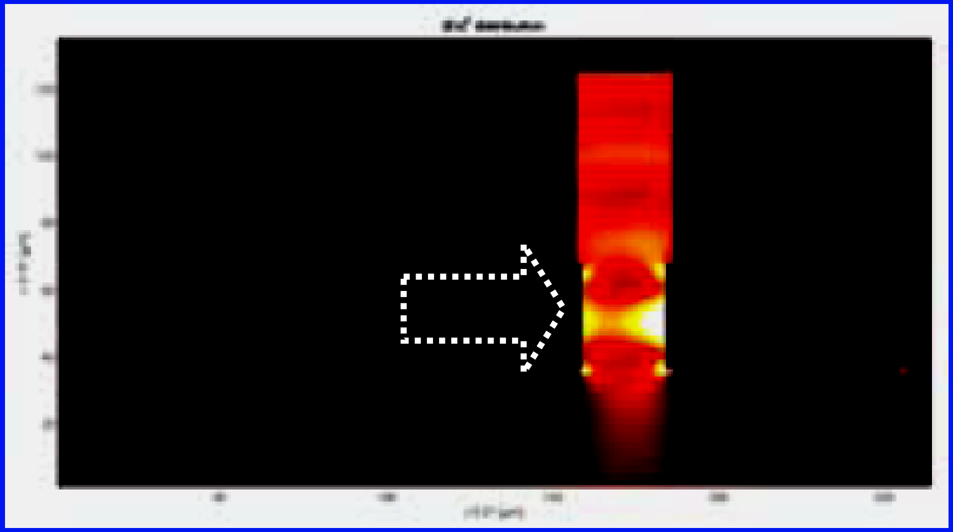
Destructive interference: *L* = 750nm

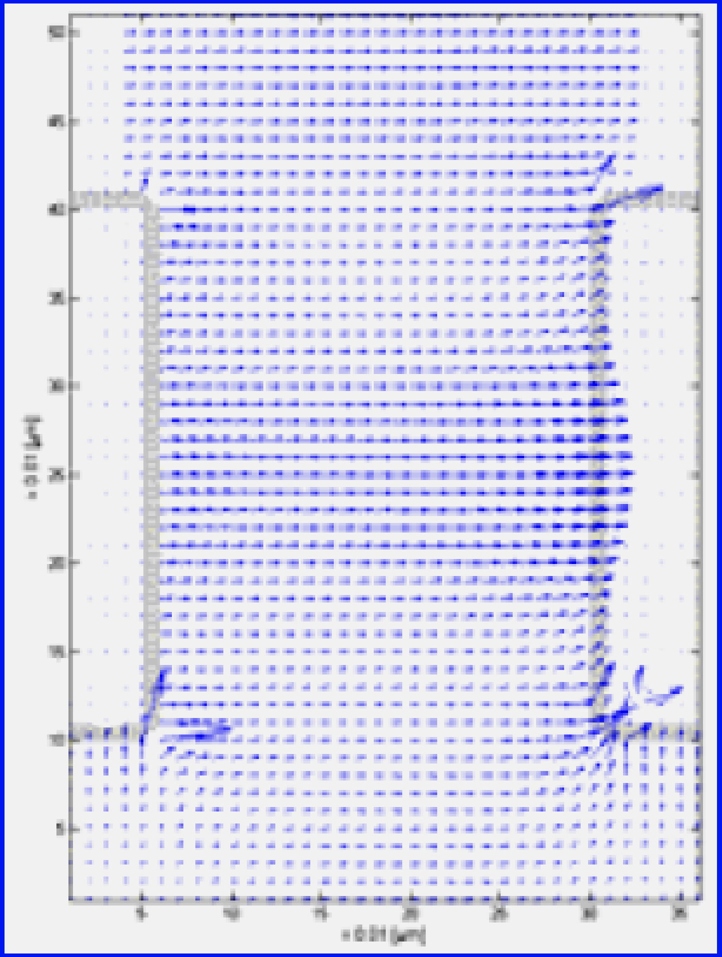


Slit width and thickness, *a* and *t*, are closed to optimal values

Induced dipoles in the slit

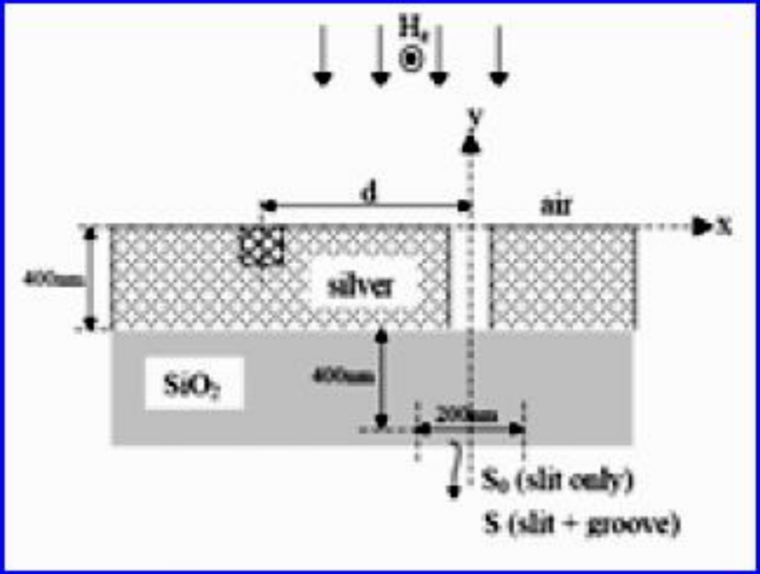


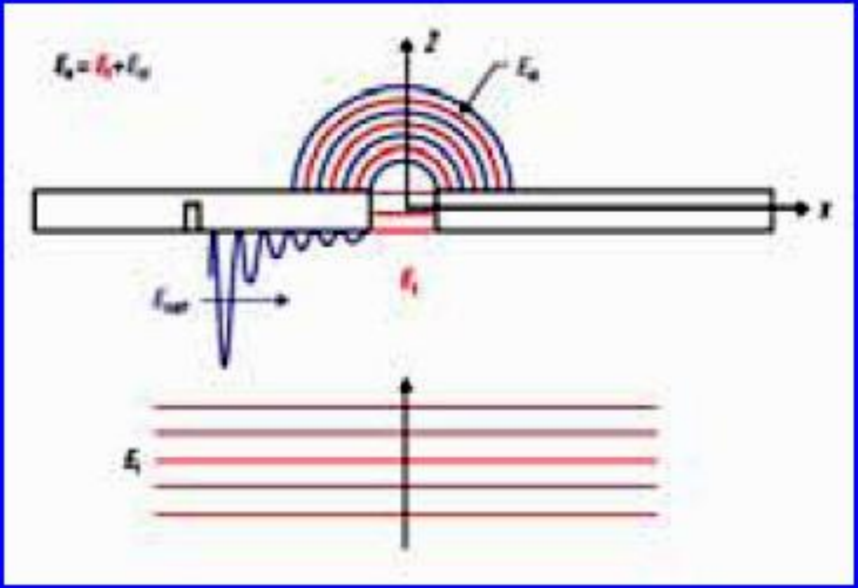


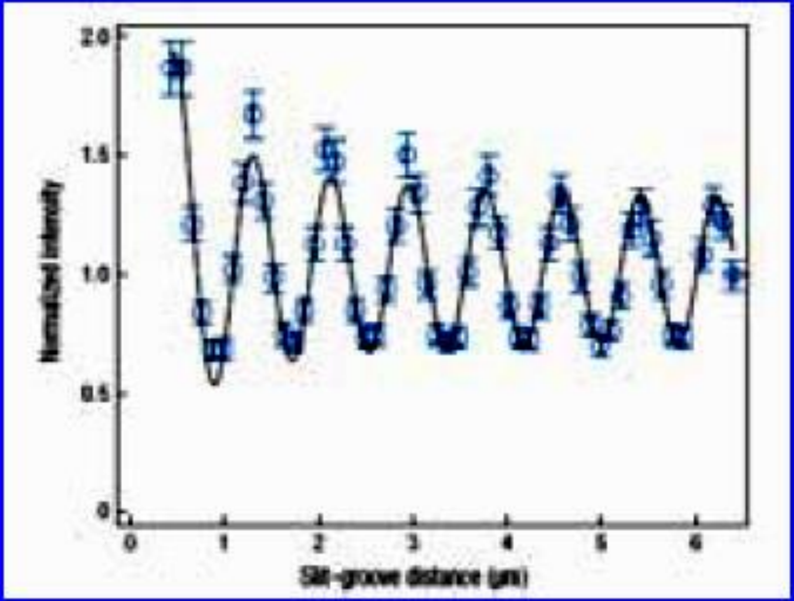


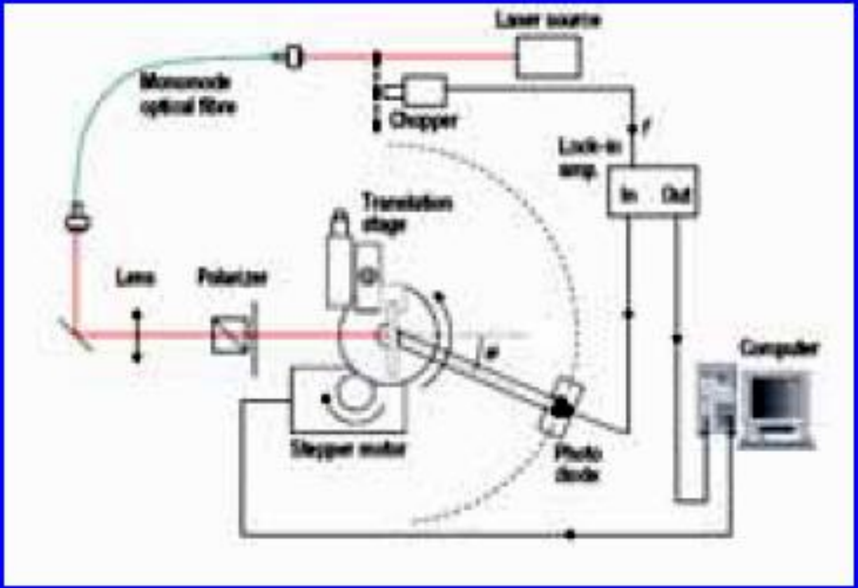
Two horizontal dipoles

Experiments of Gay Nature Physics 2006









RCWA的不足

- 理论演绎复杂，难以求解形状复杂的纳金属结构。
- 对金属材料的特殊色散问题考虑的不够。
- 当考虑的波长涵盖较多波长点时，频域的计算方法需要大量计算资源和时间。

Finite-Difference and Time-Domain (FDTD) Algorithm

FDTD 简单概念介绍

- **FDTD算法**：K.S.Yee于1966年提出的，它直接对麦克斯韦方程作差分处理，来解决电磁脉冲在电磁介质中传播和反射、透射等问题的一种算法.

- **基本思想**：基于有限元的思路，采用Yee元胞的方法计算域空间节点，同时电场和磁场节点空间与时间上都采用交错抽样；使得麦克斯韦旋度方程离散后构成显式差分方程。与前面的波动方程求解相比较，计算得到大大简化。

- **具体实现方法**：

  FDTD算法直接将有限差分式代替麦克斯韦时域场旋度方程中的微分式，得到关于场分量的有限差分式，用具有相同电参量的空间网格去模拟被研究体，选取合适的场初始值和计算空间的边界条件，得到包括时间变量的麦克斯韦方程的四维数值解，通过傅里叶变换可求得三维空间的频域解。

FDTD 简单概念介绍

FDTD基本原理

6个标量方程：

Maxwell方程组

矢量方程：

$$\begin{cases} \dfrac{\partial \vec{H}}{\partial t} = -\dfrac{1}{\mu}\left[\nabla \times \vec{E} + s\vec{H}\right] \\ \dfrac{\partial \vec{E}}{\partial t} = \dfrac{1}{\varepsilon}\left[\nabla \times \vec{H} - \sigma\vec{E}\right] \end{cases}$$

即

$$\begin{cases} \nabla \times \vec{H} = \dfrac{\partial \vec{D}}{\partial t} + \sigma\vec{E} \\ \nabla \times \vec{E} = -\dfrac{\partial \vec{B}}{\partial t} - s\vec{H} \end{cases}$$

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu}\left(\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - sH_x\right)$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu}\left(\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - sH_y\right)$$

$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu}\left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - sH_z\right)$$

$$\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon}\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \sigma E_x\right)$$

$$\frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon}\left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - \sigma E_y\right)$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z\right)$$

*Maxwell*旋度方程可以推出此六个耦合方程

FDTD 简单概念介绍

FDTD 基本方程

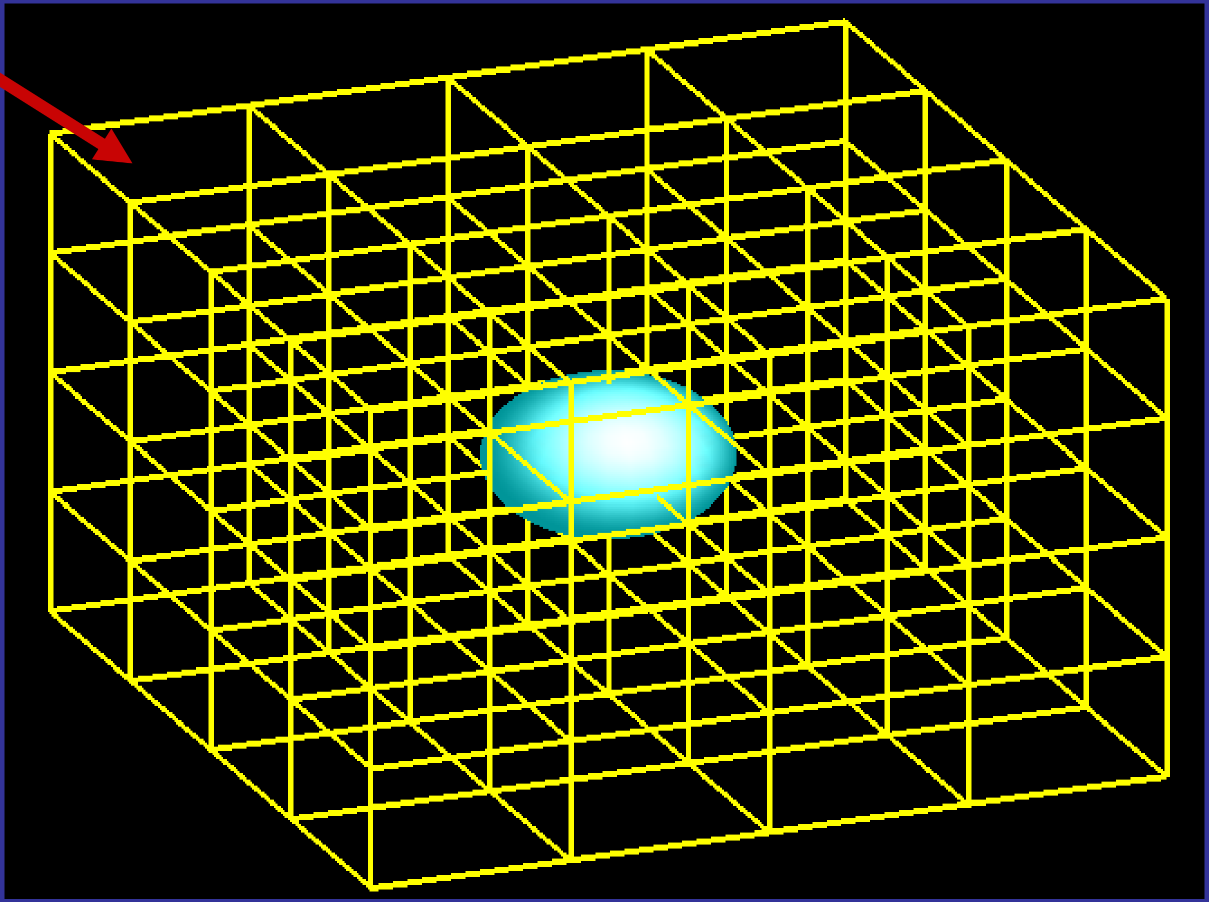
$$\frac{H_{z(t;x,y+\Delta y,z)}-H_{z(t;x,y-\Delta y,z)}}{2\Delta y}-\frac{H_{y(t;x,y,z+\Delta z)}-H_{y(t;x,y,z-\Delta z)}}{2\Delta z}=\tilde{\varepsilon}(x,y,z)\frac{E_{x(t+\Delta t;x,y,z)}-E_{x(t-\Delta t;x,y,z)}}{\Delta t}$$

$$\frac{H_{y(t;x+\Delta x,y,z)}-H_{y(t;x-\Delta x,y,z)}}{2\Delta x}-\frac{H_{x(t;x,y+\Delta y,z)}-H_{x(t;x,y-\Delta y,z)}}{2\Delta y}=\tilde{\varepsilon}(x,y,z)\frac{E_{z(t\,\_\Delta t;x,y,z)}-E_{z(t-\Delta t;x,y,z)}}{\Delta t}$$

$$\frac{H_{x(t;x,y,z+\Delta z)}-H_{x(t;x,y,z-\Delta z)}}{2\Delta z}-\frac{H_{z((t;x+\Delta x,y,z)}-H_{z(t;x-\Delta x,y,z)}}{2\Delta x}=\tilde{\varepsilon}(x,y,z)\frac{E_{y(t+\Delta t;x,y,z)}-E_{y(t-\Delta t;x,y,z)}}{\Delta t}$$

Maxwell Equations on a mesh

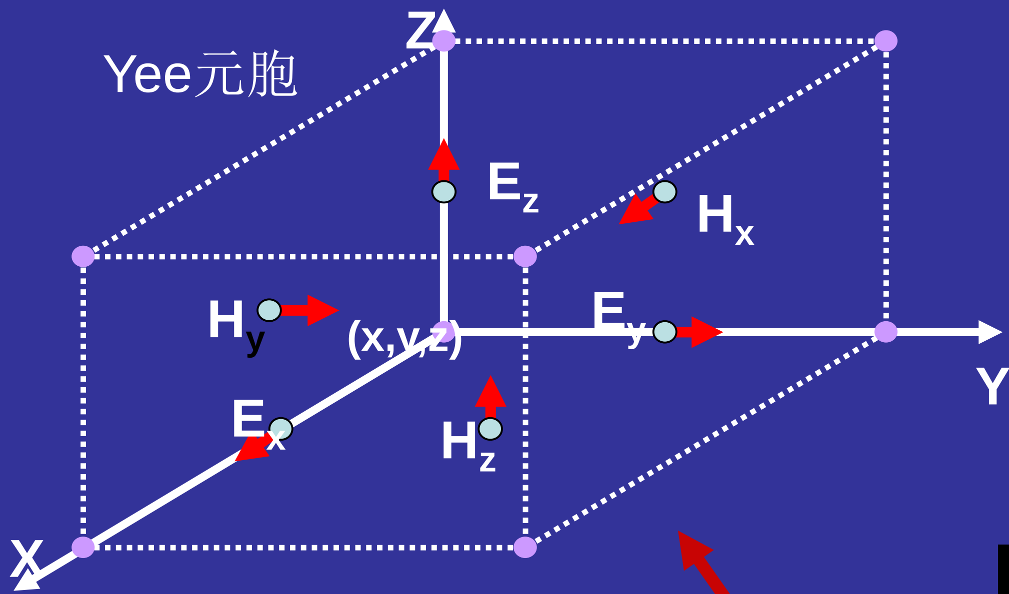
Yee cell



⇨ **E** and **H** are discrete in space

Originating from FEM

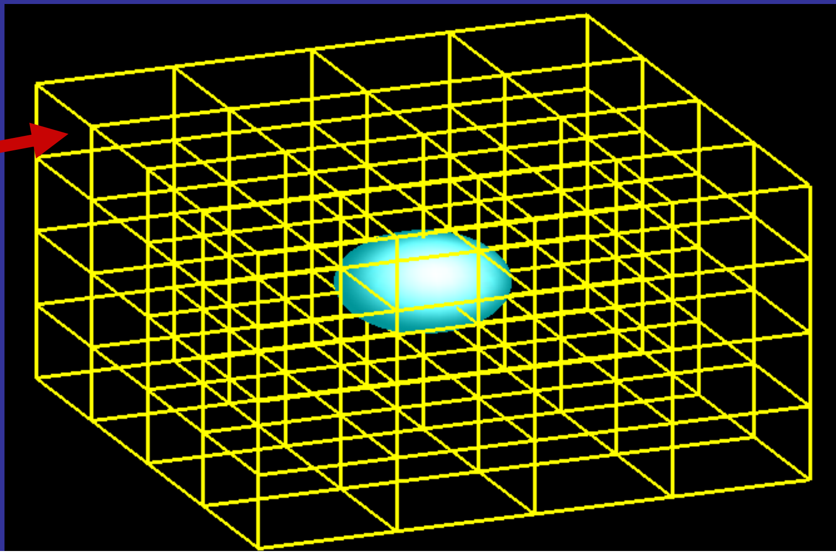
FDTD—Finite-Difference Time-Domain method



在空间上，E矢量和H矢量的各个分量（对称地）交错排列。常用的YEE 方法为二次方精度。也可以用高次近似法，但其精度对不同的网格（或波长）来说，并非高次方精度就越高！

⇨ E and H 在空间上离散

Yee cell



要把上述算法编程，并应用于各种器件的模拟设计，有许多的挑战和棘手的问题。

Kane Yee (1966). "Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media". *Antennas and Propagation, IEEE Transactions on* **14**: 302–307.

How the FDTD method works?

FDTD直接求解麦克斯韦方程: 全矢量法

$$\frac{\partial B}{\partial t} = -\nabla \times E \qquad \frac{\partial D}{\partial t} = \nabla \times H \qquad \nabla \bullet D = \rho \qquad \nabla \bullet B = 0 \qquad D = \varepsilon E \qquad B = \mu H$$

首先E和H在时域离散化

$$\vec{E}(t) \to \vec{E}^{n\Delta t} \qquad \vec{H}(t) \to \vec{H}^{(n+1/2)\Delta t}$$

FDTD 最基本的时间步进关系:

$$\vec{E}^{n+1} = \vec{E}^{n} + \alpha \vec{\nabla} \times \vec{H}^{n+1/2}$$

$$\vec{H}^{n+3/2} = \vec{H}^{n+1/2} + \beta \vec{\nabla} \times \vec{E}^{n+1}$$

蛙跳式—数据直接迭代,
不需要求解矩阵

$$\vec{E}^{0} \longrightarrow \vec{H}^{1/2} \longrightarrow \vec{E}^{1} \longrightarrow \vec{H}^{3/2} \longrightarrow \cdots$$

时间上是二次方精度: $\sim \Delta t^2$

How the FDTD algorithm works?

为确保算法在较长时间步长上运行的稳定性，时间增量**Δt**应满足下列关系式：

$$\Delta t = \frac{(\Delta x, \Delta y, \Delta z)min.}{c}$$

即：当沿三个轴向的网格单元是可变时，则应取每个轴向上的最小值，再选三者之中最小者。

FDTD Solution中有“Auto shutoff’功能来保证。

What are Dispersive Materials?

- Dispersive materials
  - ✓ have electrical parameters (permittivity and conductivity) which vary significantly as a function of frequency

- Examples include water, metals, body tissue, glass and more

- Many typical materials are **frequency-independent** and the dispersive models are not needed, *e.g.* air, dielectric, polymers.

When to use Dispersive Material Capabilities in FDTD?

- **Broad-band** output is desired from a geometry containing this type of material such as spectrum.

- In any simulation (broad-band or single frequency) in which the electrical parameters for the material would cause the calculation to become unstable (*e.g.* negative permittivity).

Why do we need dispersion models?

λ(μm)	εAg			
	Real	Imaginary	n	k
0.3	-0.86	0.13317	-0.92736	-0.06175
0.31	-1.1894	0.13895161	-1.0906	-0.07577
0.32	-1.5296	0.14486528	-1.23677	-0.08958
0.33	-1.8806	0.15091527	-1.37135	-0.10348
0.34	-2.2424	0.15710584	-1.49746	-0.11763
0.35	-2.615	0.16344125	-1.6171	-0.13215
0.36	-2.9984	0.16992576	-1.73159	-0.14712
0.37	-3.3926	0.17656363	-1.8419	-0.16261
0.38	-3.7976	0.18335912	-1.94874	-0.17866
0.39	-4.2134	0.19031649	-2.05266	-0.19533
0.4	-4.64	0.19744	-2.15407	-0.21265
0.41	-5.0774	0.20473391	-2.25331	-0.23066
0.42	-5.5256	0.21220248	-2.35066	-0.24941
0.43	-5.9846	0.21984997	-2.44634	-0.26891
0.44	-6.4544	0.22768064	-2.54055	-0.28922
0.45	-6.935	0.23569875	-2.63344	-0.31035
0.46	-7.4264	0.24390856	-2.72514	-0.33234
0.47	-7.9286	0.25231433	-2.81578	-0.35523
0.48	-8.4416	0.26092032	-2.90544	-0.37904
0.49	-8.9654	0.26973079	-2.99423	-0.40382
0.5	-9.5	0.27875	-3.08221	-0.42958
0.51	-10.0454	0.28798221	-3.16945	-0.45637
0.52	-10.6016	0.29743168	-3.25601	-0.48422
0.527	-10.997366	0.30417786	-3.31623	-0.50436
0.53	-11.1686	0.30710267	-3.34195	-0.51316
0.54	-11.7464	0.31699944	-3.4273	-0.54323
0.55	-12.335	0.32712625	-3.51212	-0.57445

Broad band calculation

$\varepsilon'(f), \varepsilon''(f)$

$\varepsilon'(\lambda), \varepsilon''(\lambda)$

Types of Dispersive Models in FDTD

- **Debye**
  - useful for materials with condensed polar molecules such as water
- **Drude**
  - similar to the Debye model
  - with an added electrical conductivity term
  - Also available for magnetic materials
- **Lorentz**
  - used to describe absorption bands
  - often in the optical frequency range

Types of Dispersive Models in FDTD (cont.)

- **Conductive**

The Conductive model is used to create a material defined by the following formula.

$$\varepsilon_{total}(f) = \varepsilon + i\frac{\sigma}{2\pi \cdot f \varepsilon_o}$$

- **Plasma**

The Plasma model is used to create a material defined by the following formula.

$$\varepsilon_{total}(f) = \varepsilon - \frac{\omega_P^2}{2\pi \cdot f\left(i\,\nu_C + 2\pi \cdot f\right)}$$

Types of Dispersive Models in FDTD (cont.)

➢ Sellmeier

The Sellmeier model is used to create a material defined by the following formula. The ***C*** coefficients have dimensions of micrometers squared (μm²).

$$\varepsilon_{total}(\lambda) = A_1 + \frac{B_1\lambda^2}{\lambda^2 - C_1} + \frac{B_2\lambda^2}{\lambda^2 - C_2} + \frac{B_3\lambda^2}{\lambda^2 - C_3}$$

➢ Kerr nonlinear

In the Kerr nonlinear model, the electric polarization field ***P*** will depend on the electric field ***E*** in the following manner.

$$\vec{P}(t) = \varepsilon_0\left(\chi^{(1)} + \chi^{(3)} \,|\, \vec{E}(t) \,|^2\right)\vec{E}(t)$$

Solving for the displacement field ***D*** gives

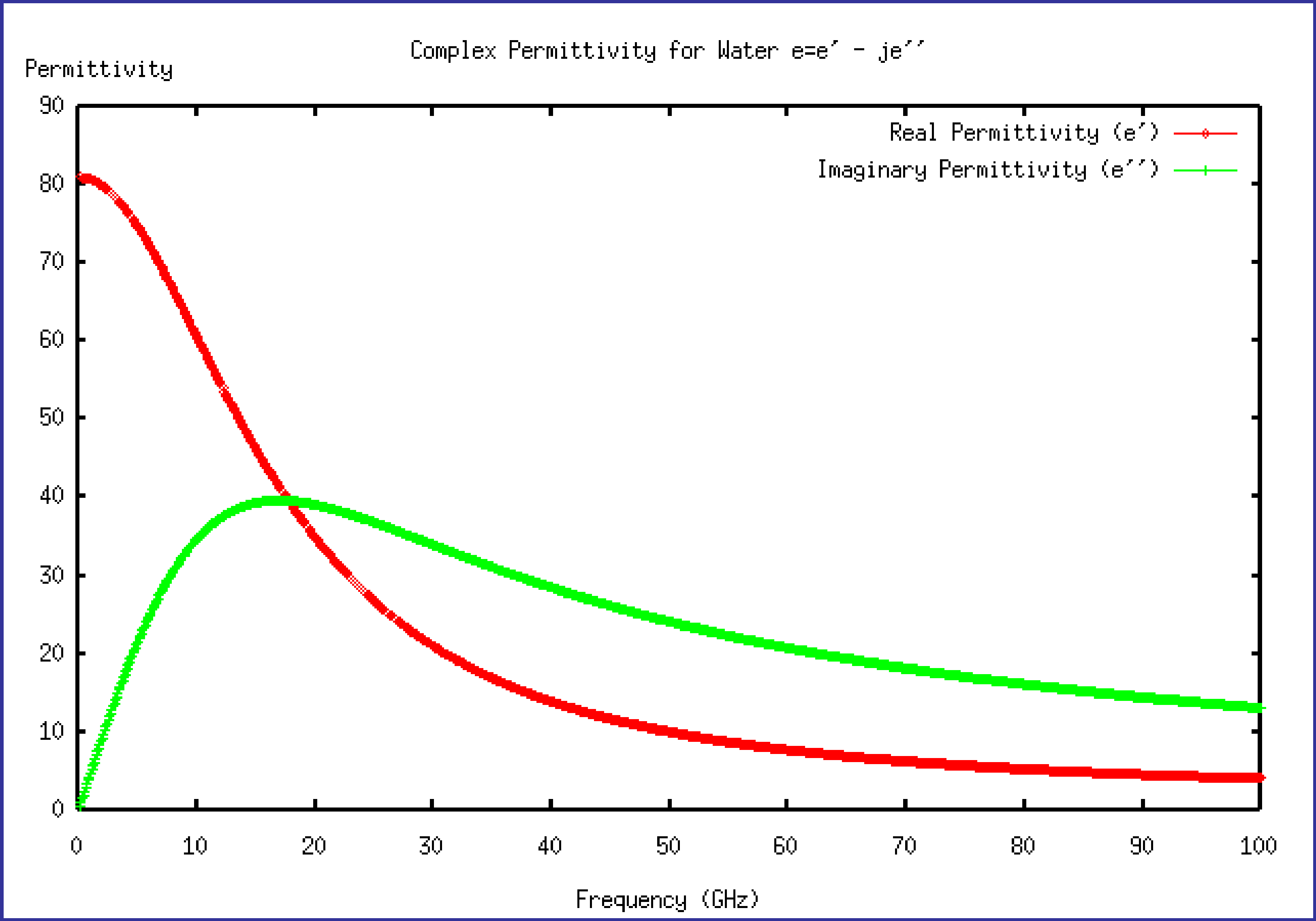
$$\vec{D}(t) = \varepsilon_0\left(\varepsilon_r + \chi^{(3)} \,|\, \vec{E}(t) \,|^2\right)\vec{E}(t)$$

The Debye Model

- The Debye permittivity is described by the equation

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + j\omega\tau_0}$$

Complex Permittivity for Water



Limits on Debye Parameters

为产生比较现实的材料并确保稳定计算，需要对参数进行如下限制：

- 介电常数的虚部不能为负
- $\varepsilon_{\infty} \geq 1$
- $\varepsilon_{static} > \varepsilon_{\infty}$

Drude Model

一般形式：

$$\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\gamma\omega}$$

其中电子的碰撞频率$\gamma=1/\tau$

τ为电子的弛豫时间。

（自由电子由振动状态恢复平衡态的时间 ）

Drude Model

Typical Plasma Frequencies

The plasma frequency for typical metals lies in the ultra-violet.

ω_p

Metal	Symbol	Plasma Wavelength	Plasma Frequency
Aluminum	Al	82.78 nm	3624 THz
Chromium	Cr	115.35 nm	2601 THz
Copper	Cu	114.50 nm	2620 THz
Gold	Au	137.32 nm	2185 THz
Nickel	Ni	77.89 nm	3852 THz
Silver	Ag	137.62 nm	2180 THz

Drude Model
$\varepsilon=\varepsilon_1+i\varepsilon_2$

The real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ parts of the dielectric function are given by:

$$\boxed{\varepsilon_1(\omega)=1(\varepsilon(\infty))-\frac{\omega_p^2}{\omega^2+\Gamma^2}}$$

and

$$\boxed{\varepsilon_2(\omega)=\frac{\omega_p^2\cdot\Gamma}{\omega\cdot\left(\omega^2+\Gamma^2\right)}}$$

Γ: 阻尼系数

公式的来历

两点假设：

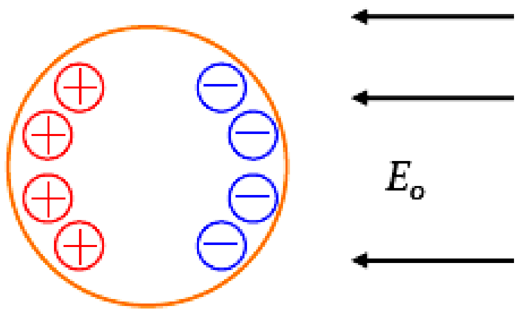
1. 一是自由电子近似（忽略金属中电子与离子之间的相互作用）和独立电子近似（忽略金属中电子与电子之间的相互作用）；

2. 二是假设电子之间的碰撞是瞬时间完成的，碰撞导致的电子动量变化也是瞬时完成的。忽略金属中电子与电子之间的相互作用。

那么在外加电磁场的作用下(例如入射光子)，金属中的自由电子将发生运动，方向与外加电场方向相反。因此，可以写出金属中自由电子在外电场作用下的**运动方程**：

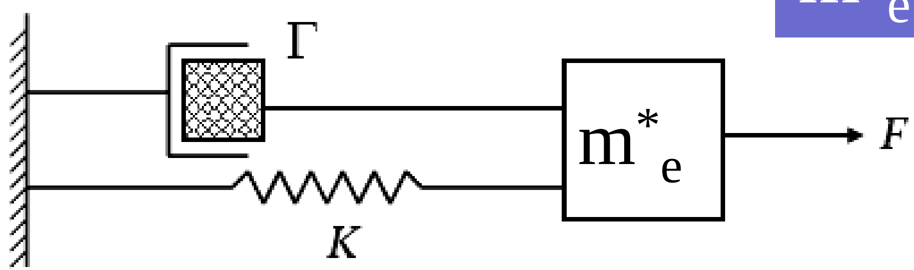
Semi Classic Model for Localized Surface Plasmon

Metal nanoparticle



振子模型

Driven, damped harmonic oscillator



Damping factor Γ:

$\Gamma \sim \gamma$， $\omega_{visible} >> \gamma = 1/\tau$;

$K \sim C = 0$ (电子未绑定某一特定的原子核)

$F \sim F_{Coulomb}$（作用在电子上的回复力，$-q\mathbf{E}$）

m^*_e: mass of electrons

$$\omega_R = K / m_e^*$$

$$FWHM = \sqrt{3}\Gamma$$

$$m_e^* \frac{\partial^2 r}{\partial t^2} + m_e^* \Gamma \frac{\partial r}{\partial t} + Kr = qE_0 e^{-i\omega t}$$

$$r_{\max} = \frac{qE_0}{m_e^* \omega_R \Gamma}$$

Drude德鲁德模型四条基本假设

1独立电子近似

自由电子之间不存在相互作用，也不存在碰撞，可以彼此独立的运动。(实际上研究证明，忽略电子间相互作用对实验结果影响不大)

2自由电子近似

晶体中的离子是固定不动的，电子可以自由运动，电子和离子之间没有静电力的相互作用。（实际上大多数情况下，电子与离子相互作用是不能忽略的。）

上述两条假设参照了理想气体的概念：理想气体中分子之间不发生碰撞，也没有相互作用。所以又把两条假设统称为自由电子气假设

3碰撞假设

电子和离子之间存在碰撞，电子和离子的碰撞是瞬时完成的，且碰撞后电子的运动速度只与温度有关，与碰撞前速度无关，电子通过这种碰撞和周围的环境达到一个热平衡。

4弛豫时间

这是Drude模型最中最重要的概念。电子完成碰撞后，距离下一次碰撞所经历时间的平均值，即两次碰撞之间的平均时间间隔称作弛豫时间。弛豫时间仅和晶体结构，即离子之间的距离有关。

$$m\frac{d^2\vec{x}}{d^2t}+m\gamma\frac{d\vec{x}}{dt}=-e\vec{E} \tag{2.1}$$

其中，$\vec{x}$，e 和 m 分别为电子的位移量、电量和质量。将公式(2.1)的特征解 $\vec{x}(t)=\vec{x}_0e^{-i\omega t}$ 代入可得：

$$x(t)=\frac{e}{m(\omega^2+i\gamma\omega)}\vec{E}(t) \tag{2.2}$$

这里引入自由电子密度 n，那么自由电子运动的电偶极矩可以表示为：

$$\vec{P}=-ne\vec{x}=-\frac{ne^2}{m(\omega^2+i\gamma\omega)}\vec{E} \tag{2.3}$$

由 $\vec{D}=\varepsilon_0\vec{E}+\vec{P}$ 可得：

$$\vec{D}=\varepsilon_0(1-\frac{\omega_p^2}{\omega^2+i\gamma\omega})\vec{E}=\varepsilon(\omega)\mathbf{E} \tag{2.4}$$

其中 ω_p 为等离子体频率。因此，可以写出金属介电常数表达式：

$$\varepsilon(\omega)=1-\frac{\omega_p^2}{\omega^2+i\gamma\omega} \tag{2.5}$$

$$\varepsilon(\omega) = \varepsilon_R + i\varepsilon_I = n^2$$

$$= (n_R + in_I)^2 = 1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma} \quad \frac{(\omega^2 - i\omega\gamma)}{(\omega^2 - i\omega\gamma)}$$

$$= \left(1 - \frac{\omega_p^2}{\omega^2 + \gamma^2}\right) + i\left(\frac{\omega_p^2\gamma}{\omega^3 + \omega\gamma^2}\right)$$

Dielectric constant at $\omega \approx \omega_{visible}$

$$\omega >> \gamma = \frac{1}{\tau} \Rightarrow \boxed{\varepsilon(\omega) = \left(1 - \frac{\omega_p^2}{\omega^2}\right) + i\left(\frac{\omega_p^2}{\omega^3 / \gamma}\right)}$$

上述公式即为Drude模型的一般表达式，常用于仿真计算中描述金属的材料特性。由于在推导的过程中进行了近似假设导致上述公式在高频波段并不能准确的表征金属的材料特性。因此，外加高频电磁场时，引入频率无穷大时的相对介电常数ε_{∞}、ε_{S}对Drude模型进行修正。

Modified Drude model for metal

$$\varepsilon_r(\omega)=\varepsilon_\infty-\frac{\omega_p^2}{\omega^2+i\omega\gamma}=\left(\varepsilon_\infty-\frac{\omega_p^2}{\omega^2+\gamma^2}\right)+i\left(\frac{\omega_p^2\gamma}{\omega^3+\omega\gamma^2}\right)$$

修正之后的Drude模型在紫外、可见光和红外波段的仿真研究中均可以表示金属材料的介电常数，得到准确的仿真结果。

General Drude Model

- The Drude model describes a material similar to the Debye model
  - with the addition of an electrical conductivity term σ
  - where σ is the conductivity.

General Drude Model Limits

Simplified limits for Drude model:

- identical to those of Debye ($\varepsilon_\infty \geq 1$, $\varepsilon_s > \varepsilon_\infty$)
- with added condition that electrical conductivity **(σ) < 0**

- **Limited set of materials fit this condition**

- More general conditions available

General Drude Model Limits

- Infinite Frequency Permittivity (ε_∞) $\geq$ 1
- If $\varepsilon_s > \varepsilon_\infty$ then $\sigma \geq 0$
- If $\varepsilon_s < \varepsilon_\infty$, then the conductivity σ must satisfy the condition of σ<0.

Applications of Drude Materials

- Isotropic Plasmas
- Metals such as gold, aluminum, and chromium at optical frequencies
- Some biological tissues
- Negative Index Materials (NIM), Double Negative (DNG) materials

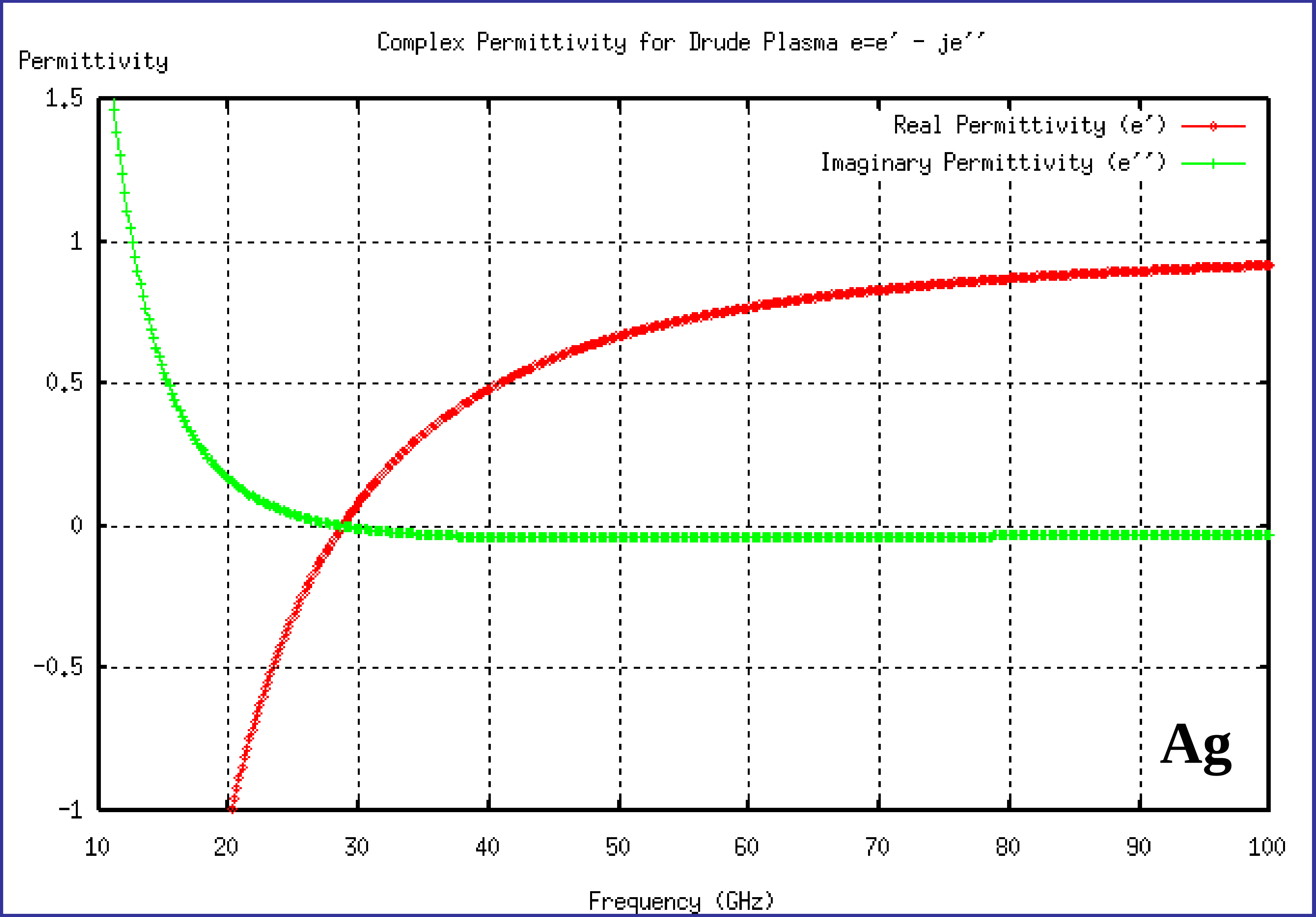
Techniques for Using Drude model

- Some materials, such as plasmas, fit the Drude model exactly at microwave region

- For the general case
  - a curve-fitting technique should be used to find the best-fit parameters for the Drude model

- Curve-fitting used for following metal examples

Complex Permittivity for Drude



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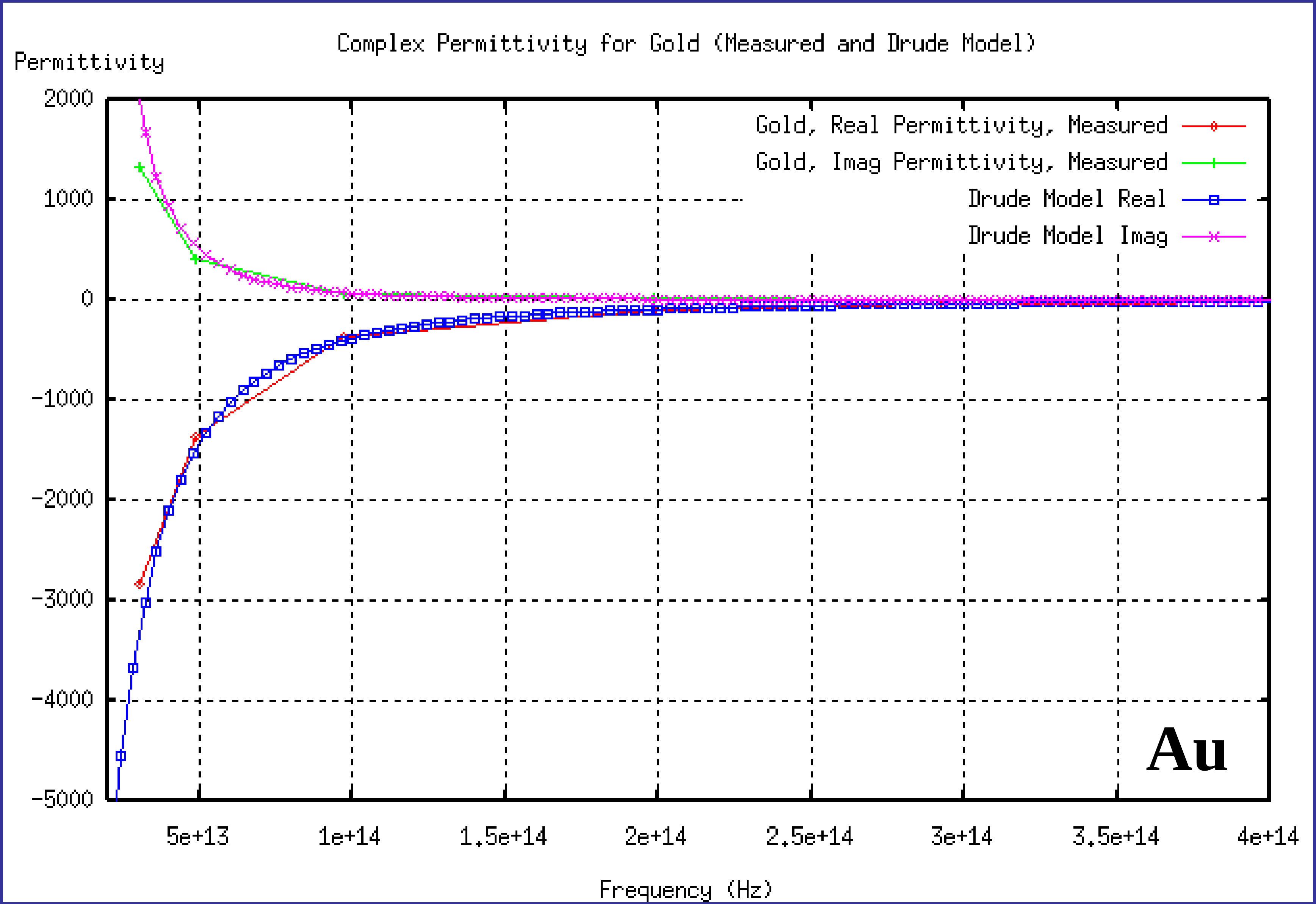
Complex Permittivity For Gold



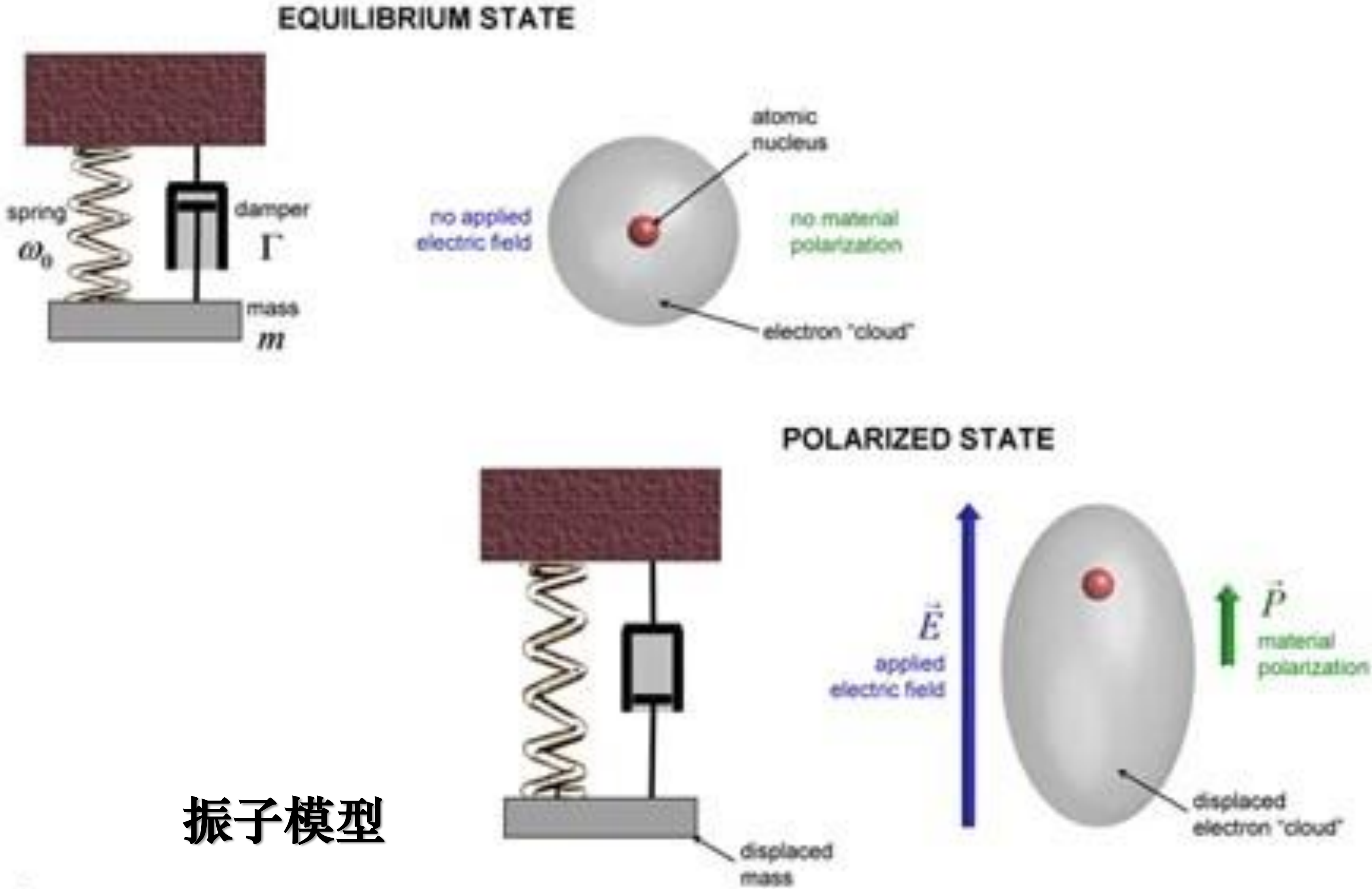
Lorentz model

数学模型表达式

$$\epsilon_r(\omega) = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma}$$

Derivation of Lorentz Oscillator Model

Lorentz Oscillator Model

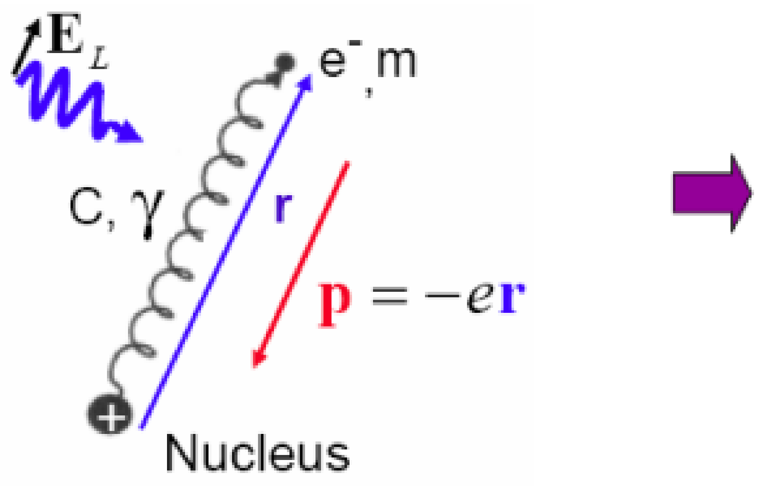


振子模型

Lorentz Model的来历推导

Linear Dielectric Response of Matter

Lorentz model (harmonic oscillator model)



Charges in a material are treated as harmonic oscillators

$$m\mathbf{a}_{el} = \mathbf{F}_{E,Local} + \mathbf{F}_{Damping} + \mathbf{F}_{Spring} \qquad \text{(one oscillator)}$$

$$m\frac{d^2\mathbf{r}}{dt^2} + m\gamma\frac{d\mathbf{r}}{dt} + C\mathbf{r} = -e\mathbf{E}_L\exp(-i\omega t)$$

Equation of Motion

$$m\frac{\partial^2 \vec{r}}{\partial t^2} + m\Gamma \frac{\partial \vec{r}}{\partial t} + m\omega_0^2 \vec{r} = -q\vec{E}$$

acceleration force

$m \Rightarrow m_e$ mass of an electron

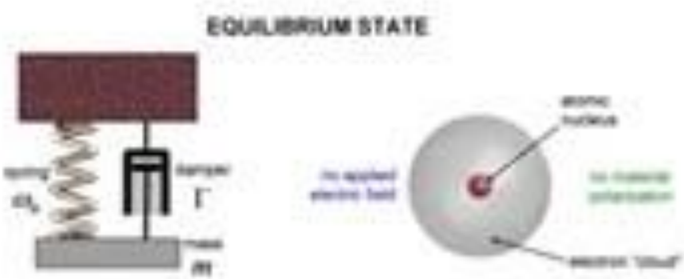
frictional force

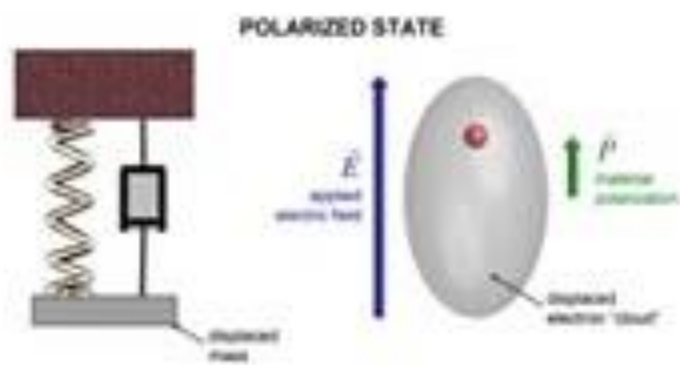
Γ damping rate (loss/sec)

restoring force

$\omega_0 = \sqrt{\frac{K}{m}}$ natural frequency

electric force





Drude模型与Lorentz模型建模时的区别

The equation of motion of a free electron (not bound to a particular nucleus; $C = 0$),

$$m_e \frac{d^2\vec{r}}{dt^2} = -C\vec{r} - \frac{m_e}{\tau}\frac{d\vec{r}}{dt} - e\vec{E} \;\Rightarrow\; m_e \frac{d^2\vec{v}}{dt^2} + m_e\gamma\vec{v} = -e\vec{E}$$

$$\left(\tau = \frac{1}{\gamma}:\ \text{relaxation time} \approx 10^{-14}\, s\right)$$

Lorentz model
(Harmonic oscillator model)

If C = 0, it is called Drude model

Fourier Transform

$$m\frac{\partial^2\vec{r}}{\partial t^2}+m\Gamma\frac{\partial\vec{r}}{\partial t}+m\omega_0^2\vec{r}=-q\vec{E}$$

$$\Big\downarrow \text{Fourier transform}$$

$$m(-j\omega)^2\,\vec{r}(\omega)+m\Gamma(-j\omega)\vec{r}(\omega)+m\omega_0^2\vec{r}(\omega)=-q\vec{E}(\omega)$$

$$\Big\downarrow \text{Simplify}$$

$$\left(-m\omega^2-j\omega m\Gamma+m\omega_0^2\right)\vec{r}(\omega)=-q\vec{E}(\omega)$$

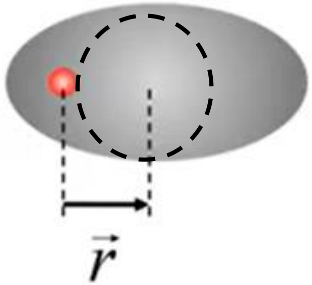
Displacement

Charge Displacement $\vec{r}(\omega)$

$$\left(-m\omega^2 - j\omega m\Gamma + m\omega_0^2\right)\vec{r}(\omega) = -q\vec{E}(\omega)$$

$$\Big\downarrow \text{Solve for } \vec{r}(\omega)$$

$$\vec{r}(\omega) = -\frac{q}{m_e}\frac{\vec{E}(\omega)}{\omega_0^2 - \omega^2 - j\omega\Gamma}$$



The displacement $\vec{r}(\omega)$ describes how far charge is displaced from its equilibrium position.

Dipole Moment

Electric Dipole Moment $\vec{\mu}(\omega)$

Definition of Electric Dipole Moment: $\vec{\mu}(\omega) = -q\vec{r}(\omega)$

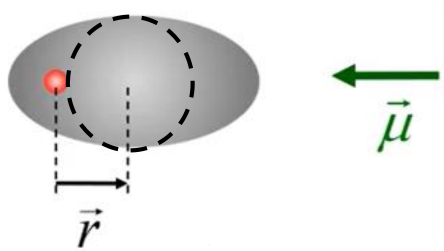
charge

distance from center

** Sorry for the confusing notation, but μ here is NOT permeability.

$$\vec{\mu}(\omega) = \frac{q^2}{m_e}\frac{\vec{E}(\omega)}{\omega_0^2 - \omega^2 - j\omega\Gamma}$$

$\alpha(\omega)$



The electric dipole moment $\vec{\mu}(\omega)$ is a measure of the strength and separation of positive and negative charges.

$$\vec{\mu}(\omega) = \alpha(\omega)\vec{E}(\omega)$$

Susceptibility (1 of 2)

Recall the following:

$$\vec{P}(\omega) = N\left\langle \vec{\mu}(\omega)\right\rangle = \varepsilon_0 \chi(\omega)\vec{E}(\omega)$$

$$\vec{\mu}(\omega) = \alpha(\omega)\vec{E}(\omega) \qquad N\alpha(\omega)\vec{E}(\omega) = \varepsilon_0\chi(\omega)\vec{E}(\omega)$$

$$\alpha(\omega) = \frac{q^2}{m_e}\frac{1}{\omega_0^2 - \omega^2 - j\omega\Gamma} \qquad \chi(\omega) = \frac{N\alpha(\omega)}{\varepsilon_0}$$

This leads to an expression for the susceptibility:

$$\chi(\omega) = \frac{N\alpha(\omega)}{\varepsilon_0} = \underbrace{\boxed{\left(\frac{Nq^2}{\varepsilon_0 m_e}\right)}}_{\omega_p}\frac{1}{\omega_0^2 - \omega^2 - j\omega\Gamma}$$

Susceptibility (2 of 2)

Susceptibility of a dielectric material:

$$\chi(\omega) = \frac{\omega_p^2}{\omega_0^2 - \omega^2 - j\omega\Gamma}$$

$$\omega_p^2 = \frac{Nq^2}{\varepsilon_0 m_e}$$ plasma frequency

$$q = 1.60217646 \times 10^{-19}\ \mathrm{C}$$

$$\varepsilon_0 = 8.8541878176 \times 10^{-12}\ \mathrm{F/m}$$

$$m_e = 9.10938188 \times 10^{-31}\ \mathrm{kg}$$

- Note this is the susceptibility of
- The location of atoms is importa this.
- Real materials have many source

ω_p

Metal	Symbol	Plasma Wavelength	Plasma Frequency
Aluminum	Al	82.78 nm	3624 THz
Chromium	Cr	115.35 nm	2601 THz
Copper	Cu	114.50 nm	2620 THz
Gold	Au	137.32 nm	2185 THz
Nickel	Ni	77.89 nm	3852 THz
Silver	Ag	137.62 nm	2180 THz

The Dielectric Function

Recall that,

$$\vec{D} = \underbrace{\varepsilon_0 \tilde{\varepsilon}_r}_{\varepsilon} \vec{E} = \varepsilon_0 \vec{E} + \vec{P} = \varepsilon_0 \vec{E} + \varepsilon_0 \chi \vec{E} = \varepsilon_0 \left(1 + \chi\right) \vec{E}$$

Therefore,

$$\tilde{\varepsilon}_r\left(\omega\right) = 1 + \chi\left(\omega\right)$$

The ~ symbol indicates the quantity is complex

The dielectric function for a material with a single resonance is then,

$$\boxed{\tilde{\varepsilon}_r\left(\omega\right) = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - j\omega\Gamma} \qquad \omega_p^2 = \frac{Nq^2}{\varepsilon_0 m_e}}$$

Real and Imaginary Parts of ε

$$\boxed{\tilde{\varepsilon}_r(\omega) = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - j\omega\Gamma} \qquad \omega_p^2 = \frac{Nq^2}{\varepsilon_0 m_e}}$$

Split into real and imaginary parts

$$\tilde{\varepsilon}_r(\omega) = \varepsilon_r'(\omega) + j\varepsilon_r''(\omega) = 1 + \frac{\omega_p^2}{\left(\omega_0^2 - \omega^2\right) - j\omega\Gamma} \frac{\left(\omega_0^2 - \omega^2\right) + j\omega\Gamma}{\left(\omega_0^2 - \omega^2\right) + j\omega\Gamma}$$

$$= 1 + \omega_p^2 \frac{\left(\omega_0^2 - \omega^2\right) + j\omega\Gamma}{\left(\omega_0^2 - \omega^2\right)^2 + \omega^2\Gamma^2}$$

$$= 1 + \omega_p^2 \frac{\omega_0^2 - \omega^2}{\left(\omega_0^2 - \omega^2\right)^2 + \omega^2\Gamma^2} + j\omega_p^2 \frac{\omega\Gamma}{\left(\omega_0^2 - \omega^2\right)^2 + \omega^2\Gamma^2}$$

$$\boxed{\varepsilon_r'(\omega) = 1 + \omega_p^2 \frac{\omega_0^2 - \omega^2}{\left(\omega_0^2 - \omega^2\right)^2 + \omega^2\Gamma^2} \qquad \varepsilon_r''(\omega) = \omega_p^2 \frac{\omega\Gamma}{\left(\omega_0^2 - \omega^2\right)^2 + \omega^2\Gamma^2}}$$

Summary of Derivation

1. We wrote the equation of motion by comparing bound charges to a mass on a spring.

$$m_e \frac{\partial^2 \vec{r}}{\partial t^2} + m_e \Gamma \frac{\partial \vec{r}}{\partial t} + m_e \omega_0^2 \vec{r} = -q\vec{E}$$

2. We performed a Fourier transform to solve this equation for ***r***.

$$\vec{r}(\omega) = -\frac{q}{m_e} \frac{\vec{E}(\omega)}{\omega_0^2 - \omega^2 - j\omega\Gamma}$$

3. We calculated the electric dipole moment of the charge displaced by ***r***.

$$\vec{\mu}(\omega) = \frac{q^2}{m_e} \frac{\vec{E}(\omega)}{\omega_0^2 - \omega^2 - j\omega\Gamma}$$

4. We calculated the volume averaged dipole moment to derive the material polarization.

$$\vec{P}(\omega) = \tfrac{1}{V} \sum \vec{\mu}_i(\omega) = N \langle \vec{\mu}(\omega) \rangle$$

5. We calculated the material susceptibility.

$$\chi(\omega) = \frac{\omega_p^2}{\omega_0^2 - \omega^2 - j\omega\Gamma} \qquad \omega_p^2 = \frac{Nq^2}{\varepsilon_0 m_e}$$

6. We calculated the dielectric function.

$$\tilde{\varepsilon}_r(\omega) = 1 + \chi(\omega)$$

$$\boxed{\tilde{\varepsilon}_r(\omega) = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - j\omega\Gamma}}$$

The Lorentz Model

引入频率无穷大时的相对介电常数ε_∞、ε_s对Lorentz模型进行修正

The Lorentz complex permittivity is defined as

$$\varepsilon(\omega) = \varepsilon_\infty + (\varepsilon_s - \varepsilon_\infty)\frac{\omega_0^2}{\omega_0^2 + 2j\omega\gamma - \omega^2}$$

where ω_0 is the resonant frequency and γ is the damping coefficient (collision frequency), both in radians/second.

The Lorentz Model

- 以单一频率对应的高共振下的ε为特征；
- 无限和静态介电常数ε_s、ε_∞值与Debye要求相同；
- **共振频率和阻尼系数值确定了ε峰值。**

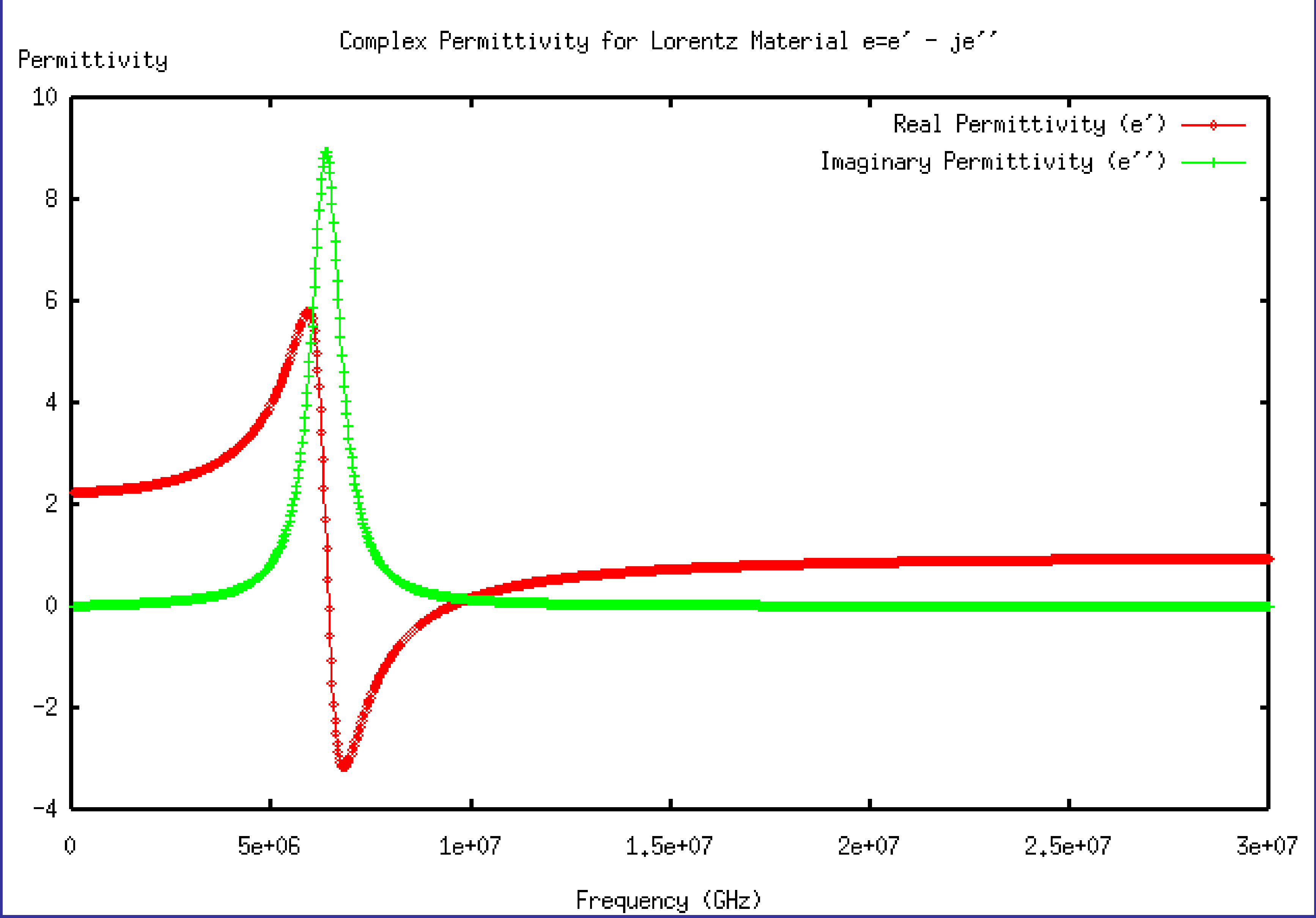
Limits on the Lorentz Parameters

- As with Debye, $\varepsilon_s > \varepsilon_\infty$
- $\omega_0 > 0$ and $\gamma > 0$
- A conductivity value (σ) is not required

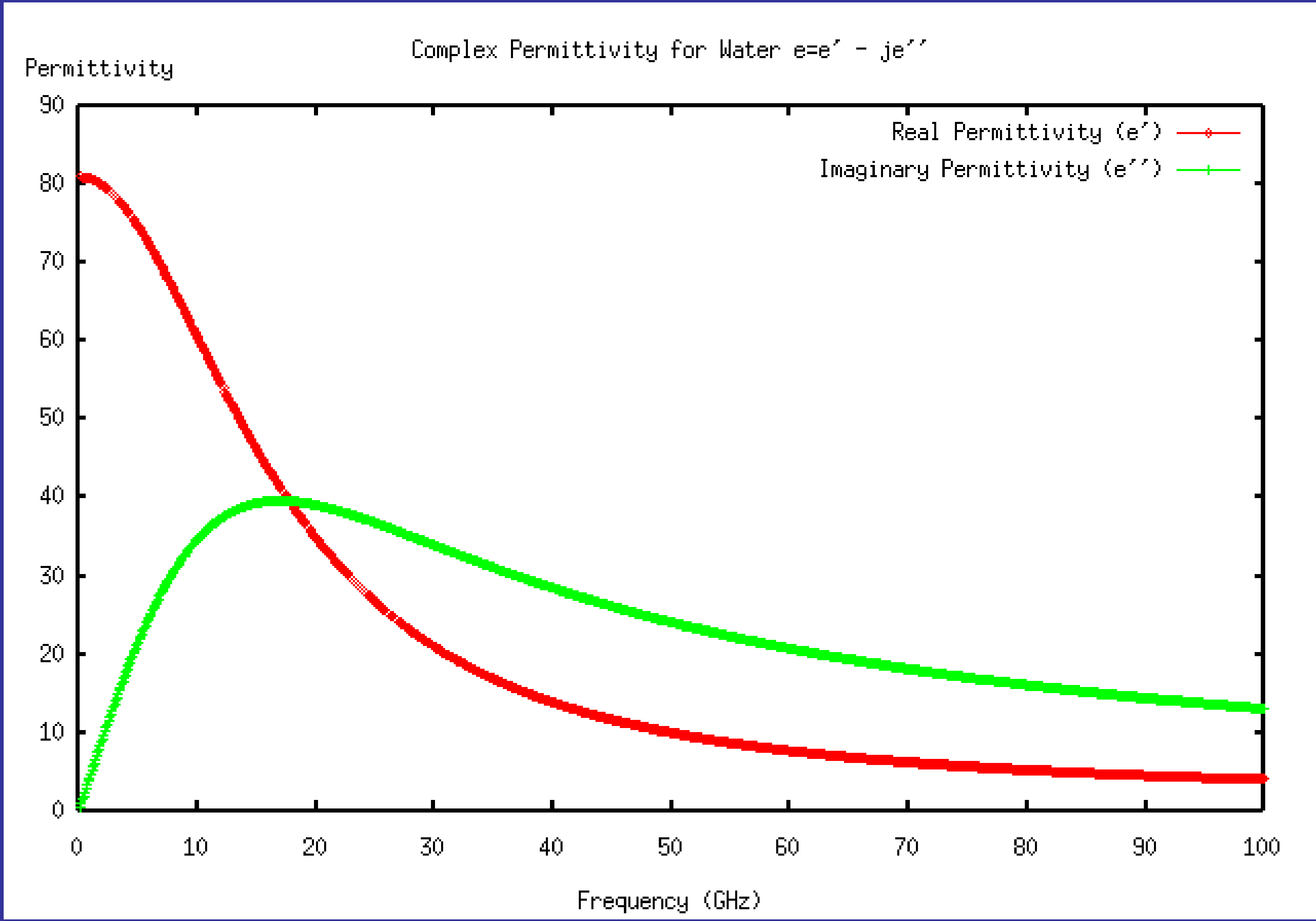
Example Lorentz Complex Permittivity

- $\varepsilon_s = 2.25$, $\varepsilon_\infty = 1.0$
- $\omega_0 = 4.0 \times 10^{16}$, $\gamma = 0.28 \times 10^{16}$

Complex Permittivity for Lorentz



Complex Permittivity for Water



In Summary

Lorentz model

$$\tilde{\varepsilon}_r(\omega) = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - j\omega\Gamma}$$

Drude model for metal in free-electron region

$$\varepsilon_r(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma} = \left(1 - \frac{\omega_p^2}{\omega^2 + \gamma^2}\right) + i\left(\frac{\omega_p^2\gamma}{\omega^3 + \omega\gamma^2}\right)$$

Modified Drude model for metal in bound-electron region

$$\varepsilon_r(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega\gamma} = \left(\varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + \gamma^2}\right) + i\left(\frac{\omega_p^2\gamma}{\omega^3 + \omega\gamma^2}\right)$$

Extended Drude (Drude-Lorentz) model

$$\varepsilon_r(\omega) = \varepsilon_\infty - \left(\frac{\omega_p^2}{\omega^2 + i\omega\gamma}\right) - \left(\frac{\Delta\varepsilon\,\Omega_L^2}{\left(\omega^2 - \Omega_L^2\right) + i\omega\,\Gamma_L}\right)$$

Also keep in mid….

n' and n'' vs χ' and χ'' vs ε' and ε''

All pairs (n' and n'', χ' and χ'', ε' and ε'') describe the same physics

For some problems one set is preferable for others another

n' and n'' used when discussing wave propagation

$$\boldsymbol{E}(z,t)=\mathrm{Re}\left\{\boldsymbol{E}(z,\omega)\exp\left(-i\beta z-\frac{\alpha}{2}z+i\omega t\right)\right\}$$ where $\underbrace{\beta=k_0 n'}_{\text{Phase propagation}}$ and $\underbrace{\alpha=-2k_0 n''}_{\text{absorption}}$

χ' and χ''
ε' and ε'' } used when discussing microscopic origin of optical effects

Inter relationships

Example: n and ε

From $n=\sqrt{\varepsilon_r}$

$\downarrow$

$n'+in''=\sqrt{\varepsilon_r'+i\varepsilon_r''}$ ➡

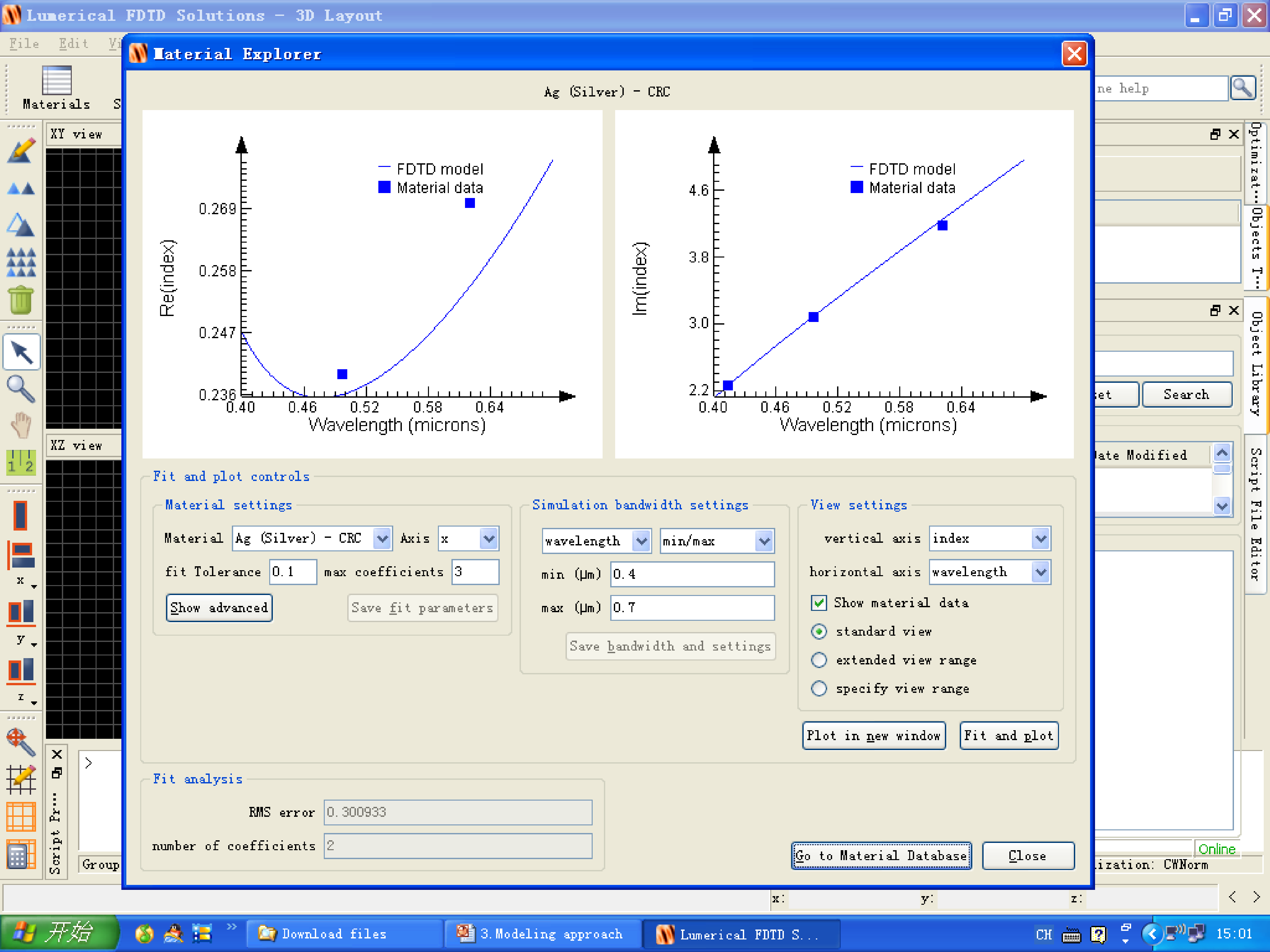
$$\boxed{\begin{aligned}\varepsilon_r'&=(n')^2-(n'')^2\\ \varepsilon_r''&=2n'n''\end{aligned}}$$

and

$$\boxed{\begin{aligned}n'&=\sqrt{\frac{\sqrt{(\varepsilon_r')^2+(\varepsilon_r'')^2}+\varepsilon_r'}{2}}\\ n''&=\sqrt{\frac{\sqrt{(\varepsilon_r')^2+(\varepsilon_r'')^2}-\varepsilon_r'}{2}}\end{aligned}}$$

Commercial softwares

- **FDTD Solution:** nanophotonics
- **XFDTD:** general EM fields
- **RSoft:** 被Synopsis收购主打BeamPr.
- **Opti-FDTD:** too slow
- **CST:** microwave/millimeter wave
- **COMSOL:** microwave/millimeter wave
- **HFSS:** microwave/millimeter wave

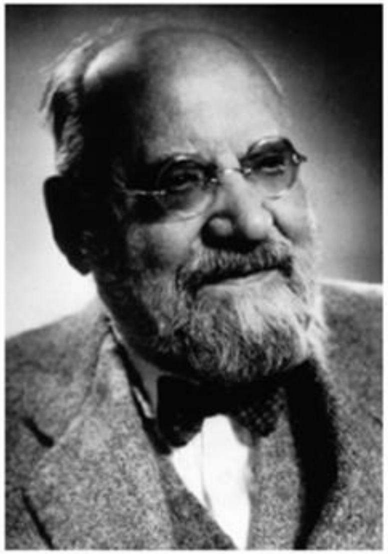


Lumerical FDTD Solutions - 3D Layout
Material Explorer
Ag (Silver) - CRC
FDTD model
Material data
Re(index)
0.269
0.258
0.247
0.236
0.40 0.46 0.52 0.58 0.64
Wavelength (microns)
Im(index)
4.6
3.8
3.0
2.2
Fit and plot controls
Material settings
Material Ag (Silver) - CRC
Axis x
fit Tolerance 0.1
max coefficients 3
Show advanced
Save fit parameters
Simulation bandwidth settings
wavelength
min/max
min (µm) 0.4
max (µm) 0.7
Save bandwidth and settings
View settings
vertical axis index
horizontal axis wavelength
Show material data
standard view
extended view range
specify view range
Plot in new window
Fit and plot
Fit analysis
RMS error 0.300933
number of coefficients 2
Go to Material Database
Close
开始
Download files
3.Modeling approach
Lumerical FDTD S...
15:01

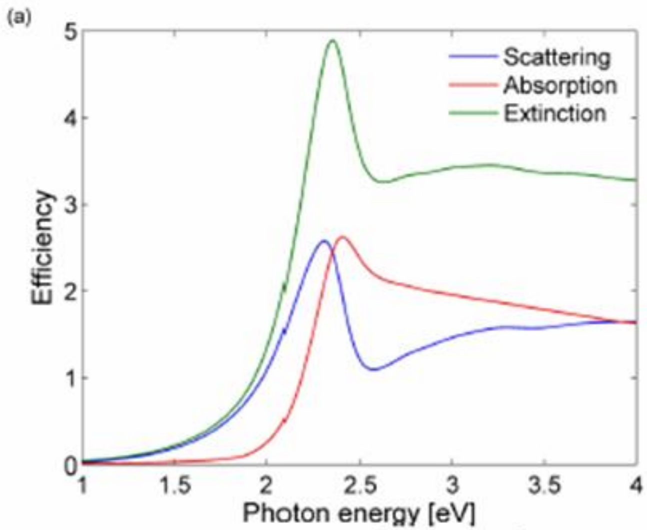
Discrete dipole approximation

(DDA)

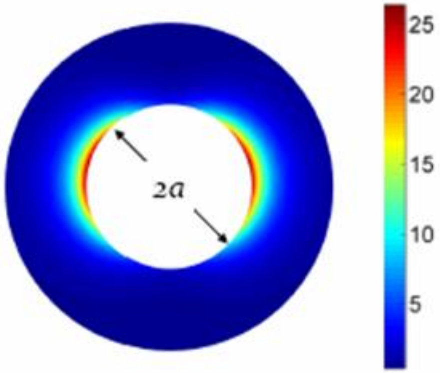
Electrodynamic Analysis of Localized Surface Plasmon



Gustav Mie

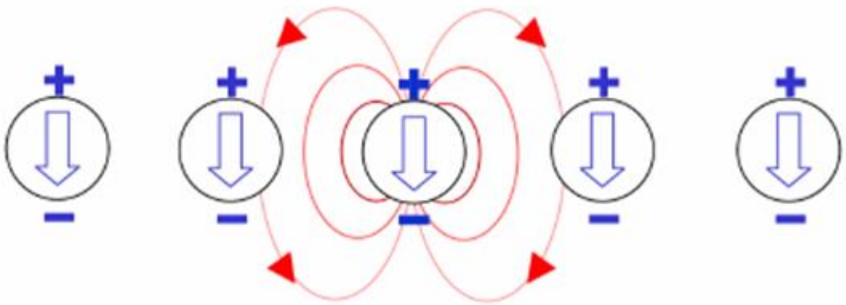


60-nm Au nanosphere in free space



Near field enhancement

Discrete Dipole Approximation
Finite Different Time Domain
T-matrix



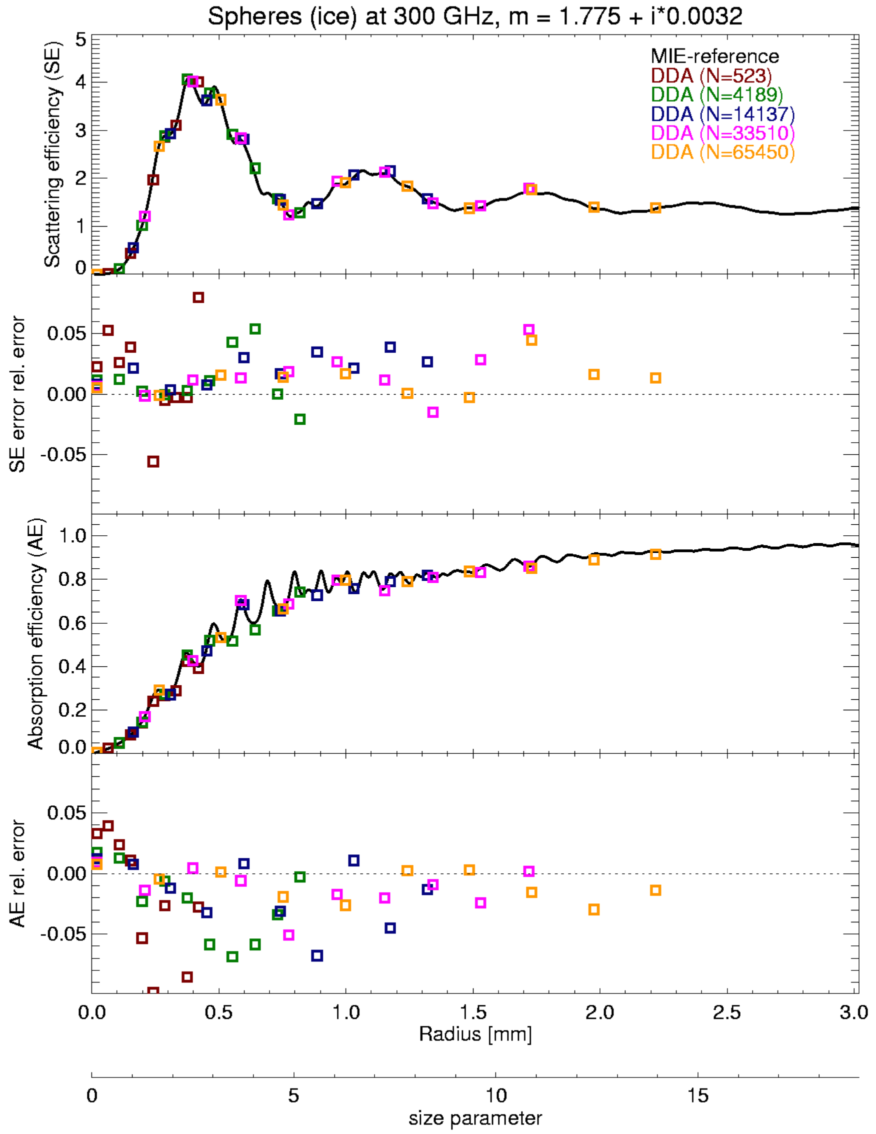
Interparticle coupling

Verification of DDA

DDA single scattering properties –

comparison to Mie calculations

DDA single scattering properties – comparison to Mie calculations



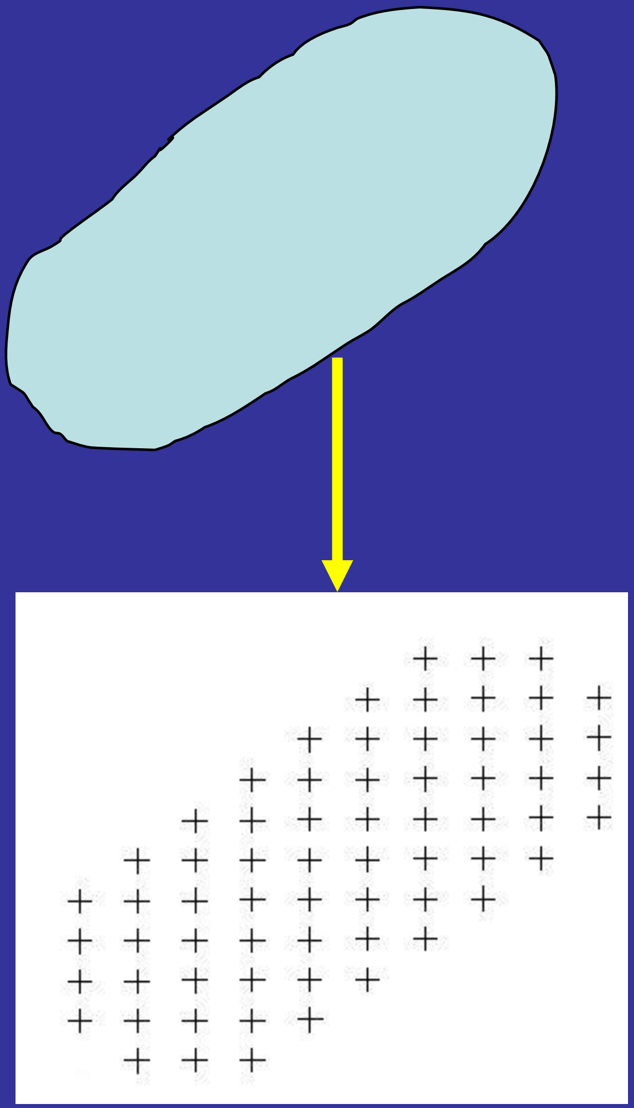
Solid ice spheres at 300 GHz

Criterion for DDA application: *mkd* < 0.5

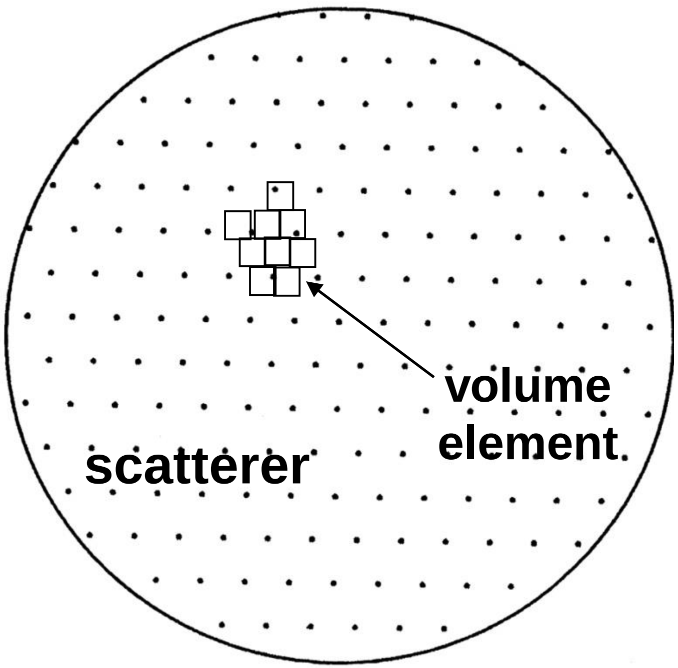
n: complex refractive index
k: wave number
d: dipole separation
N: number of dipoles,N ~ 1/d

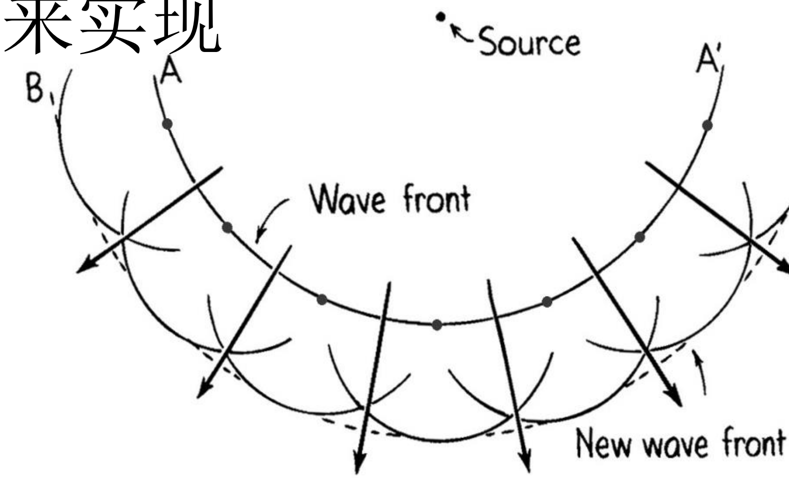
Discrete dipole approximation

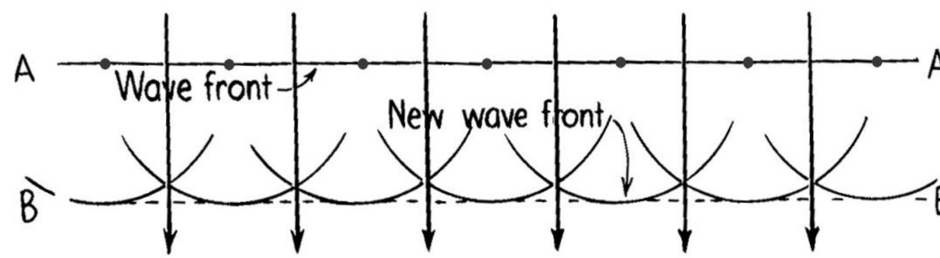
- 适用于极性分子　PPT
- 将点散射体当做偶极子处理
- 用偶极子阵列代替立方晶格
- 对每个偶极子求解电场E→进一步分析散射场



一个颗粒的散射可通过将其细分为无数小的含有偶极子的体积元素来实现







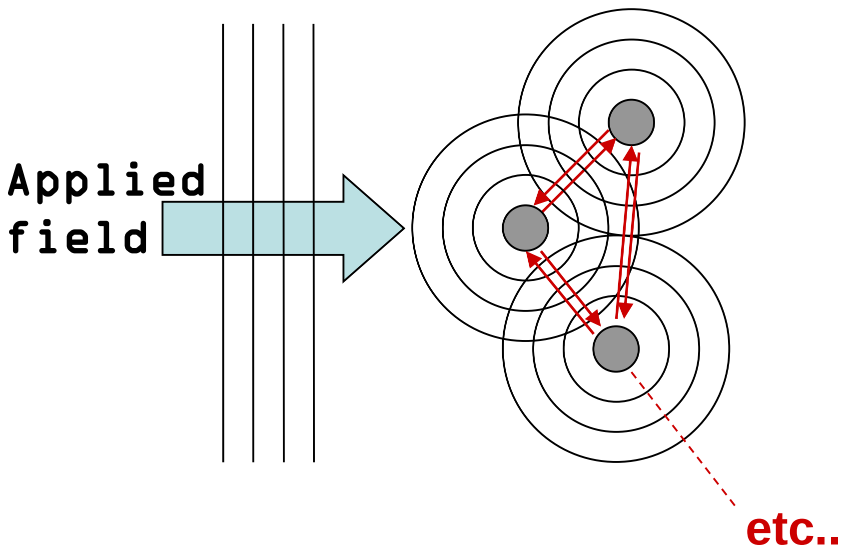
这些体积元素扮演者散射波源的角色

这与惠更斯原理的思路是一致的，除了下面几种更一般的情况:

- ✓ 波的偏振
- ✓ 颗粒成分的变化
- ✓ 任意复杂颗粒形状
- ✓ 开发更直观地描述散射的方法

DDA continued…

- Model complex particle with many point dipoles
- Each has a dipole moment of $p_j = 3\mathrm{d}vK(\varepsilon)\mathbf{E}_j$ ($\mathbf{E}_j$ is field at j$^{\text{th}}$ dipole)
- Every dipole sees every other dipole, *i.e.* total field at the ***l*** $^{\text{th}}$ dipole is:



So need a self-consistent solution for $\mathbf{E}_j$ at every dipole

$$\mathbf{E}(\mathbf{r}_j) = \mathbf{E}_{applied}(\mathbf{r}_j) + \sum_{k \neq j} \mathbf{A}_{jk}\left(\alpha_k \mathbf{E}(\mathbf{r}_k)\right)$$

Electric field at *j*

Applied field at *j*

Tensor characterising of the E field from dipole *k*, as measured at *j*

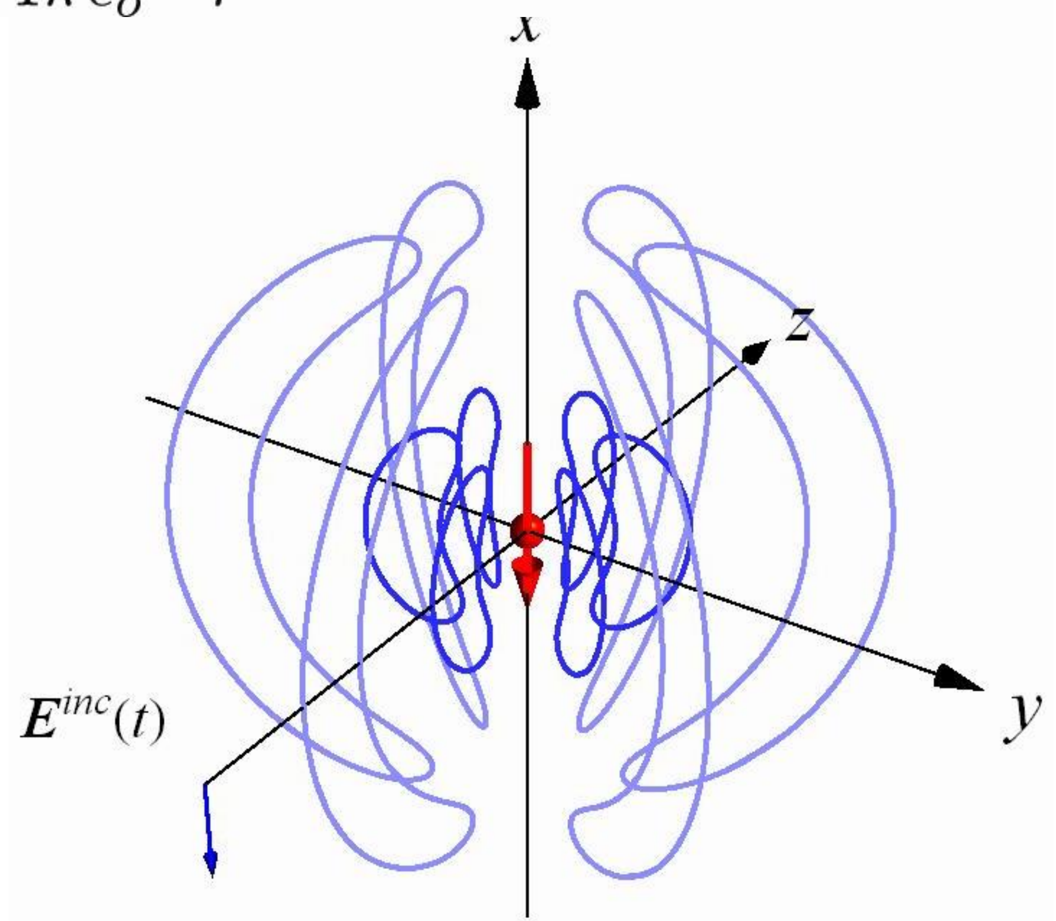
polarisability of dipole *k*

偶极子辐射

当偶极子与外界入射光子形成震荡时，将产生与自身相关的电磁波

$$\mathbf{E}^{dip}(\mathbf{r},t)=\frac{k^2}{4\pi\epsilon_o}\frac{e^{ikr}}{r}\left[\hat{\mathbf{r}}\times\mathbf{p}(t)\right]\times\hat{\mathbf{r}}$$

so the volume element radiates…

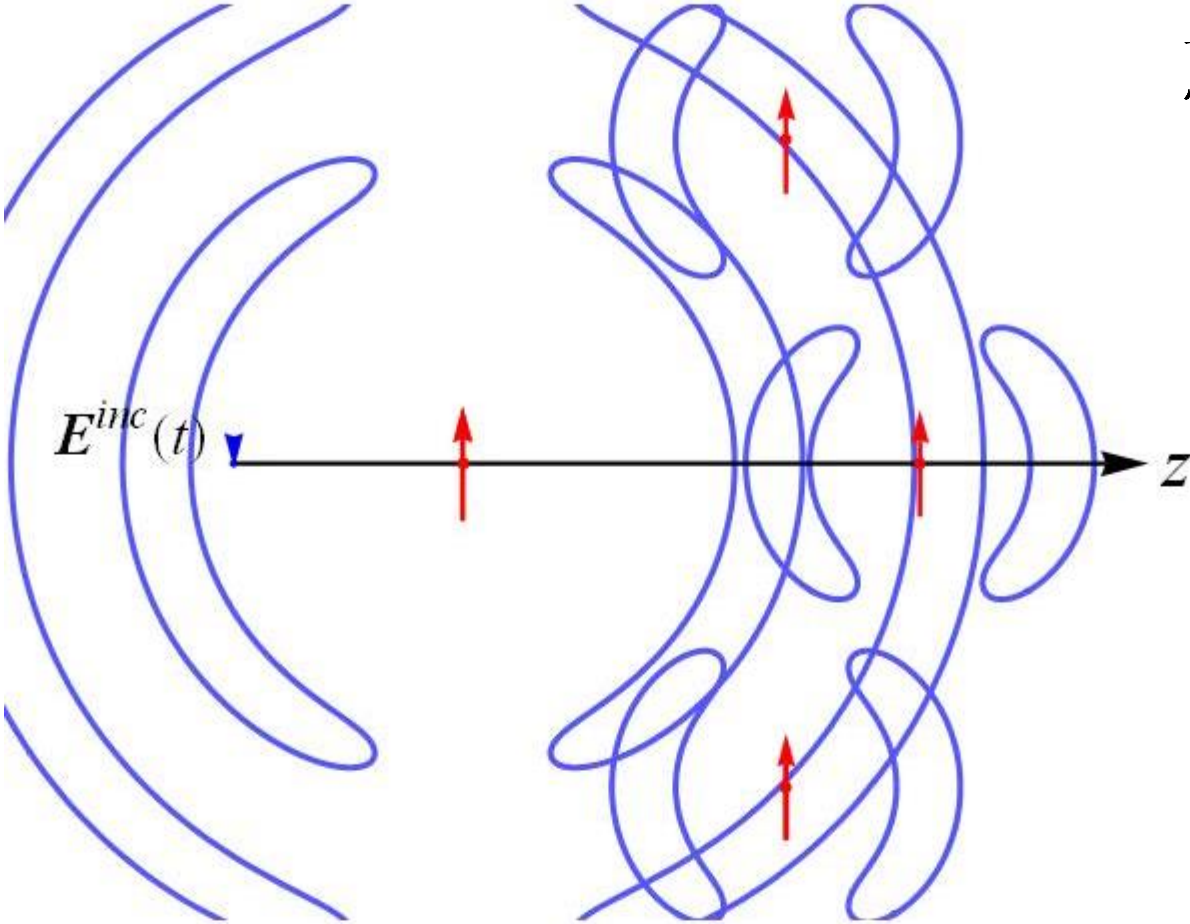


波沿着径向向外传播

辐射波长与入射光一致

偶和情况下

邻近体积元素将响应入射场以及附近其它体积元素的场辐射



一个元素的辐射影响到其它的元素,反之亦然。

The elements are ***coupled*** together.

The simple, diffraction / Fourier transform description scattering neglects this.

通过求解整个系统的线性代数方程我们即可知道颗粒中的偶极子是如何响应入射光波及其耦合。

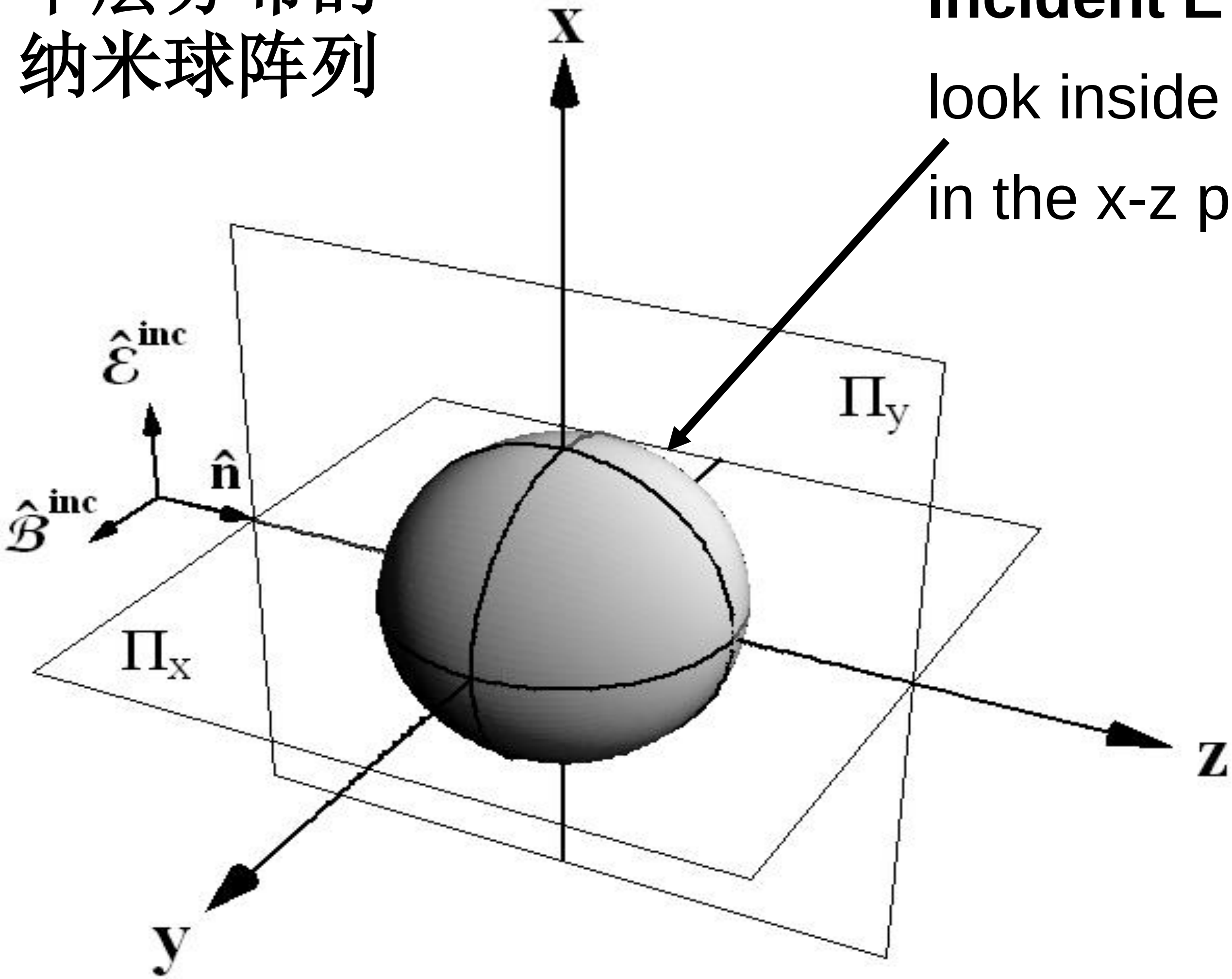
耦合效应举例: 单个球颗粒

单层分布的
纳米球阵列

Incident E field:

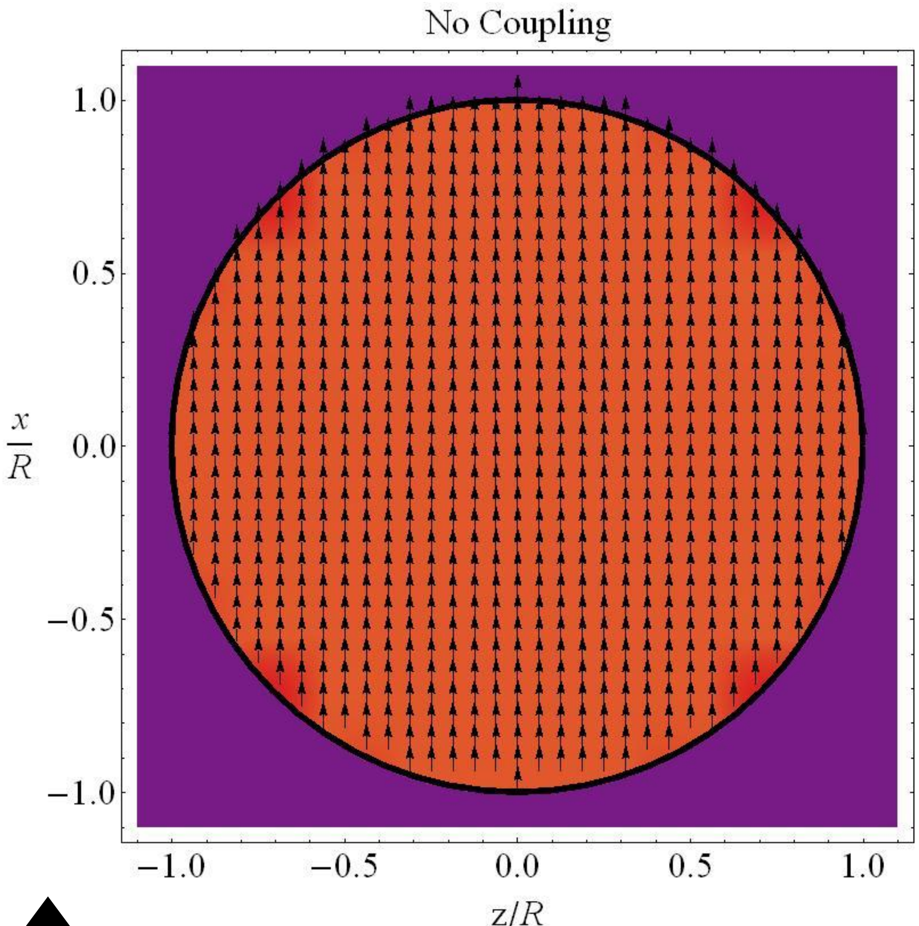
look inside of a sphere

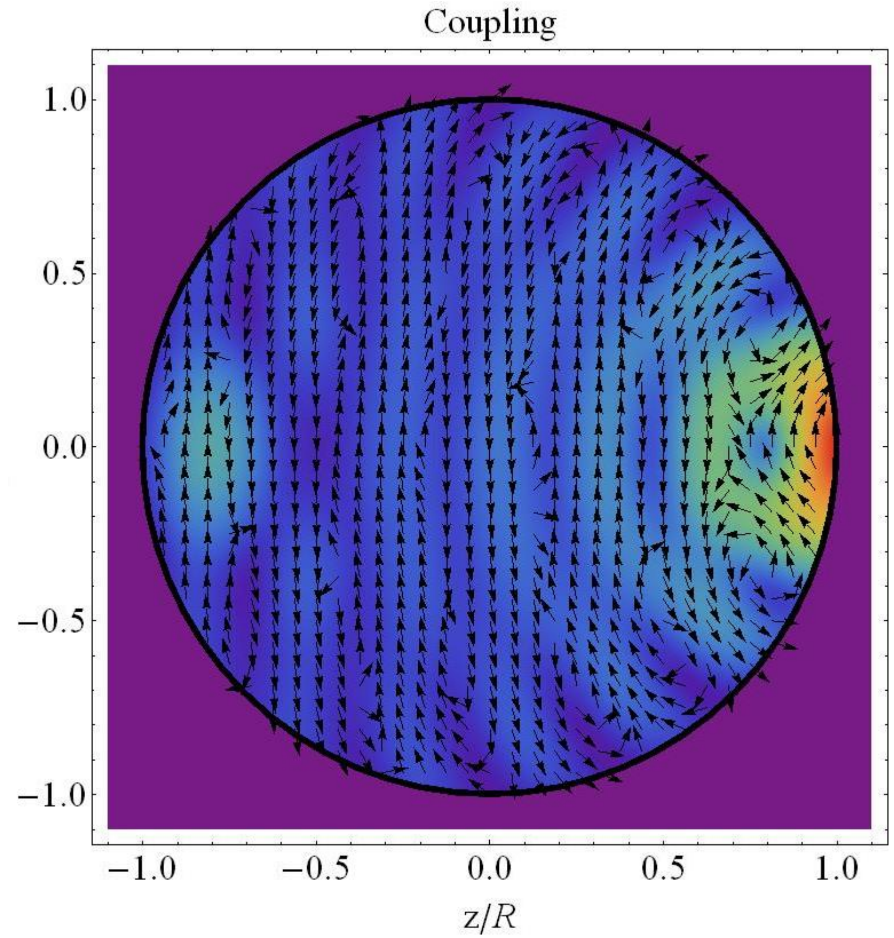
in the x-z plane



What coupling does

the effects of coupling…





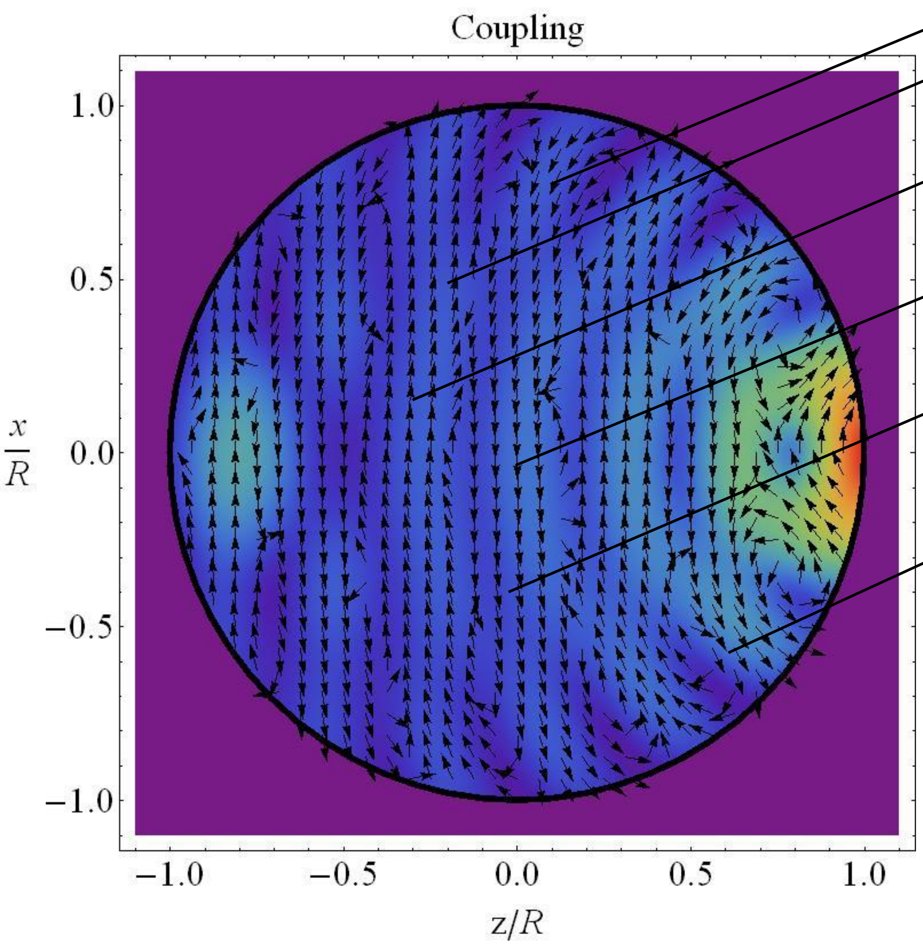
polarization

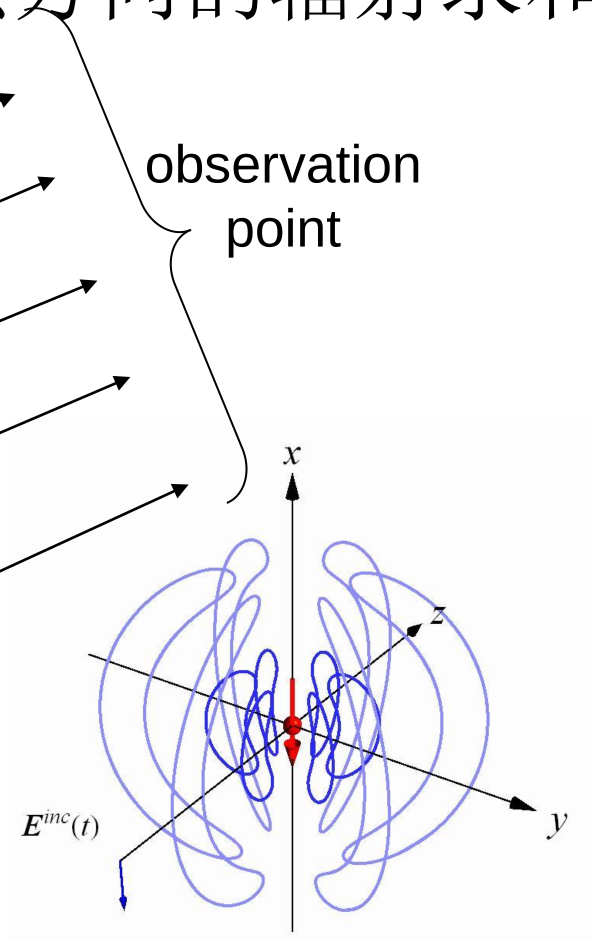
polarization

Coupling changes the direction & magnitude of the dipole moments from what they would be if they had responded to the incident wave only.

DDA

一旦知道所有偶极子的耦合，整个颗粒的散射波即为每个偶极子的散射波沿着观察点方向的辐射求和。





This description of scattering is the ***Discrete Dipole Approximation*** (DDA)

DDA 的严格理论求解

$$\nabla \cdot \mathbf{D}(\mathbf{r}) = \rho(\mathbf{r})$$
$$\nabla \cdot \mathbf{B}(\mathbf{r}) = 0$$
$$\nabla \times \mathbf{E}(\mathbf{r}) = -\partial_t \mathbf{B}(\mathbf{r})$$
$$\nabla \times \mathbf{H}(\mathbf{r}) = \mathbf{J}(\mathbf{r}) + \partial_t \mathbf{E}(\mathbf{r})$$

Maxwell's equations

wave equation

electric field inside of the particle – this is where the dipoles enter

$$\mathbf{E}^{sca}(\mathbf{r}) = k^2\left(m^2-1\right)\left(\bar{\bar{\mathbf{I}}} + \frac{1}{k^2}\nabla \otimes \nabla\right) \cdot \int_V \mathbf{E}^{int}(\mathbf{r}') \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}\mathrm{d}\mathbf{r}'$$

Volume Integral Equation (VIE)

Dividing the particle into its volume elements discretize the VIE which generates a system of algebraic equations that can be solved to yield the dipole coupling.

Special case

This corresponds to ***neglecting the coupling*** between the volume elements. The VIE then reduces to

如果入射光场用颗粒内部电场代替，可得颗粒的散射场：

$$\mathbf{E}^{int}(\mathbf{r}) \rightarrow \mathbf{E}^{inc}(\mathbf{r})$$

FFT

$$\mathbf{E}^{sca}(\mathbf{r}) \propto \int_V e^{i\mathbf{q}\cdot\mathbf{r}'} \mathrm{d}\mathbf{r}'$$

颗粒体积积分方程的傅里叶变换形式

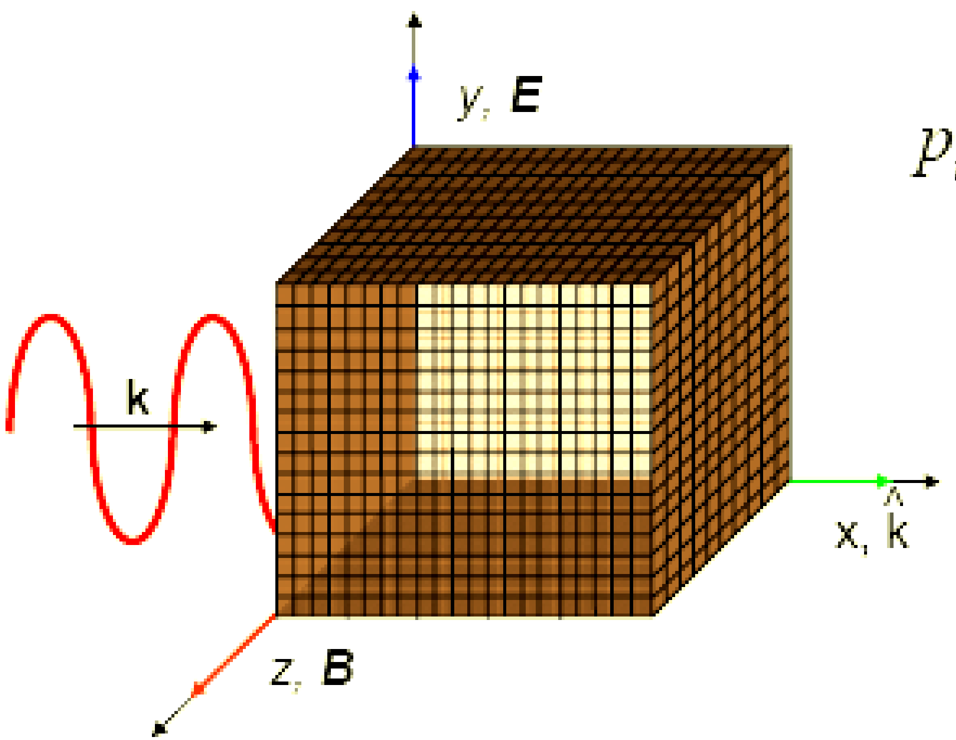
简单的FFT变换描述= 无耦合限制的散射

DDA simulation details

Neal, Palffy-Muhoray

- Discrete dipole approximation (DDA) simulation determines susceptibilites

颗粒分子在电场作用下发生极化并产生感应电偶极矩**p**



Simulation Solves:

$$p_i = \alpha_i \left(E_{inc,i} - \sum_{j \neq k}^{N} A_{jk} p_k\right)$$

Algebraic equations

If

$$\alpha_i^{-1} = A_{ii}$$

then

$$\sum_{i=1}^{N} A_{ij} p_i = E_{inc,j}$$

分子极化率

α_i— polarizability

- Consider N dipoles, the ith dipole $\mathbf{p}_i$ located at $\mathbf{r}_i$ and having polarizability α_i.

- $\mathbf{p}_i = \alpha_i \mathbf{E}_{loc,i}$ 电偶极矩$\mathbf{p}_\mathrm{i}$、分子极化率α_i与电场$\mathbf{E}$之间的关系

- $\mathbf{E}_{loc,i} = \mathbf{E}_0 e^{\mathbf{k}\cdot\mathbf{r}-i\omega t} - \sum_{j\neq i} \mathbf{A}_{ij} \cdot \mathbf{p}_j$

- $\mathbf{A}_{ij} \cdot \mathbf{p}_j$ = dipole field (near-field + far-field contribution) at $\mathbf{r}_j$ due to $\mathbf{p}_i$.

- Solve for $\mathbf{p}_i$. Then extinction coefficient C_{ext} is given by

$$C_{ext} = \frac{4\pi k}{|\mathbf{E}_0|^2} \mathrm{Im} \sum_{\mathrm{j=1}}^{\mathrm{N_{par}}} \mathbf{E}_0^* \exp(-\mathrm{i}\omega \mathrm{t}) \cdot \mathbf{p}_\mathrm{j} \tag{1}$$

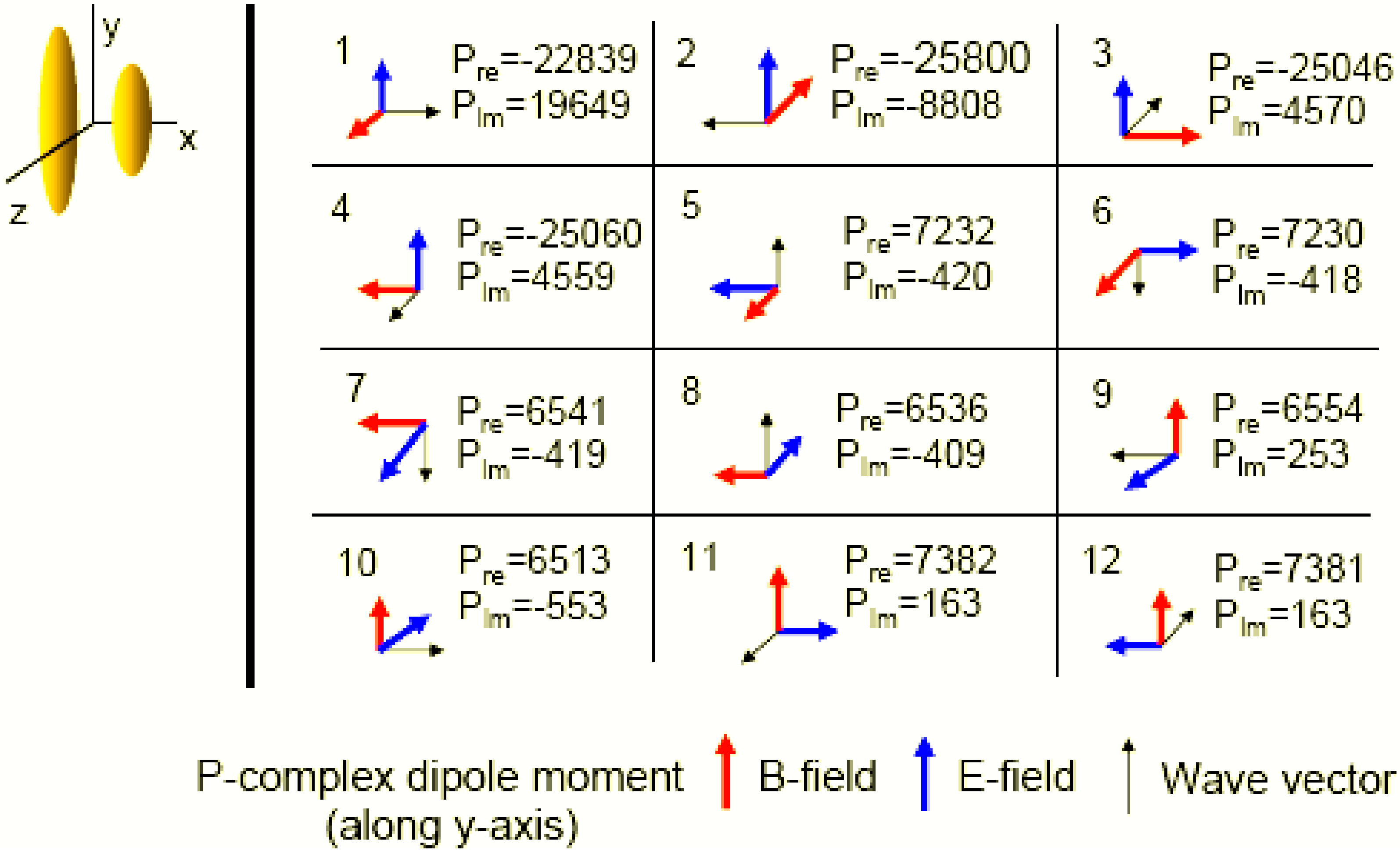
  by optical theorem. (N_{par} is the number of particles in the cluster.)

- α_i is related to ϵ_i of the i^{th} particle by requiring that it given the correct first scattering coefficient in the Mie expansion.

Refs. for DDA: E. M. Purcell and C. R. Pennypacker, Ap. J. 186, 705 (1973); J. J. Goodman *et al*, Opt. Lett. 16, 1198 (1991).

Results: computed dipole moments for Au NRs

Neal, Palffy-Muhoray



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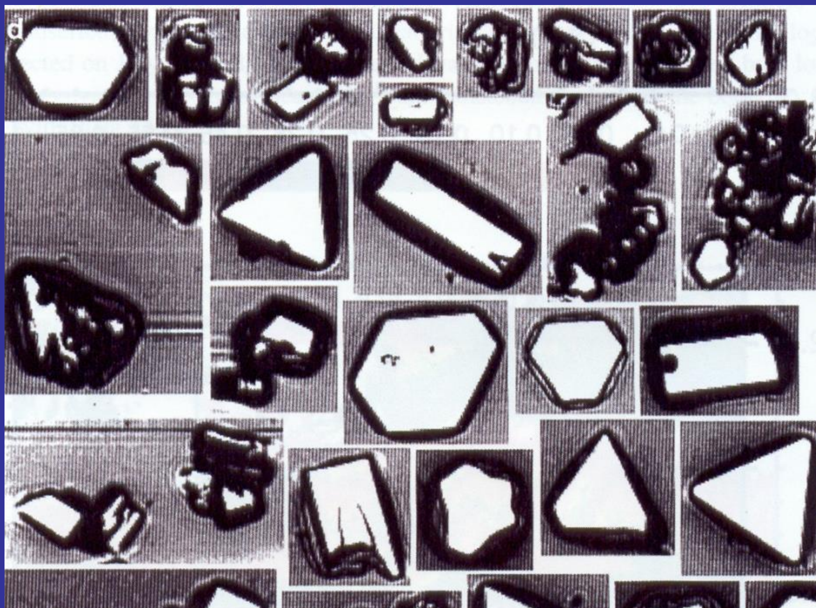
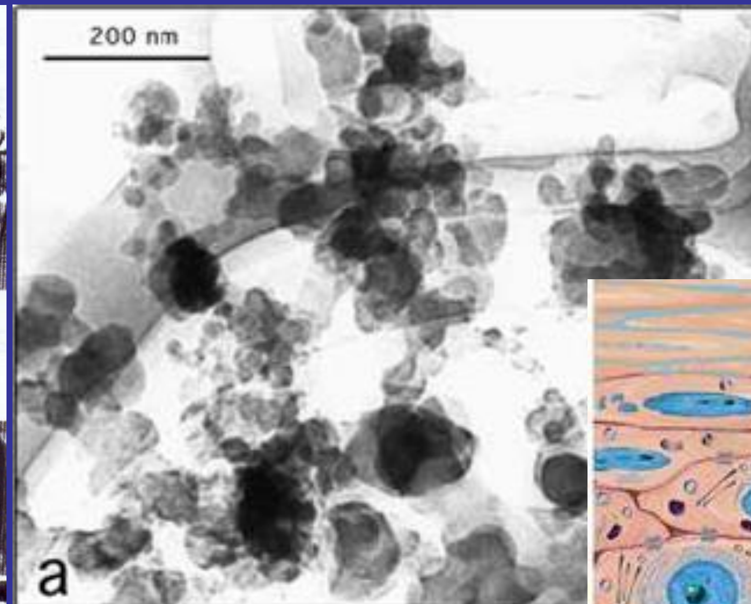
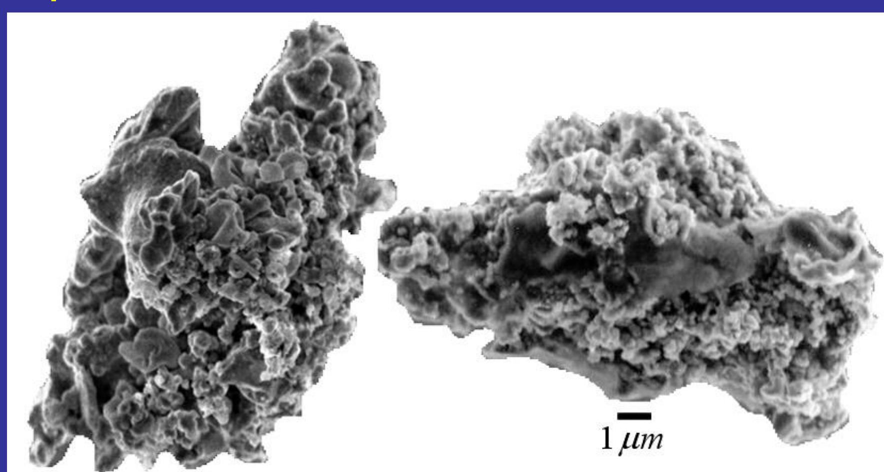
What is this good for ?

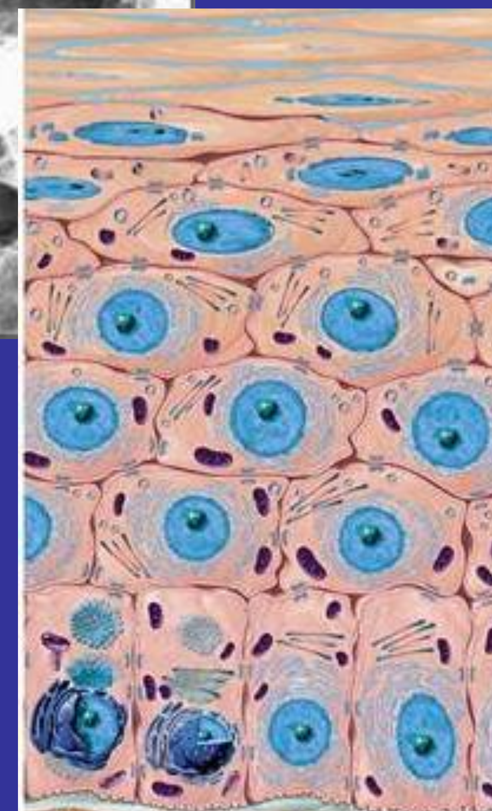
the DDA is well suited to model scattering from complex, particles since there are no restrictions on the particle shape & composition:



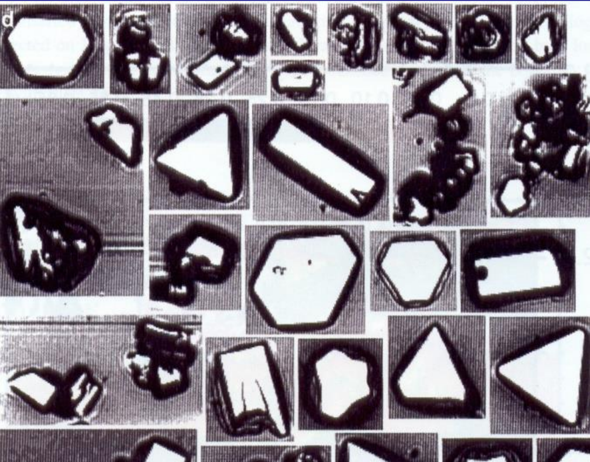


atmospheric particles: water, ice, carbon soot, dust



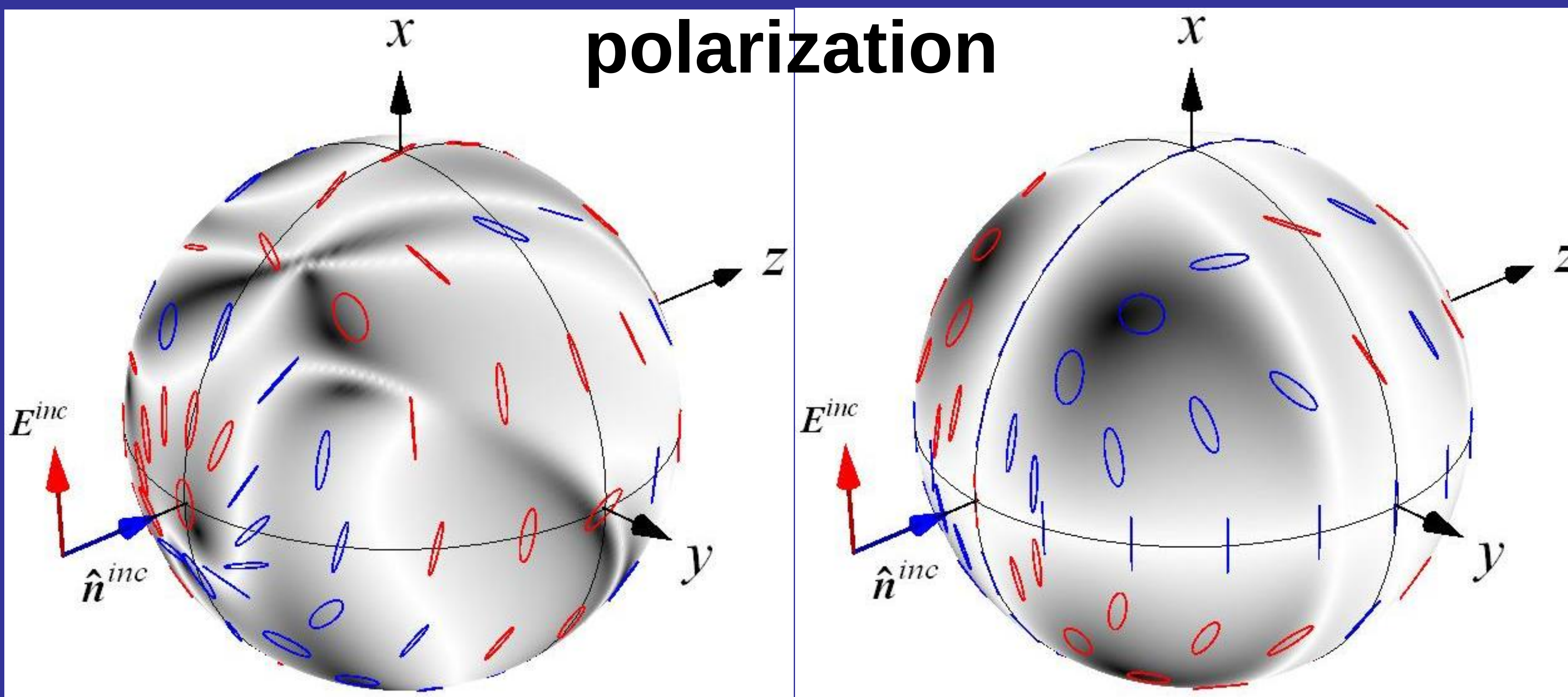


biological particle



An application:

回向散射波的偏振态可标示非球形颗粒的存在, ***e.g.*** 云中的冰颗粒和水滴。



Ice: no symmetry　　　　**Water**: sphere - symmetry

Discrete Dipole Approximation (DDA)

Approximation:

– 用偶极子点阵描述实际目标颗粒;

– 只考虑电偶极子, 忽略*磁性偶极子*。

Required conditions:

– **Best results** if targets have sizes comparable to wavelength (*i.e.* Mie-region, $a \sim \lambda$).

– Materials should have $|\boldsymbol{n}\textbf{-1}|$: $\mathbf{1 \sim 3}$, n = complex refractive index.

– d: “interdipole separation“ should be smaller than structural lengths and wavelength λ, $\boldsymbol{d}<\boldsymbol{\lambda}$.

– numerical studies indicate $|\boldsymbol{n}|\boldsymbol{kd} < \mathbf{1}$, $k=2\pi/\lambda$ (wave number)

DDA source code

- ✓ DDSCAT6.1 (Draine and Flatau, 2003), publicy available (GNU)
- ✓ FORTRAN (77) software package (highly portable)
- ✓ **Calculation of** :

  - 吸收, 散射, 消光系数

  - 散射强度矩阵、散射函数振幅
- ✓ **可变量:**

  - 目标类型/方位 (随机/非随机)

  - 散射角度

  - 偶极子数量

  - 频率、复折射率
- ✓ 尺寸参数: *SP*< 15, |*mkd*| < 0.5 (see Draine and Flatau, 2003)


Have a nice day!

Supplementary Information

T-matrix

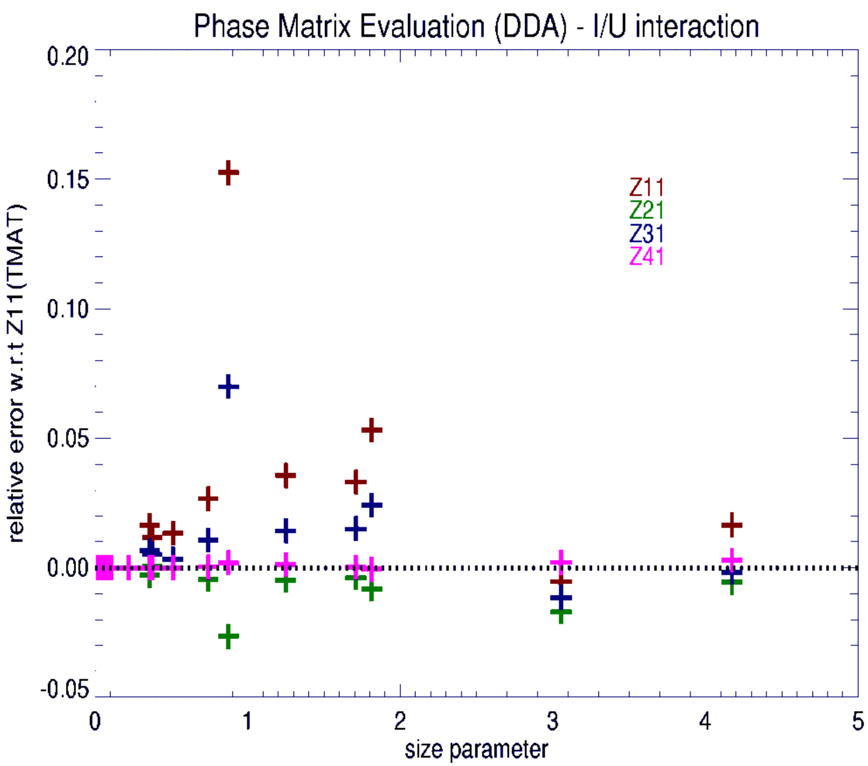
- ✓ Expand incident, transmitted and scattered fields into a series of spherical vector wave functions, then find the relation between incident (a,b) and scattered (p,q) coefficients
- ✓ Once know transition matrix **T,** then can compute the complete scattered field
- ✓ Elements of **T** essentially 2D integrals over the particle surface
- ✓ Easy for rotationally symmetric particles (spheroids, cylinders, etc)
- ✓ **But…**
  - ◆ Less straightforward for arbitrary shapes
  - ◆ Numerically unstable as *kR* gets big
- ✓ Up to *kR*~50 if the shape isn't too extreme

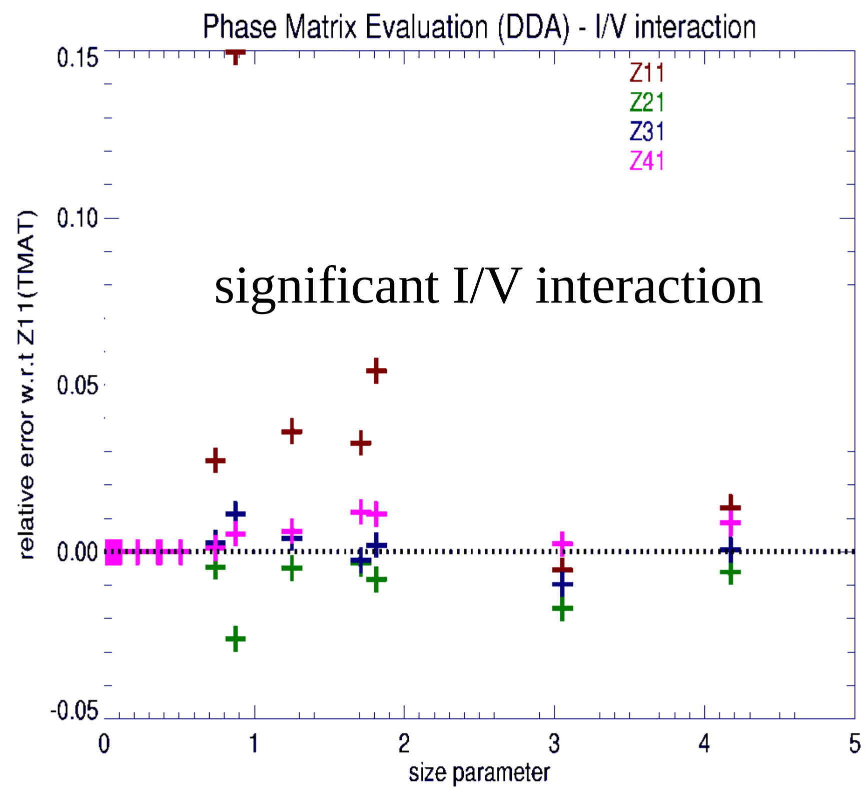
$$\begin{bmatrix} \mathbf{p} \\ \mathbf{q} \end{bmatrix} = \begin{bmatrix} \mathbf{T}_{11} & \mathbf{T}_{12} \\ \mathbf{T}_{21} & \mathbf{T}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}$$

DDA single scattering properties – comparison to T-matrix

- The evaluation was performed for all combinations of possible incoming and scattered directions on a 10° angle grid
- Frequencies considered are in the range from 183 - 875 GHz
- Effective radii range from 5 - 230 μm.
- Refractive index was calculated corresponding to a temperature of 250K (Warren, 1984)
- Number of dipoles chosen corresponding to mkd criterion, although minimum $N = 1000$

DDA single scattering properties – comparison to T-matrix





→ Phase matrix elements all lie within the accuracy of ~ +-15% with respect to Mishchenko.

Conclusion: DDA is better than T-matrix

Classical equations in **scalar diffraction optics**

- Helmholtz's equation
- Green's function
- Green's formula
- Kirchhoff's formula

光通过双缝时的双缝干涉条件

a)同一光源发出的光。

b)它们的频率必须相同。

c)两列波的光程差不能太大。

d)两列波的振幅不能悬殊太大。

上述四个干涉条件，在物理光学中叫做相干条件(Condition of coherence)。

3、电磁波的衍射

当电磁波在传播过程中遇到障碍物或者透过屏幕上的小孔时，会导致偏离原来入射方向的出射电磁波，这种现象称为衍射(**diffraction phenomenon**)。衍射现象的研究对于光学和无线电波的传播都是很重要的。

衍射　：　　不能用反射或折射来解释的，光线对直线光路的任何偏离。衍射是光传播的普遍属性，是光的波动性的表现。

衍射问题的解决方式:

1，考虑光波的矢量性，用矢量波方法求解。（数学上很复杂，但是在某些问题（如研究高分辨率光栅时）必须要用这个方法。

2，标量的方法（基尔霍夫标量衍射理论），把光作为标量来处理，只考虑电磁场一个分量的复振幅。适用范围：衍射孔径比波长大的多，观测点离衍射孔径比较远。

§ 1. 衍射现象概述

c. 惠更斯(F. M. Huygens)子波源假设理论

波前上每一点起着一个次级波源(子波源)的作用，每一个次级波源发出次级球面波(子波)，它向着四面八方扩展，所有这些次级波的包络面便是新的波前。

可解释”衍射”现象，但无法定量分析

d. 18世纪牛顿在科学领域处于权威地位，由于他摒弃了光的波动理论，使得这一理论停滞了近一个世纪。

§ 1. 衍射现象概述

e. 1801年，杨氏干涉原理(T. Young)证实了光的波动性——振幅叠加

f.1818年，菲涅耳(A. J. Fresnel)提出惠更斯-菲涅耳原理。

可定性分析衍射现象，提出了定量初步模型。

g.基尔霍夫(G. Kirchhoff)提出了基尔霍夫衍射理论，完善了惠更斯-菲涅耳理论。

可定性、定量分析衍射现象。

衍射规律的频域表达式

a. 衍射规律的频域描述

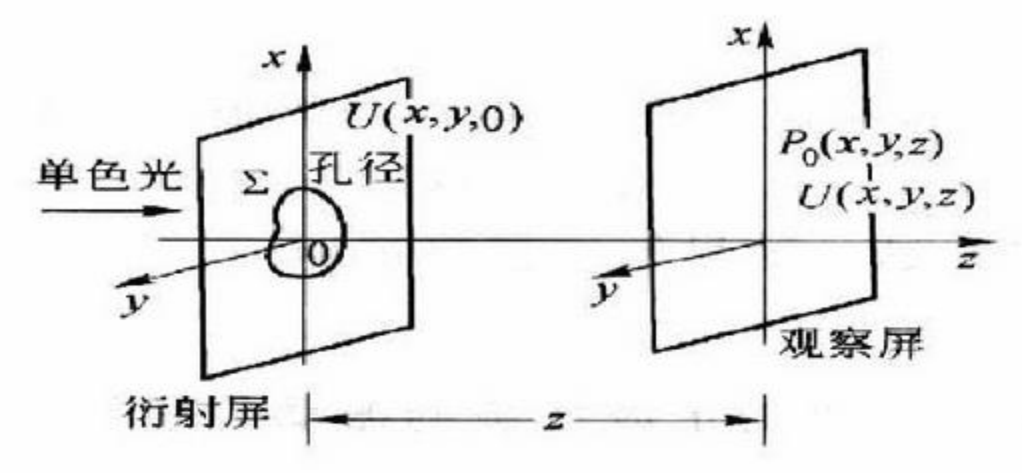


图2.3.1 计算角谱用的坐标系

令

$$G_0(\xi,\eta)=F\{U(x,y,0)\},G_Z(\xi,\eta)=F\{U(x,y,z)\}$$

则由

$$U(x,y,z)=\int\int_{-\infty}^{+\infty}G_Z(\xi,\eta)e^{j2\pi(\xi x+\eta y)}\mathrm{d}\xi\mathrm{d}\eta$$

菲涅耳衍射与夫琅和费衍射

用普遍形式下的标量衍射理论来计算具体衍射问题时，在数学上是非常困难的。因此有必要讨论某些近似。按照近似条件的不同，分为菲涅耳近似和夫琅和费近似两种，从而有菲涅耳衍射和夫琅和费衍射。

a. 旁轴近似

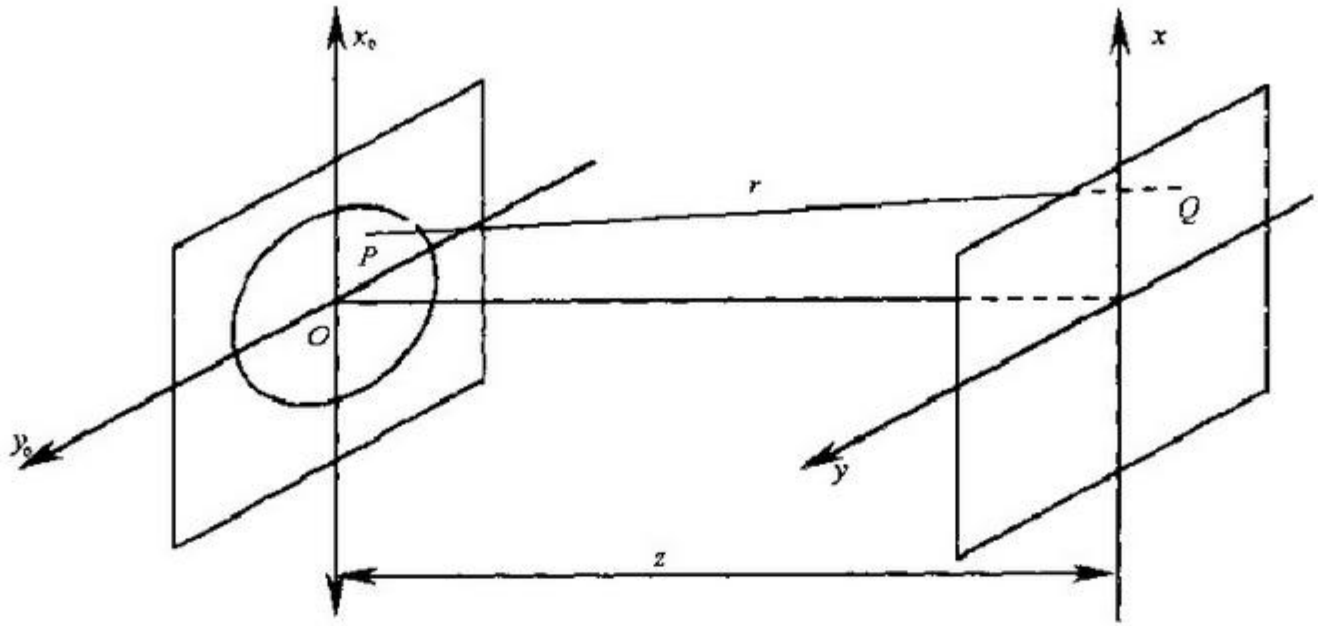


图2.4.1 讨论衍射用的几何示意图

菲涅耳衍射与夫琅和费衍射

由基尔霍夫衍射公式

$$U(p)=\frac{1}{j\lambda}\iint_s \frac{U(p_1)}{r}\cdot\exp(jkr)[\frac{\cos(\vec{n}\cdot\vec{r})-\cos(\vec{n}\cdot\vec{r}_0)}{2}]dS$$

当**观察屏足够远**，**衍射区相对小时**，可得：

$$cos(\vec{n}\cdot\vec{r})=1 \qquad cos(\vec{n}\cdot\vec{r}_0)=-1$$

此时：

$$r=z[1+\frac{(x-x_0)^2+(y-y_0)^2}{z^2}]^{1/2}$$

$$=z\{1+\frac{(x-x_0)^2+(y-y_0)^2}{2z^2}-\frac{[(x-x_0)^2+(y-y_0)^2]^2}{8z^4}+\cdots\}$$

菲涅耳衍射与夫琅和费衍射

在 $z^2 >> (x-x_0)^2+(y-y_0)^2$ 时

$$r \approx z\left[1+\frac{(x-x_0)^2+(y-y_0)^2}{2z^2}\right]$$

称为<u>旁轴近似条件</u>

菲涅耳衍射与夫琅和费衍射

b. 菲涅尔衍射

在直角坐标系中，在旁轴近似条件下（非指数项中r近似为z）基尔霍夫衍射公式可近似表示为

$$U(x,y)=\frac{\exp(jkz)}{j\lambda z}\iint_s U_0(x_0,y_0)\cdot\exp[jk\frac{(x-x_0)^2+(y-y_0)^2}{2z}]dx_0dy_0$$

称为菲涅耳衍射公式

菲涅耳近似条件

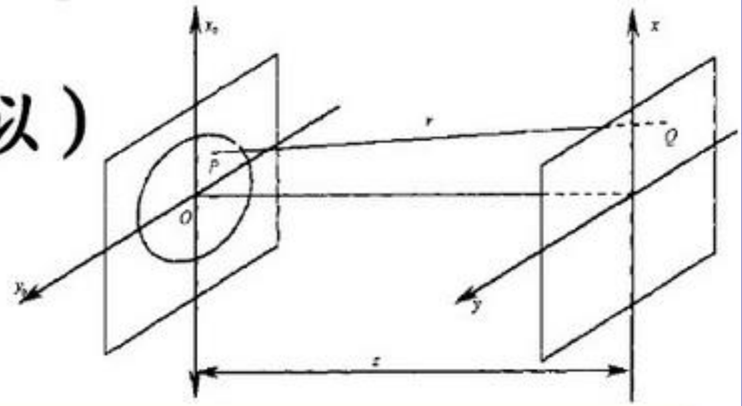
菲涅耳衍射与夫琅和费衍射

c. 夫琅和费衍射

由旁轴近似条件:

$$r \approx z[1+\frac{x^2+y^2}{2z^2}+\frac{x_0^2+y_0^2}{2z^2}-\frac{xx_0+yy_0}{z^2}]$$

当 $z^2 >> x_0^2+y_0^2$ 时（远场近似）



$$r \approx z[1+\frac{x^2+y^2}{2z^2}-\frac{xx_0+yy_0}{z^2}]$$

$$U(x,y)=\frac{\exp(jkz)}{j\lambda z}\exp(jk\frac{x^2+y^2}{2z})\iint_s U_0(x_0,y_0)\cdot\exp[-j\frac{2\pi}{\lambda z}(x_0x+y_0y)]dx_0dy_0$$

称为夫琅禾费衍射公式　　夫琅禾费近似条件

菲涅耳和夫琅和费衍射

f. 夫琅和费衍射与菲涅耳衍射的关系

菲涅耳衍射区

$$r = z + \frac{x^2 + y^2}{2z} + \frac{x_0^2 + y_0^2}{2z} - \frac{x_0 x + y_0 y}{z}$$

夫琅和费衍射区：

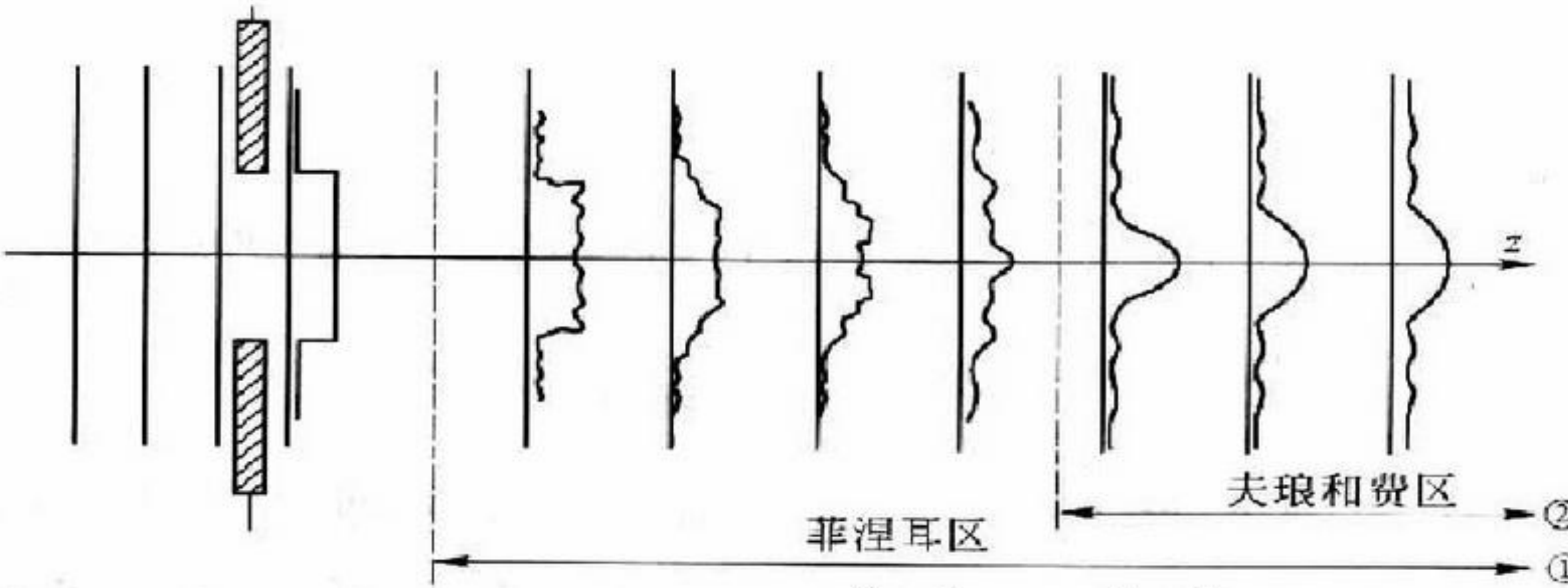
$$r = z + \frac{x_0^2 + y_0^2}{2z} - \frac{x_0 x + y_0 y}{z}$$

夫琅和费衍射区包含在菲涅耳衍射区之内。

但夫琅和费近似从形式上破坏了菲涅耳衍射的卷积关系(空间不变特性)，故不存在专门的传递函数。不过，由于菲涅耳衍射区包含了夫琅和费衍射区，故其衍射过程的传递函数也适用于夫琅和费衍射。

菲涅耳和夫琅和费衍射

夫琅和费衍射与菲涅耳衍射的关系



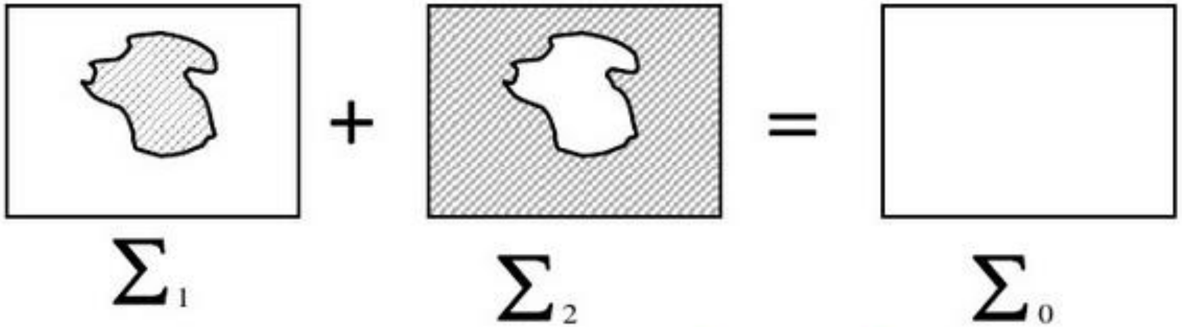
$$r_{01} = \frac{x_1^2+y_1^2}{2z} + z + \frac{x_0^2+y_0^2}{2z} - \frac{x_0x_1+y_0y_1}{z}$$

① ②

讨论两类衍射用的几何示意图

菲涅耳和夫琅和费衍射

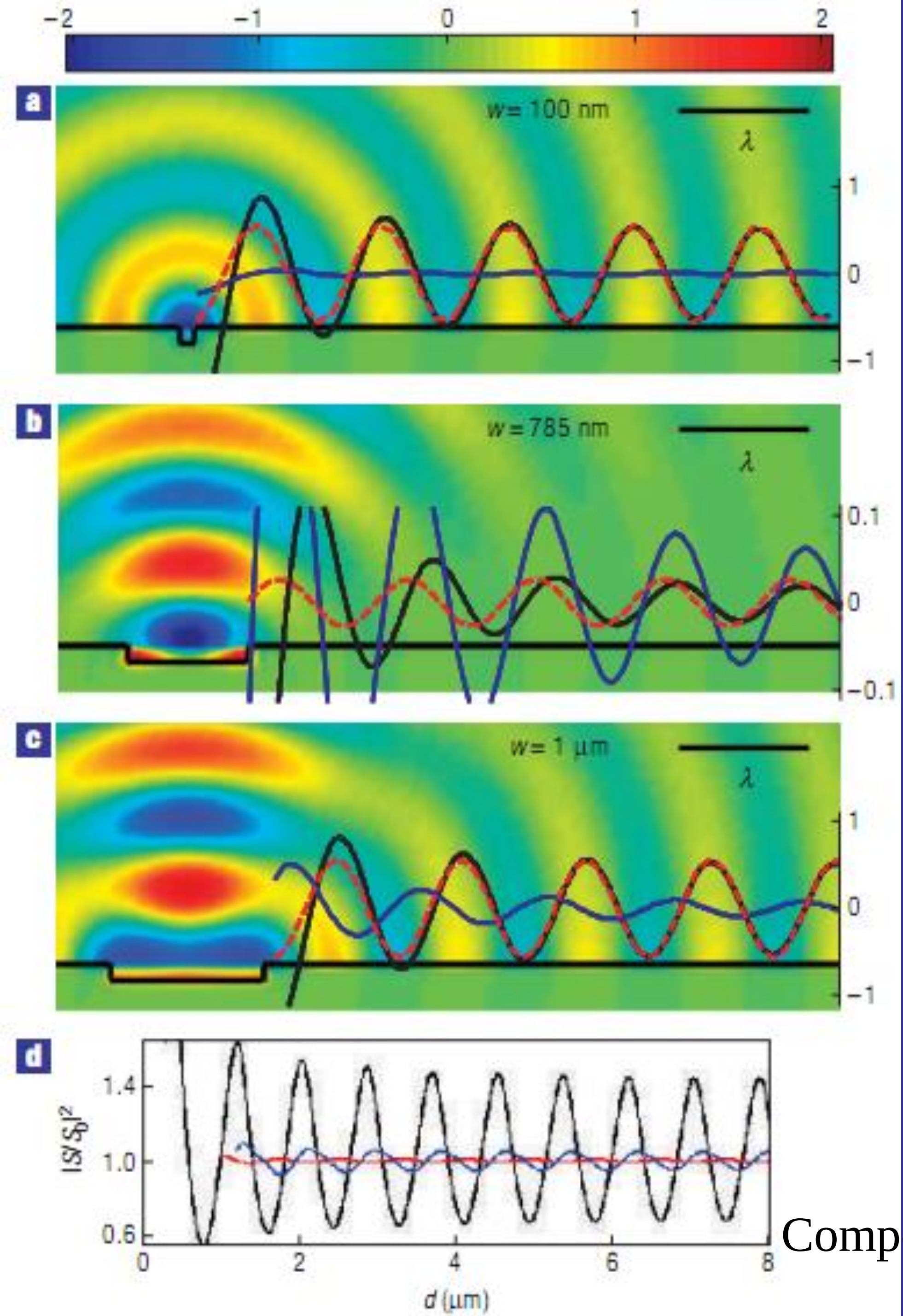
巴俾涅原理



互补屏 Σ_1 和 Σ_2 各自在衍射场中产生的复振幅之和等于衍射屏 Σ_0 产生的复振幅，这种现象称为巴俾涅原理。

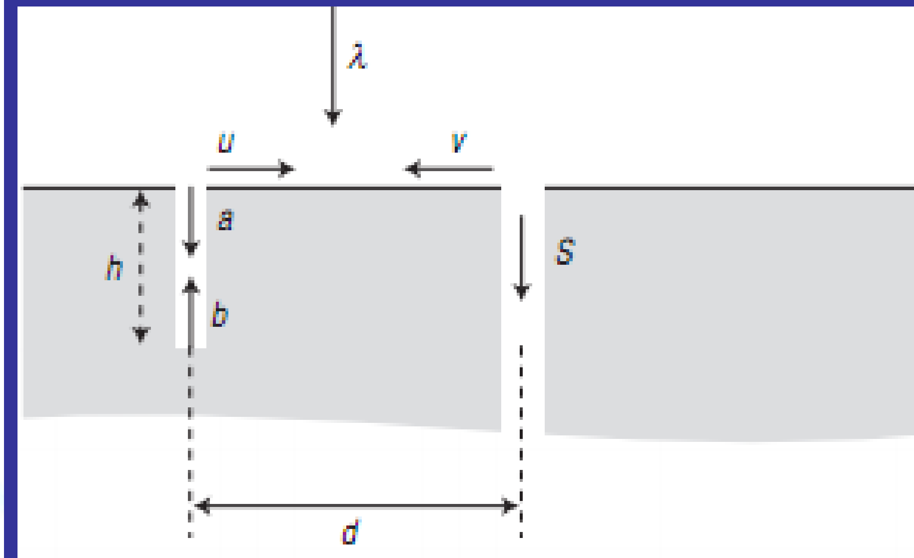
巴俾涅原理可用基尔霍夫衍射公式证明：

$$\iint_{\Sigma_1}[\cdots]dS+\iint_{\Sigma_2}[\cdots]dS=\iint_{\Sigma_0}[\cdots]dS$$



Creeping waves

Nature Physics 2, 551 (2006).



Black line: RCWA calculated curve

Red line: SPP-model

Blue line: CDEW-model which completely fails at predicting either the magnitude of oscillations, or their phase, particularly for the small-width case.

Composite diffracted evanescent waves (CDEW)

等离激元的经典描述

设电子气相对与正电背景的位移为x，则产生的电场为：

$$E = nex/\varepsilon_0$$

作用在每个电子上的恢复力为$-eE$，电子气的运动方程为：

$$nm\frac{d^2x}{dt^2} = -neE = -\frac{n^2e^2x}{\varepsilon_0}$$

$$\frac{d^2x}{dt^2} + \varpi_p^2 x = 0$$

其中：$\varpi_p = (\frac{ne^2}{m\varepsilon_0})^{1/2}$ $\qquad \omega_p^2 = \frac{ne^2}{\varepsilon_0 m}$

对应于频率为 ω_p的简谐振动的运动方程！

在量子理论中，其振荡的能量ω_p是量子化的，其能量量子称为等离激元。