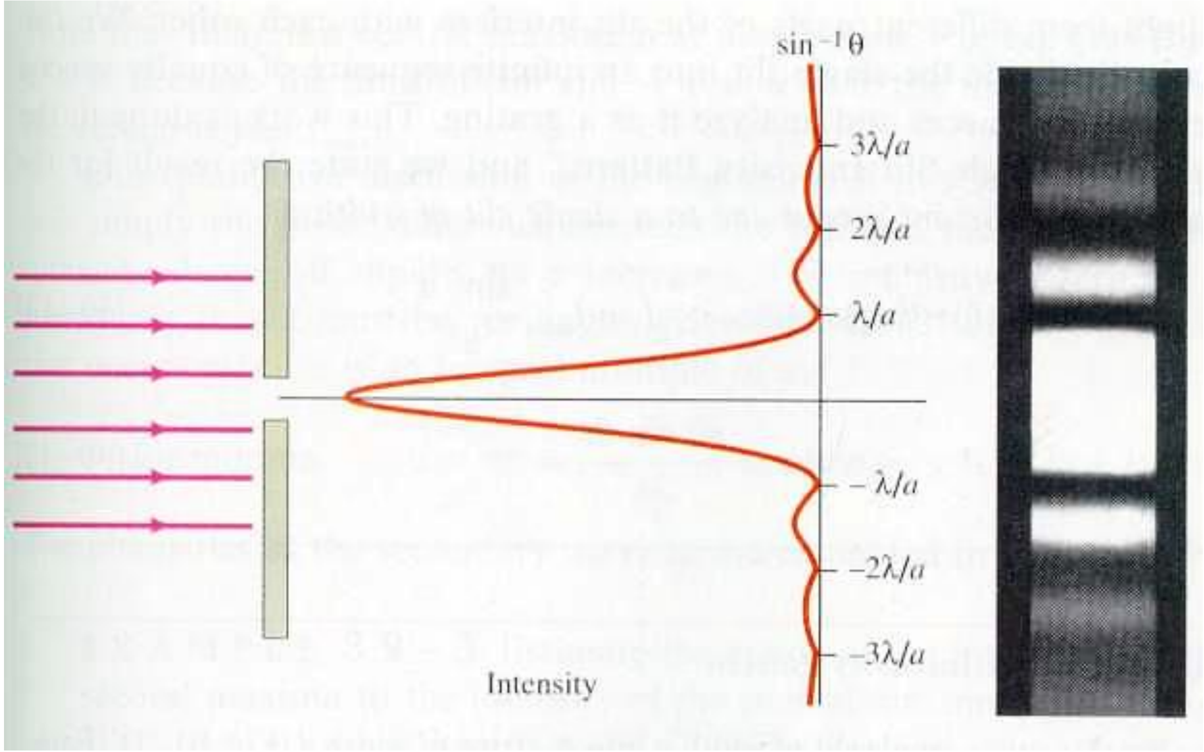
X-射线衍射在材料晶体结构解析中的应用

刘志国

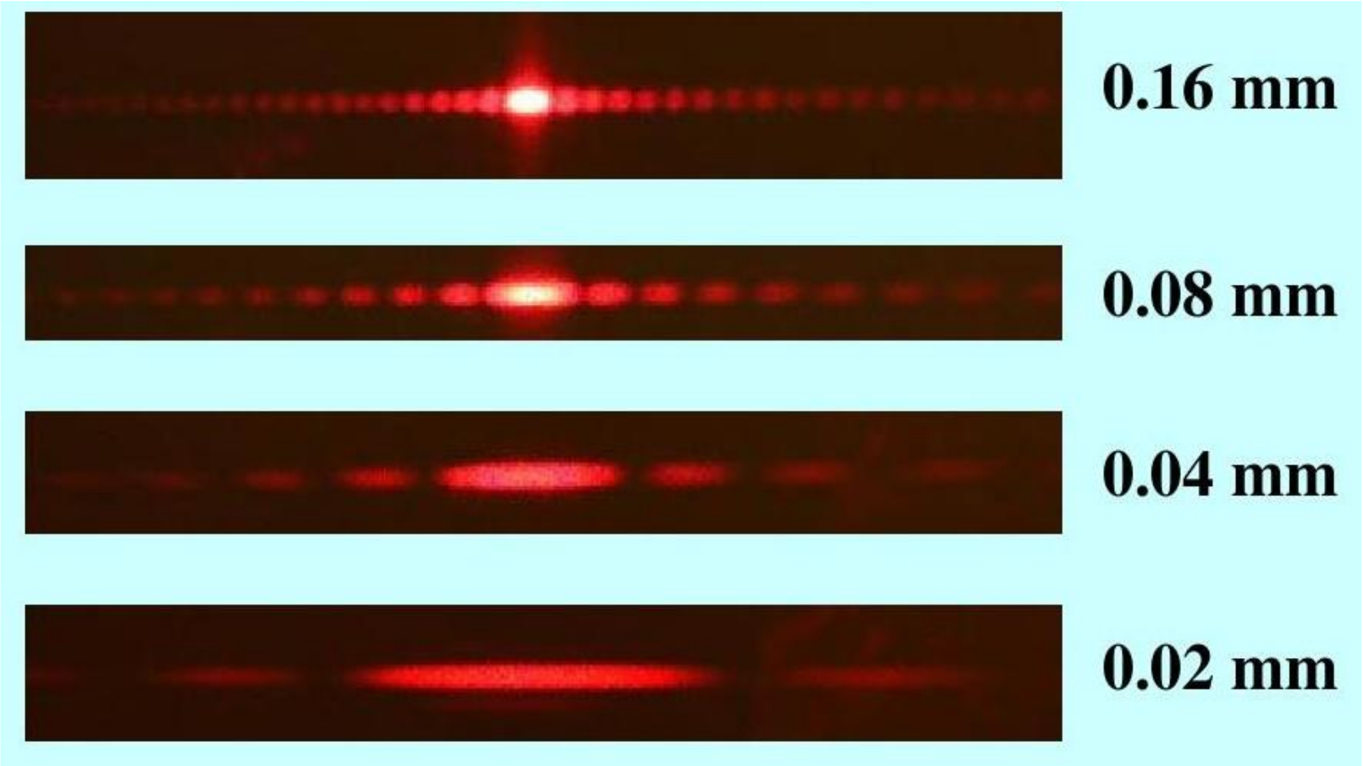
单缝衍射



暗纹条件 $a\sin\theta = k\lambda \quad k = \pm 1, \pm 2, \pm 3, \ldots\ldots$

中央明纹的角宽度 $\Delta\theta_1 = 2\arcsin\dfrac{\lambda}{a} \approx 2\dfrac{\lambda}{a}$

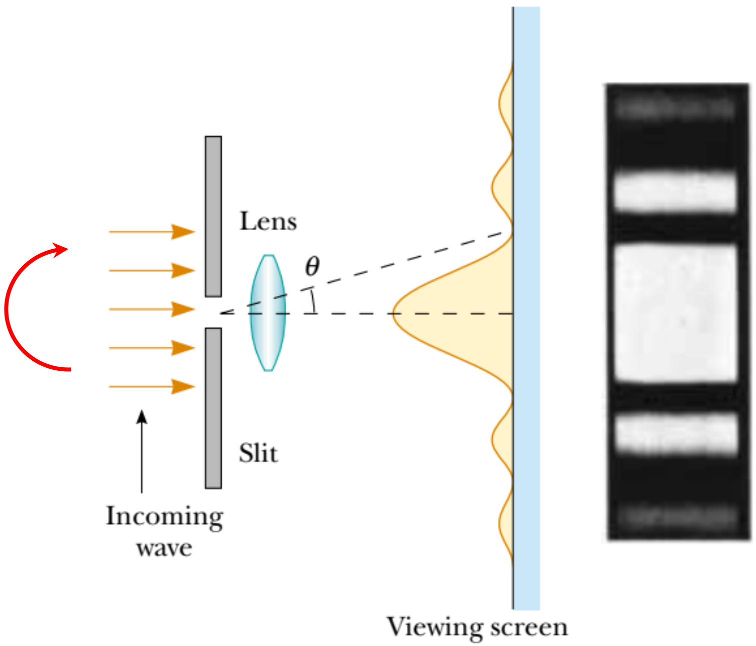
单缝宽度对衍射条纹的影响

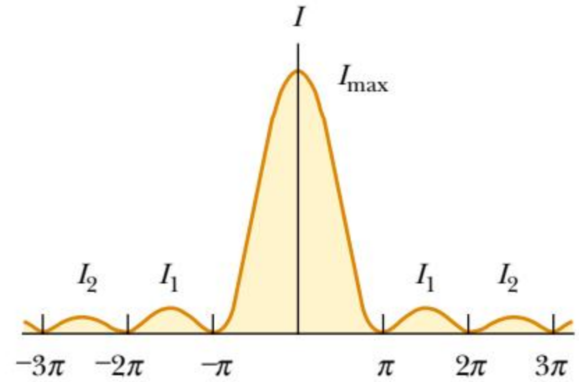


随着单缝宽度的减小，衍射条纹的宽度逐渐增加。通过中央明纹的宽度Δx、透镜的焦距f和光的波长λ，可以计算出单缝的宽度。

$$\Delta\theta_1 = \frac{\Delta x}{f} \approx 2\frac{\lambda}{a} \qquad a = 2\frac{f\lambda}{\Delta x}$$

单缝方向对衍射条纹的影响

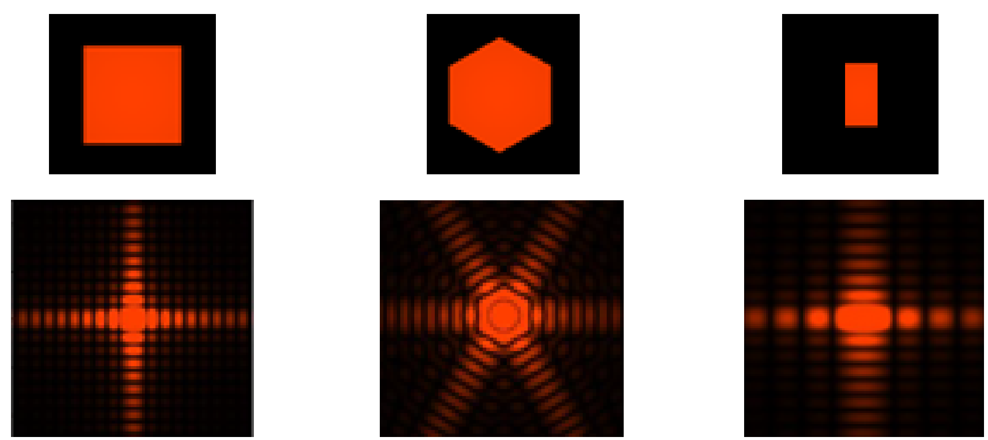




如果单缝绕着透镜的光轴转过90°，衍射条纹也会转过90°。

衍射只会沿着受单缝限制的方向发生，根据衍射条纹可判断单缝的方向。

从衍射图案可以判断衍射屏的形状



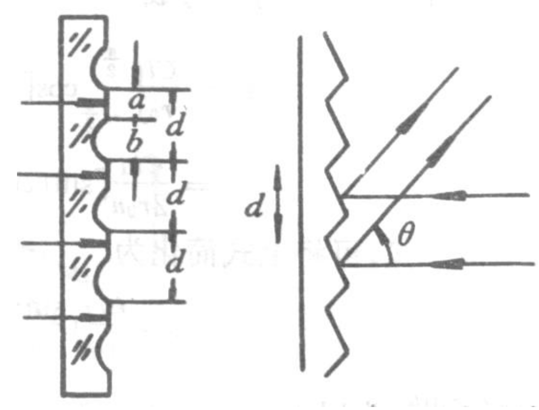
光栅衍射

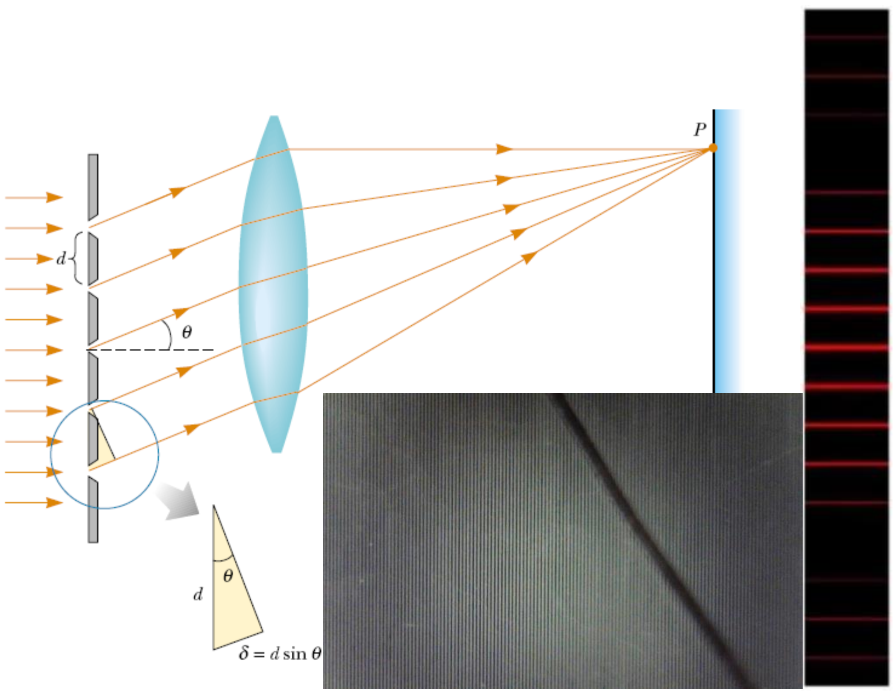
光栅：具有空间**周期性**的衍射装置

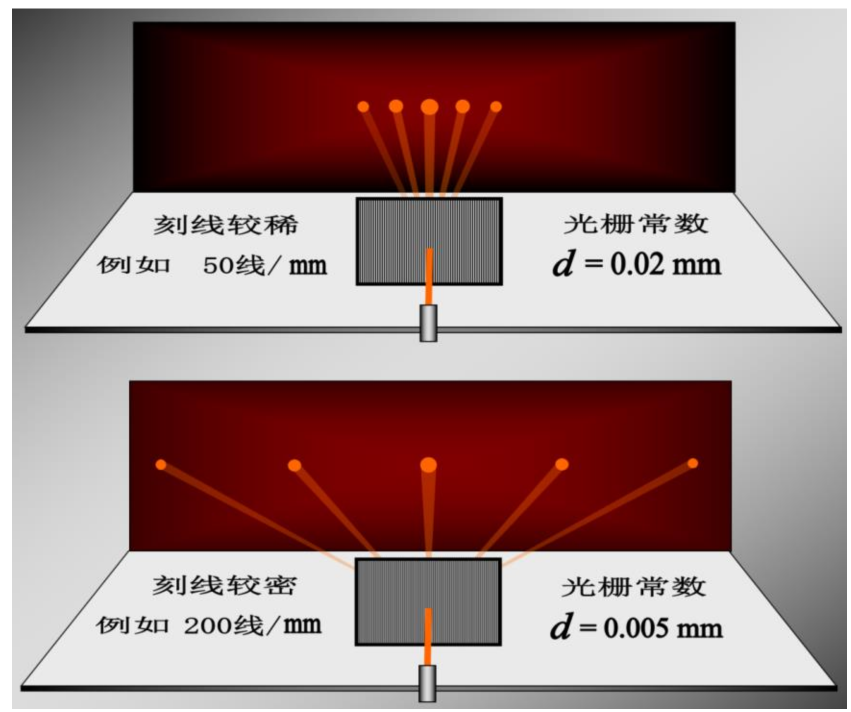
缝间距为d，$\boldsymbol{d = a + b}$ 称为**光栅常数**

光栅方程 $(a+b)\sin\theta = k\lambda \qquad k = 0, \pm1, \pm2, \ldots$

根据衍射图案可计算出光栅常数（周期）







光栅的缺级现象

光栅方程

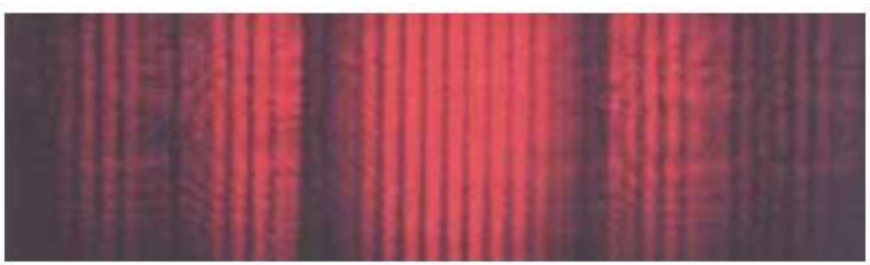
$$(a+b)\sin\theta = k\lambda \qquad k=0,\pm1,\pm2,\ldots$$

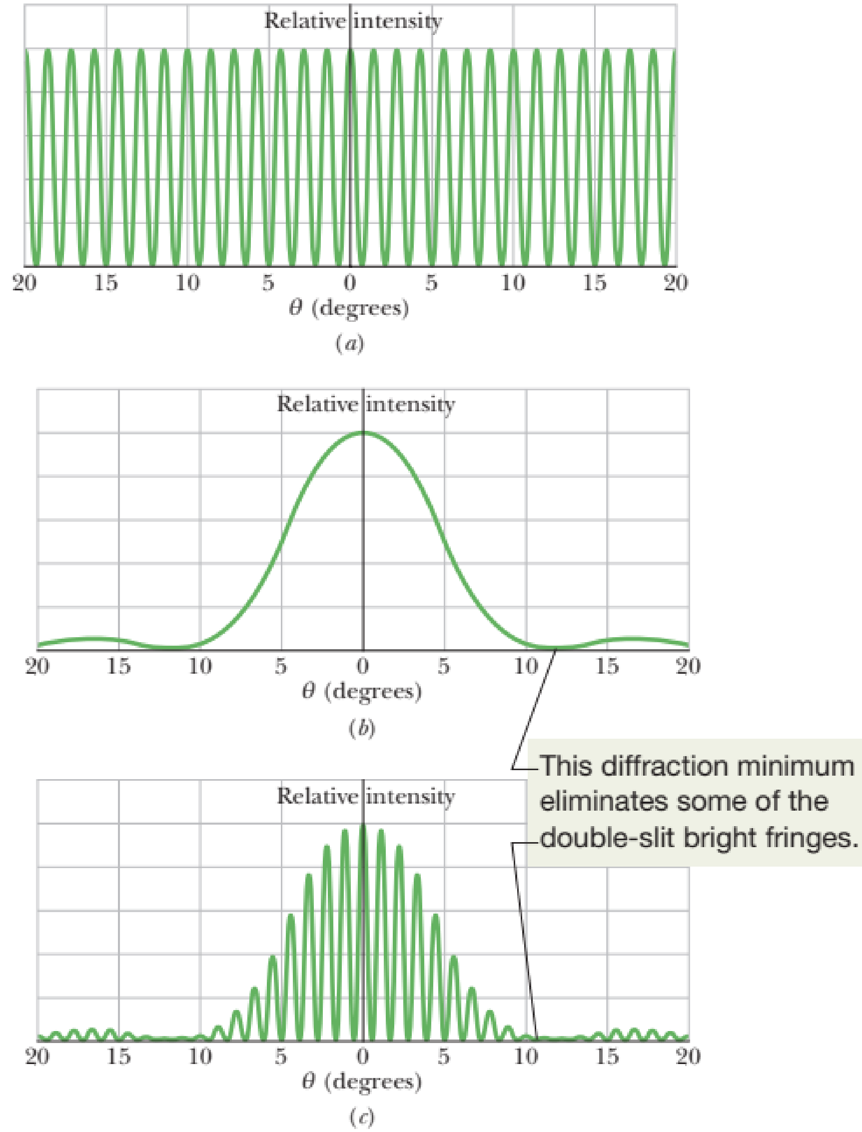
单缝衍射暗纹条件

$$a\sin\theta = k'\lambda \qquad k'=\pm1,\pm2,\ldots$$

同时满足，则第k级亮条纹**缺级**。

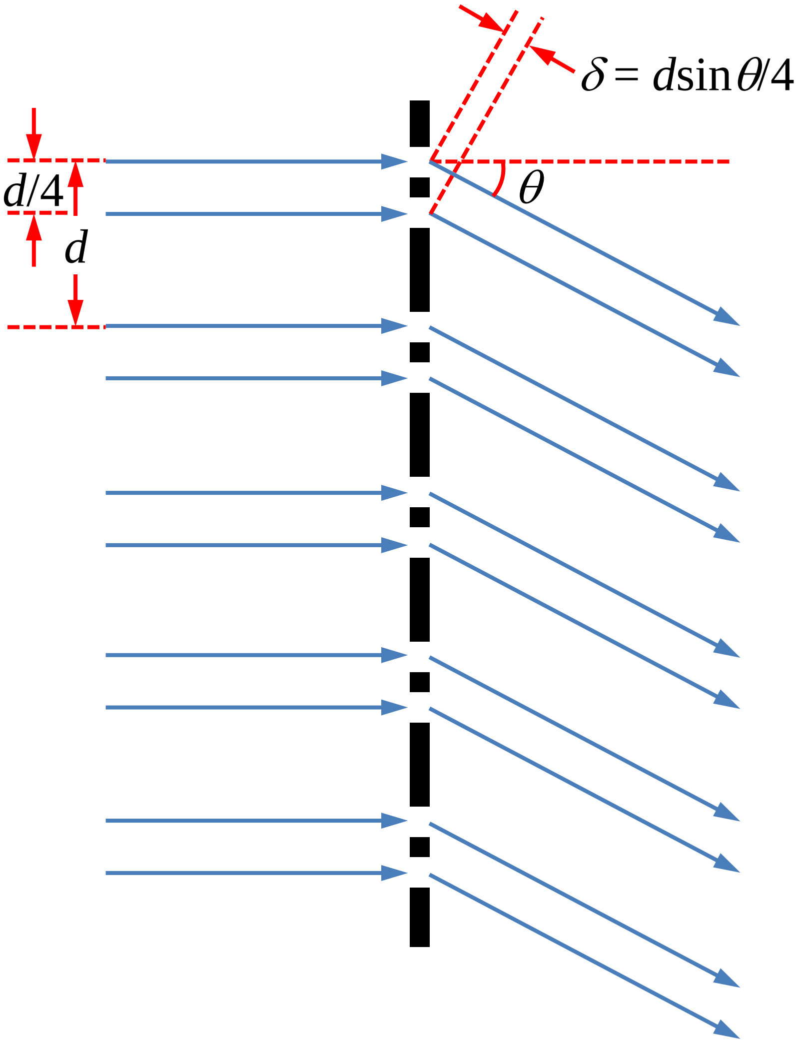
$$\frac{a+b}{a}=\frac{k}{k'}$$





从缺级现象可判断a与$a+b$的关系

光栅的缺级现象



如果光栅存在一些细节结构，也可能造成缺级现象

光栅方程

$$d\sin\theta = k\lambda \qquad k = 0, \pm 1, \pm 2, \ldots$$

$$\frac{d}{4}\sin\theta = \frac{k}{4}\lambda$$

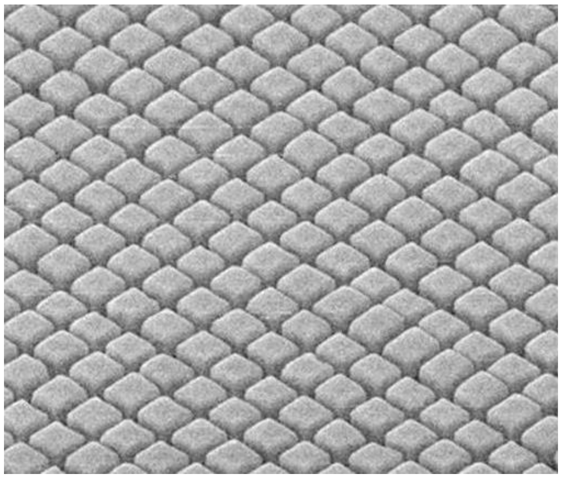
当*k* = ±2，±6，……时

$$\frac{d}{4}\sin\theta = \pm\frac{1}{2}\lambda, \pm\frac{3}{2}\lambda, \ldots\ldots$$

第*k*级缺级

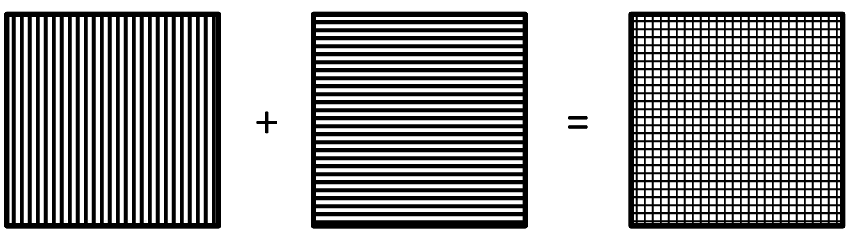
二维光栅

二维的空间周期性结构



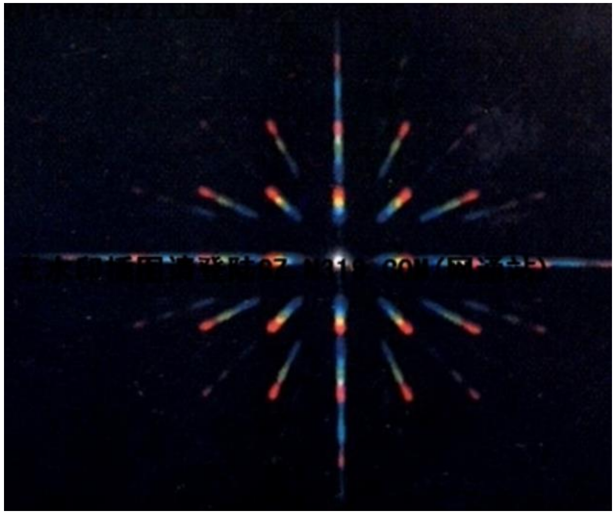
手机屏幕

相当于把两个一维光栅叠起来

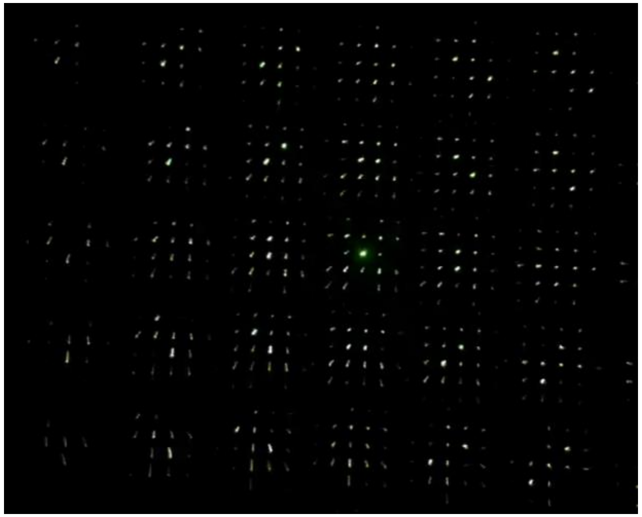


“满天星”激光笔

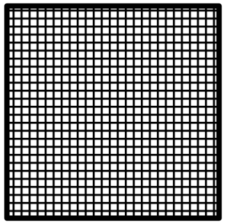
衍射图案和光栅常数的关系



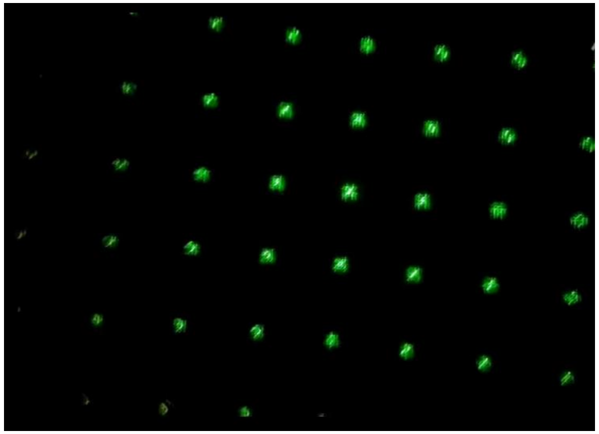
白光



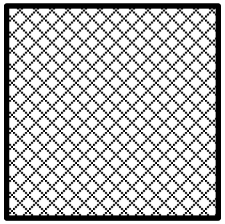
$$d\sin\theta = k\lambda \qquad k = 0, \pm 1, \pm 2, \ldots$$

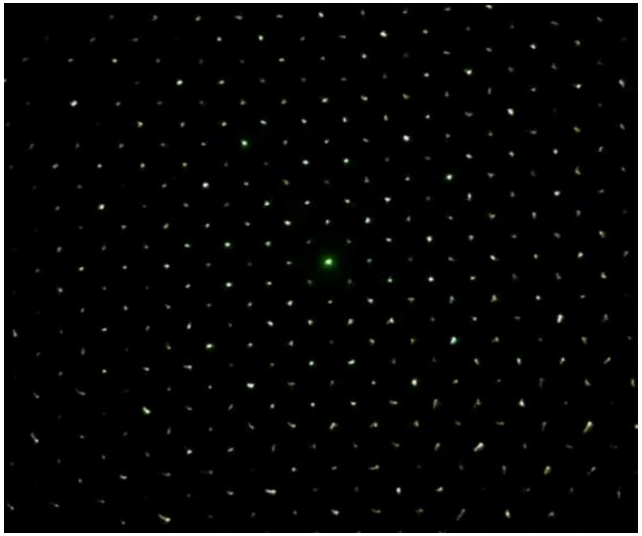


***d*小**



***d*大**





晶体——天然的三维光栅

问题的引出——X-射线是波还是粒子流？

1895年，德国物理学家伦琴发现了X射线；

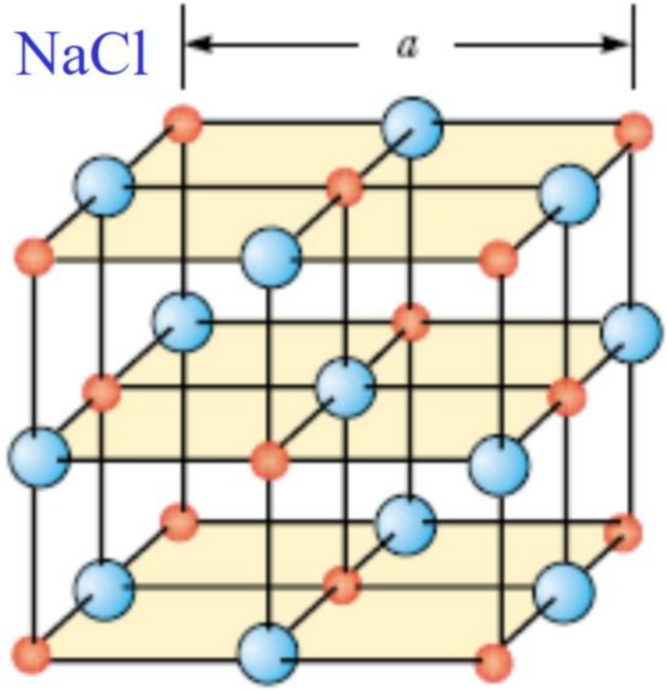
普通光栅看不到衍射现象，无法确定其属性；

只有障碍物尺寸和波长差不多时，衍射现象才明显！

$$(a+b)\sin\theta = k\lambda \qquad k = 0,\pm1,\pm2,\ldots$$

1912年，德国物理学家劳厄提出，利用晶体作为三维光栅，来观察X-射线的衍射现象，并获得了成功。

NaCl



X-射线波长：Cu K_α线，

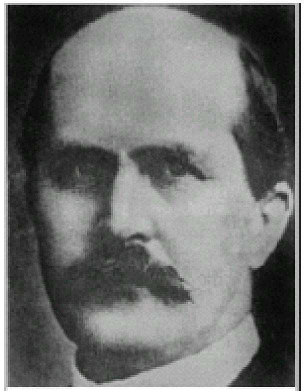
λ = **0.15418 nm**

晶体中原子间距：

$d \sim$ **0.1 nm**量级

布拉格公式

1913年，英国物理学家布拉格父子注意到了劳厄的工作，并提出了著名的布拉格公式



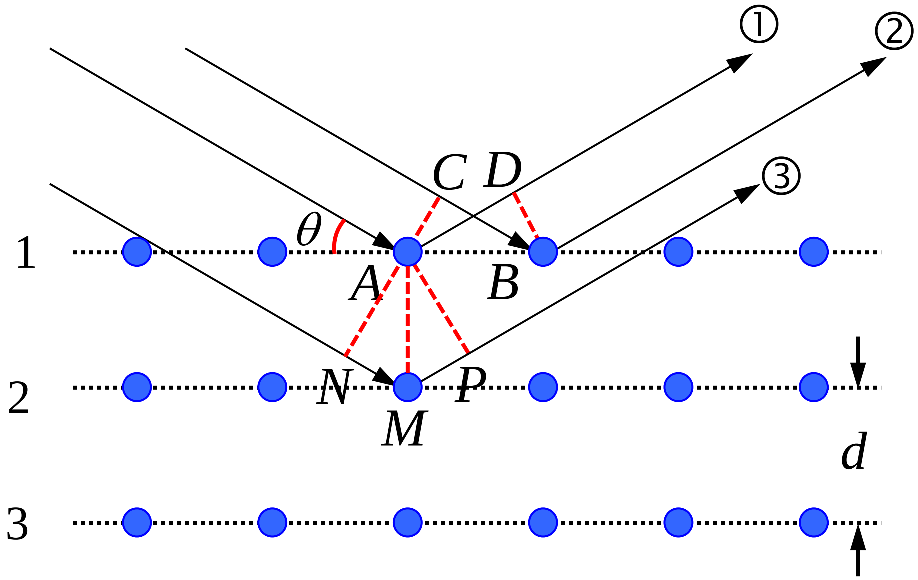
布喇格，W. H.

布喇格，W. L.

晶体由许多晶面组成

$$2d\sin\theta = n\lambda \quad n = 1,2,3,\ldots\ldots$$

干涉相长



a. 同一晶面散射的光，反射线方向加强

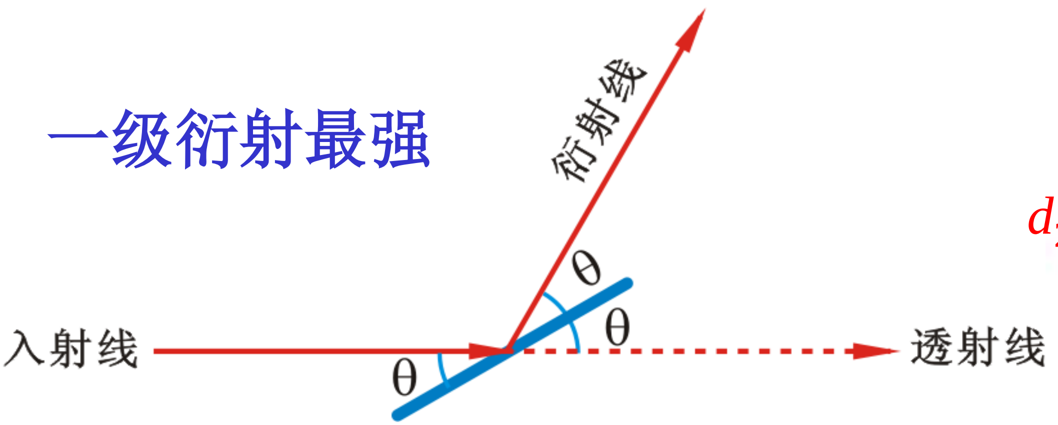
b. 不同晶面反射光的光程差

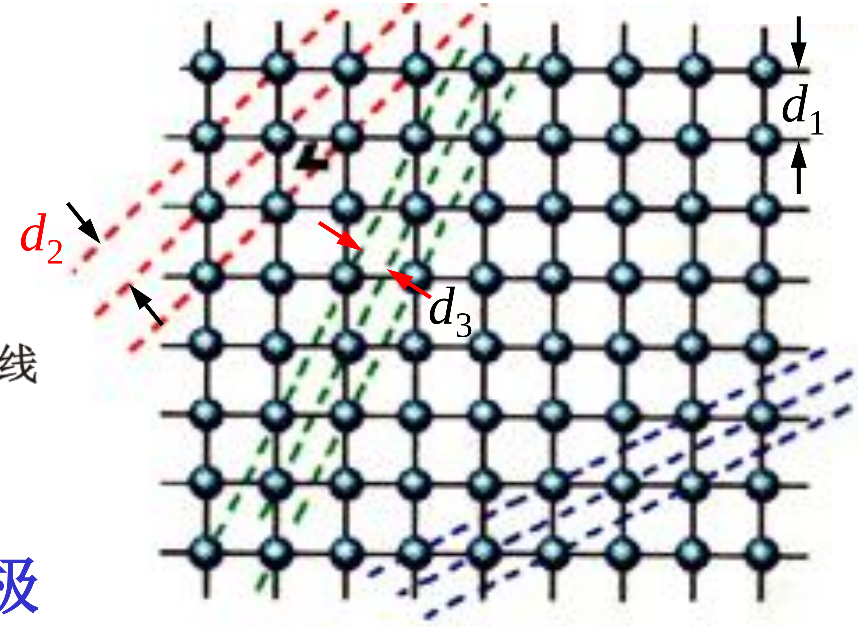
$$\delta = NM + MP = 2d\sin\theta = n\lambda$$

$$n = 1, 2, 3, \ldots\ldots$$

晶体结构解析

一级衍射最强





固定入射X-射线的方向，转动晶体，在与入射线成**2*θ***方向观察到衍射主极

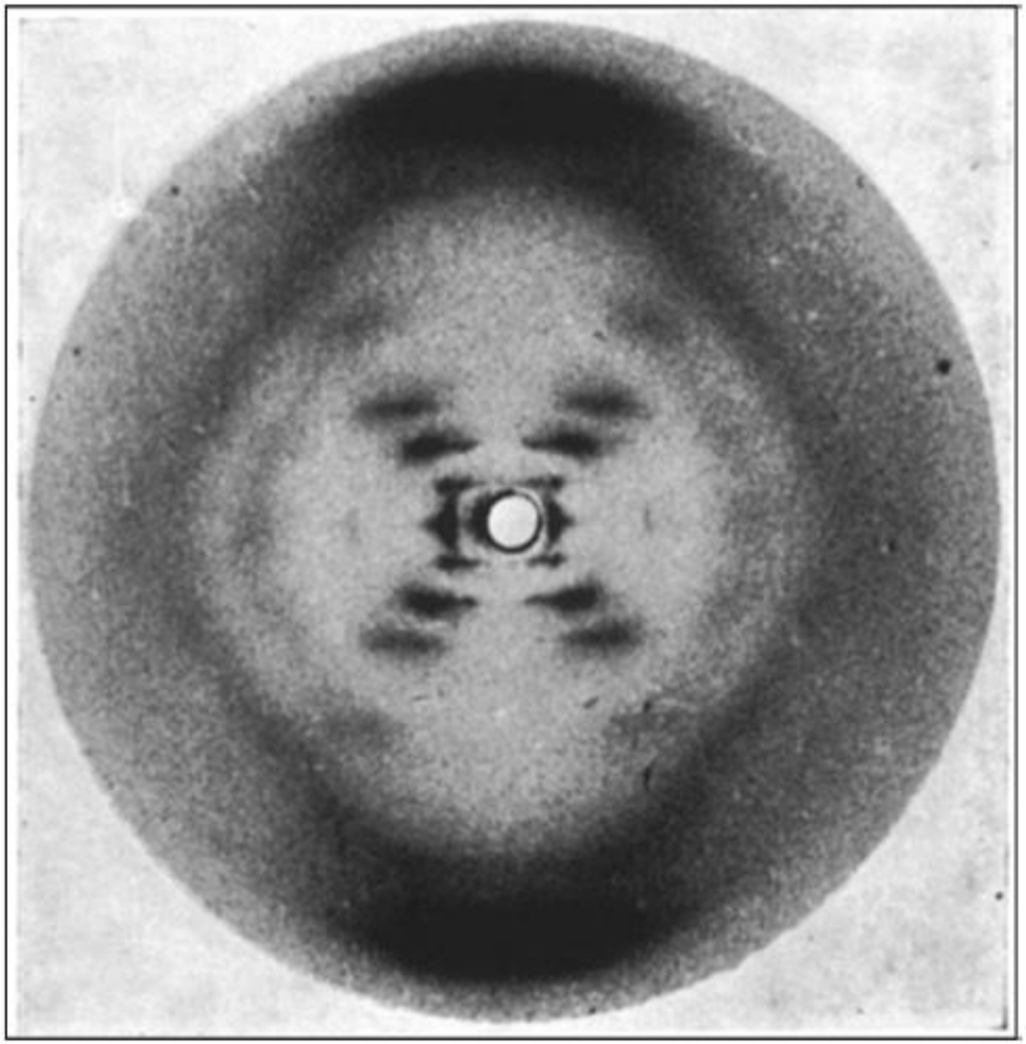
$$\boxed{\begin{aligned} d_2 &= d_1/\sqrt{2} \\ d_3 &= d_1/\sqrt{5} \end{aligned}}$$

$$2d_1\sin\theta_1 = \lambda \qquad 2d_2\sin\theta_2 = \lambda \qquad 2d_3\sin\theta_3 = \lambda$$

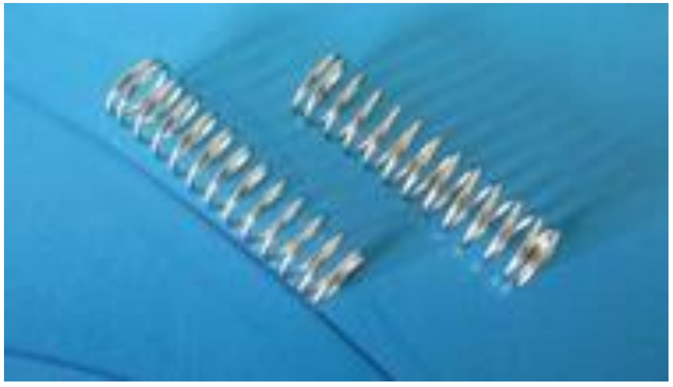
$$d_1 : d_2 : d_3 = \frac{1}{\sin\theta_1} : \frac{1}{\sin\theta_2} : \frac{1}{\sin\theta_3}$$ 测得 ***θ*₁**、***θ*₂**、 ***θ*₃**

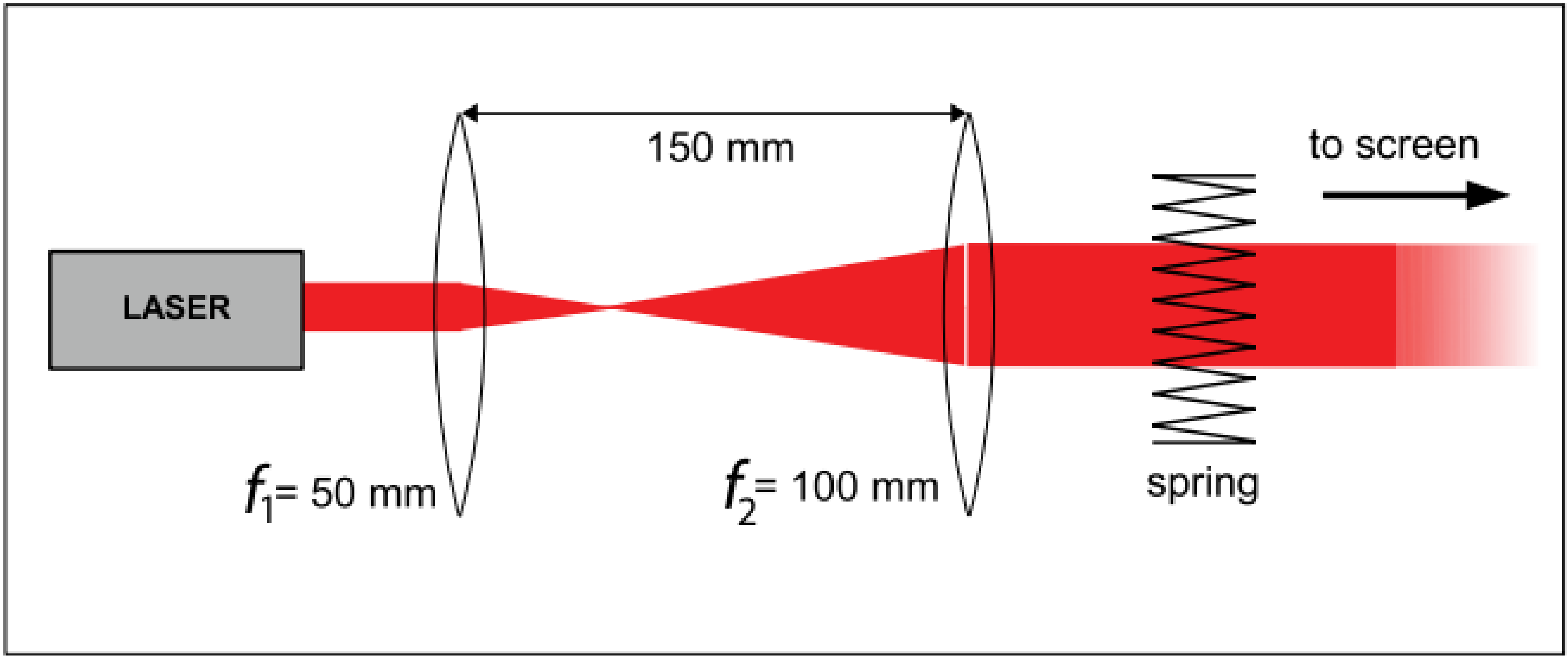
若 $d_1 : d_2 : d_3 : \ldots\ldots = 1 : \dfrac{1}{\sqrt{2}} : \dfrac{1}{\sqrt{5}} : \ldots\ldots$ 则晶体结构为立方

一个实例——某种有机分子的X-射线衍射

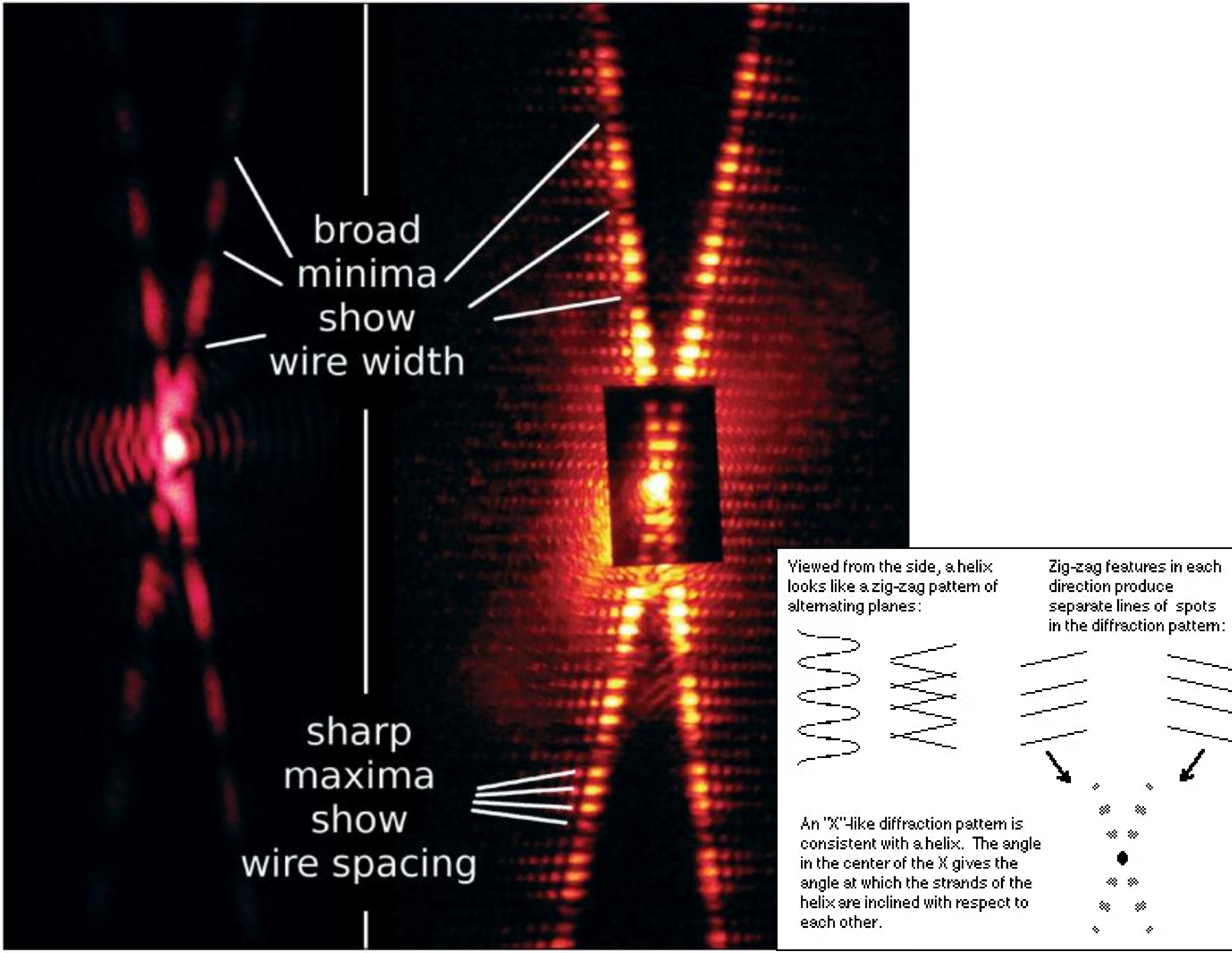


弹簧的衍射



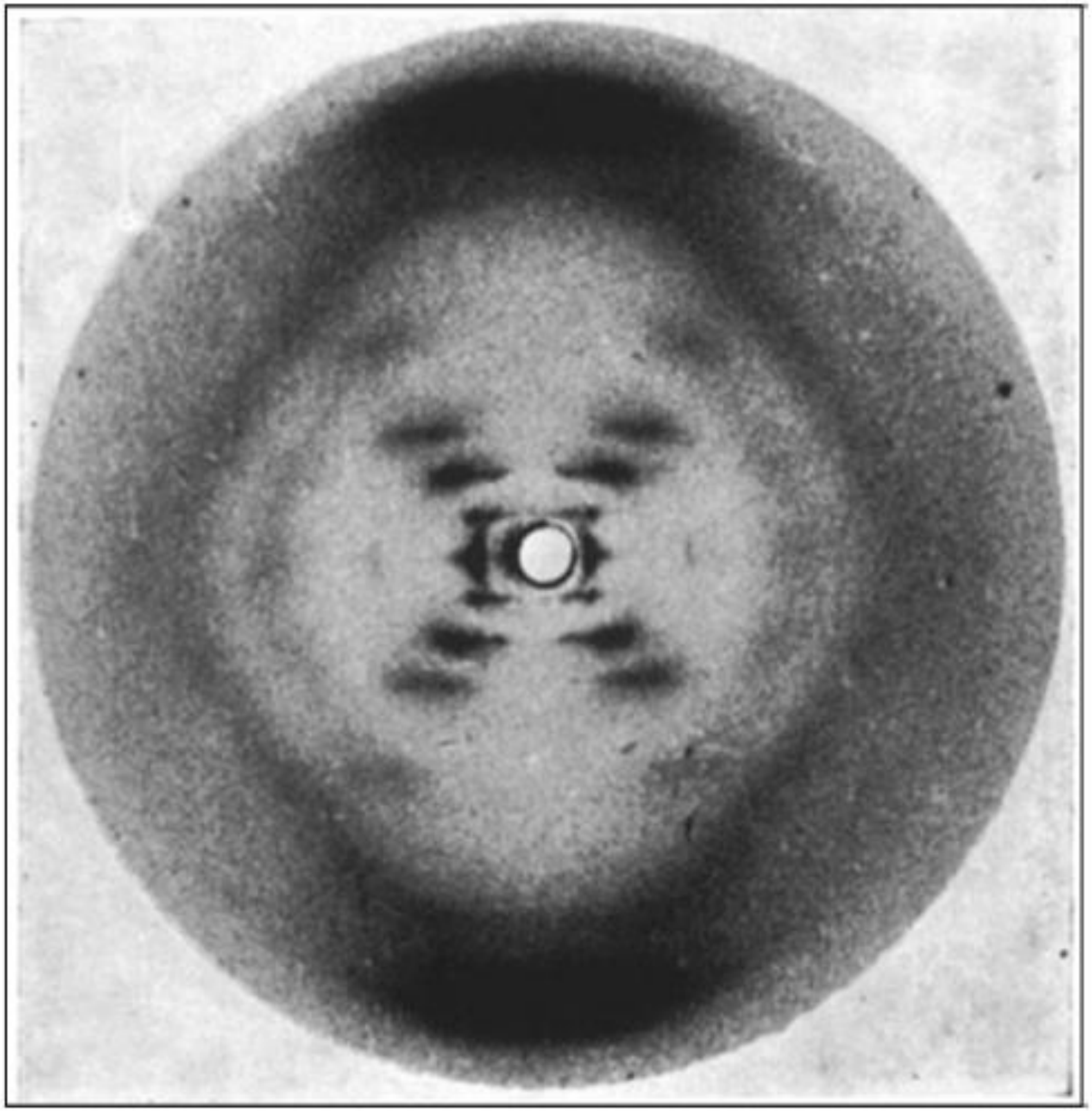


LASER
150 mm
to screen
f_1= 50 mm
f_2= 100 mm
spring

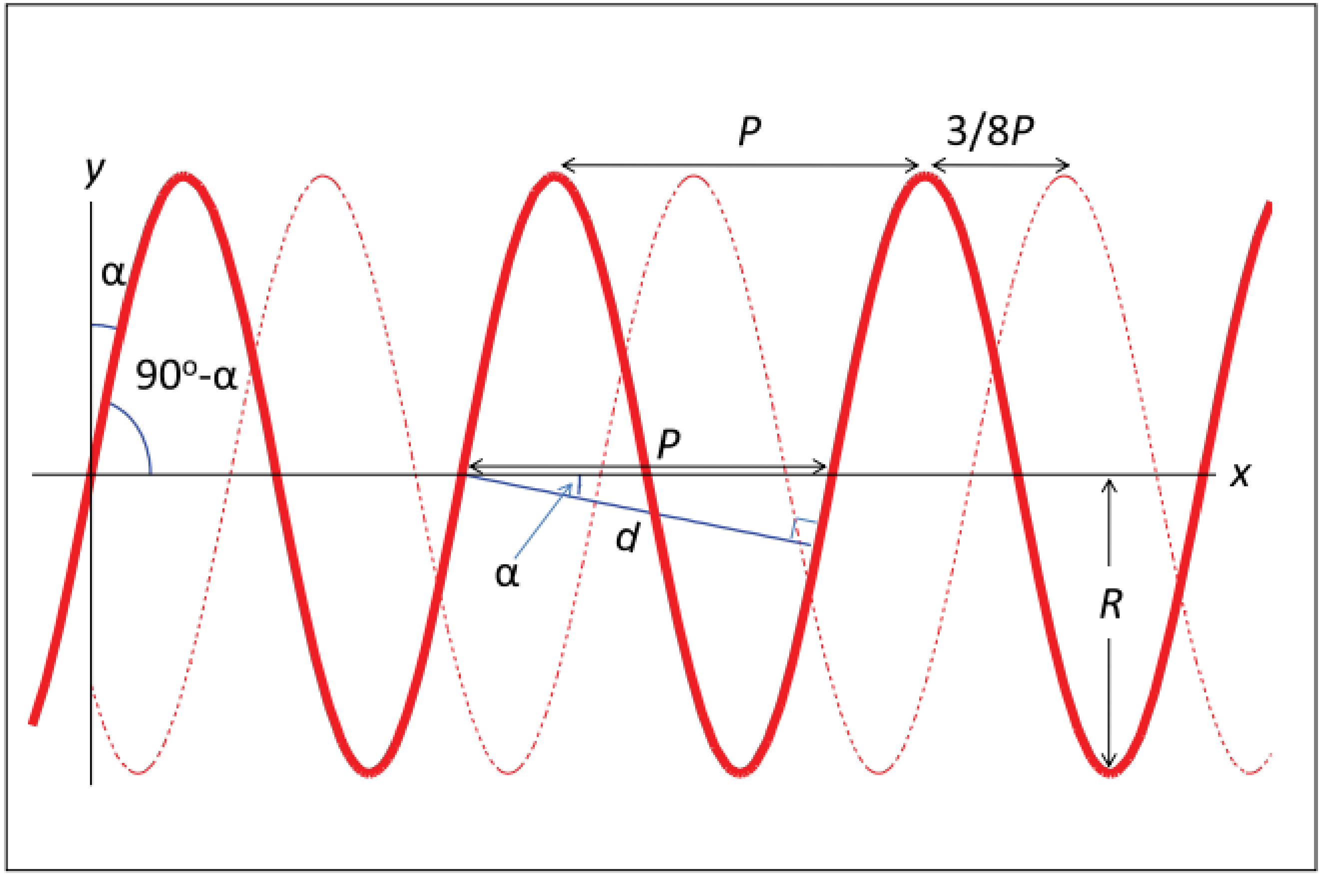


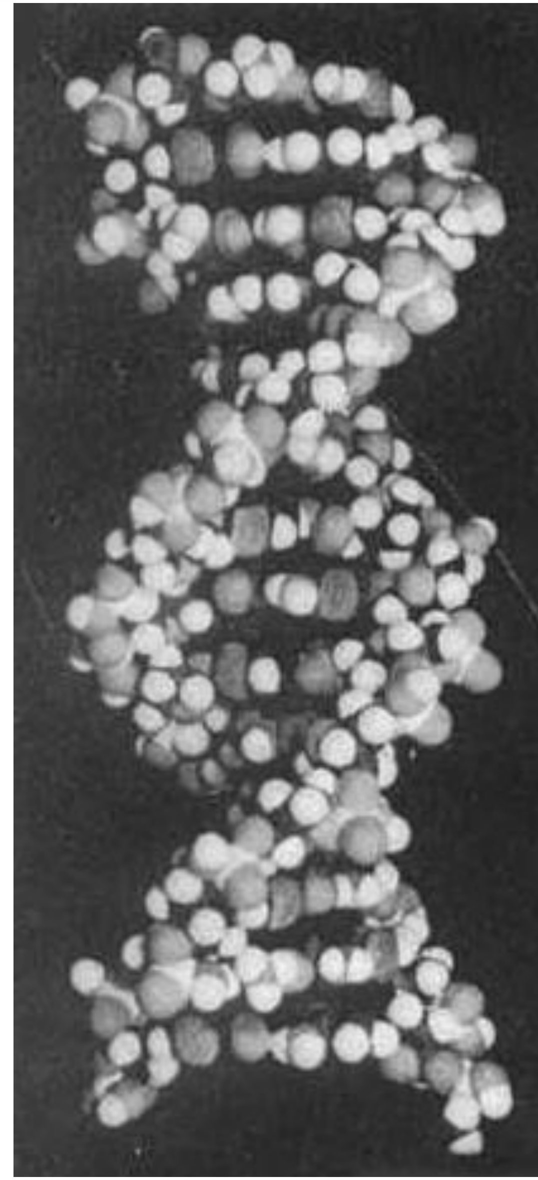
broad minima show wire width
sharp maxima show wire spacing
Viewed from the side, a helix looks like a zig-zag pattern of alternating planes:
Zig-zag features in each direction produce separate lines of spots in the diffraction pattern:
An "X"-like diffraction pattern is consistent with a helix. The angle in the center of the X gives the angle at which the strands of the helix are inclined with respect to each other.

第4级缺级



缺级——双弹簧结构





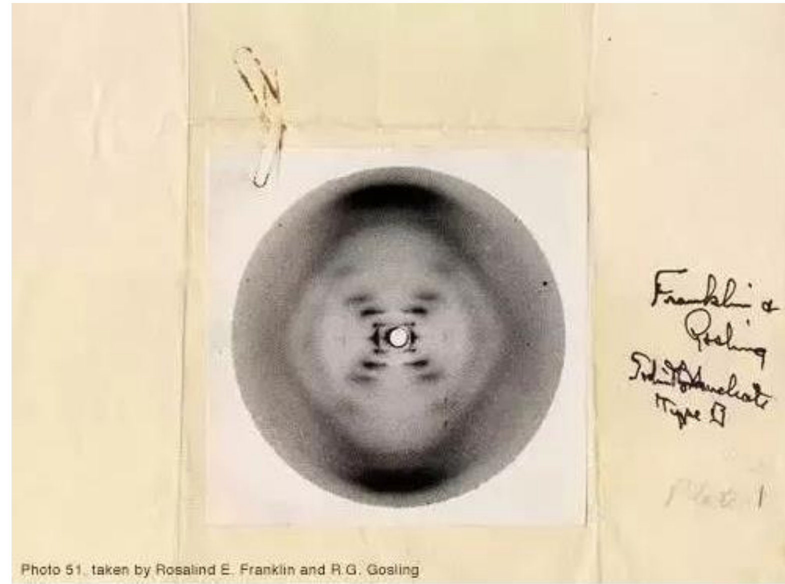
$$P\sin\theta = \pm k\lambda,\ \ \frac{3}{8}P\sin\theta = \pm\frac{3}{8}k\lambda,\ \ k = 1,2,3,\ldots\ldots$$

当k = 4,12,……时, 缺级

Nobel奖级的工作

——DNA分子的双螺旋结构

罗莎琳·富兰克林



B型DNA的X射线晶体衍射照片——“照片51号”

Photo from the Nobel Foundation archive.

Francis Harry Compton Crick

Prize share: 1/3

Photo from the Nobel Foundation archive.

James Dewey Watson

Prize share: 1/3

Photo from the Nobel Foundation archive.

Maurice Hugh Frederick Wilkins

Prize share: 1/3

1962年诺贝尔生理学或医学奖由Francis Harry Compton Crick，James Dewey Watson和Maurice Hugh Frederick Wilkins共同授予“关于核酸分子结构及其对生物材料信息传递的重要性的发现”。

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