像差校正电子显微镜

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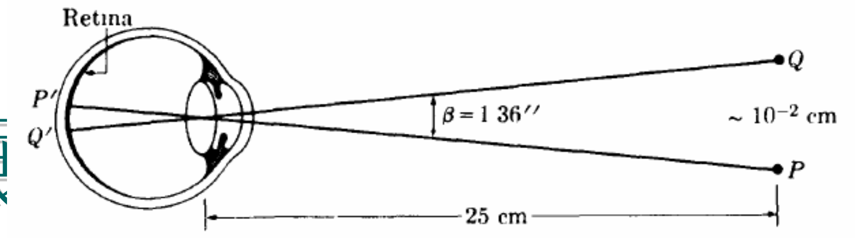
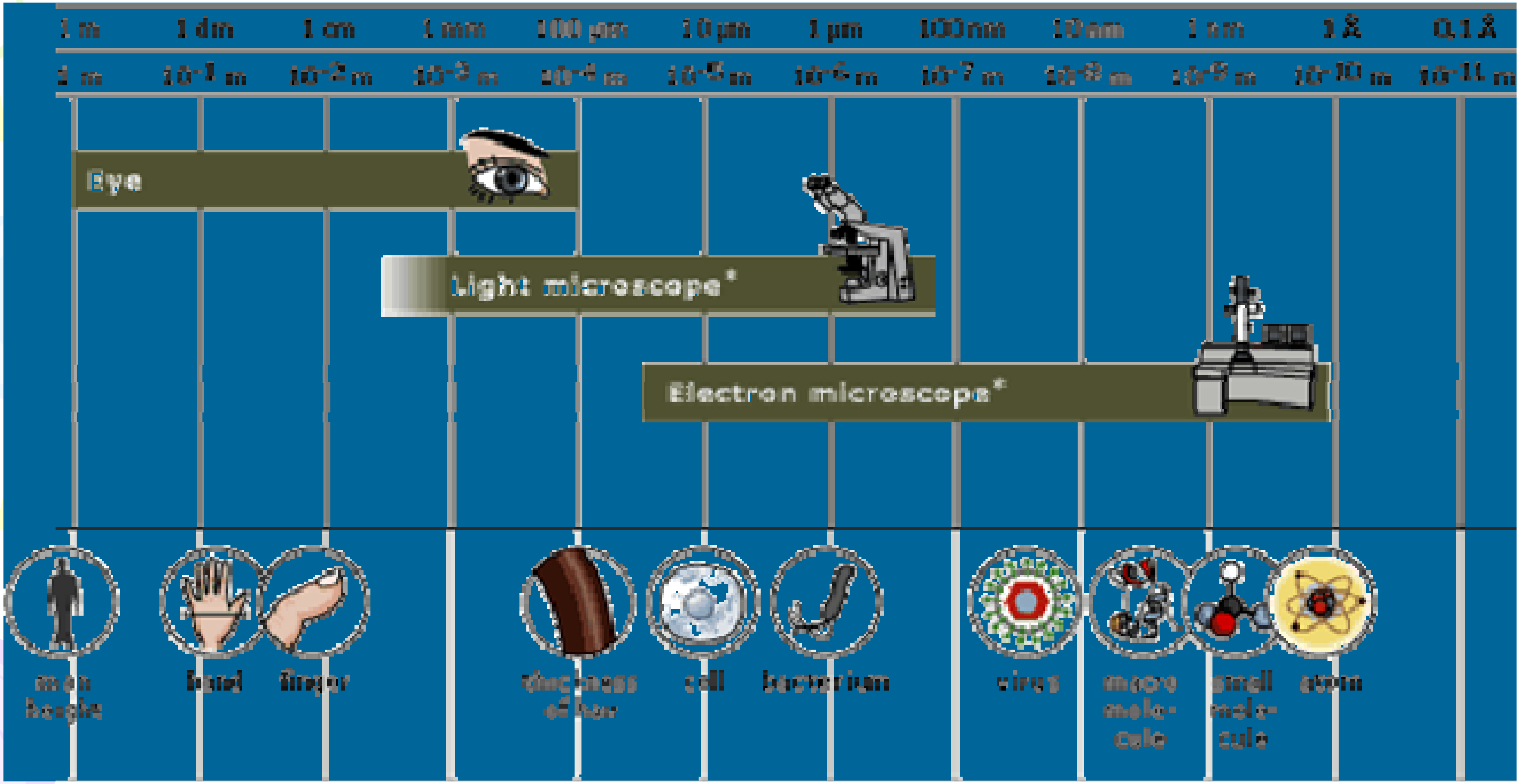
显微能力发展

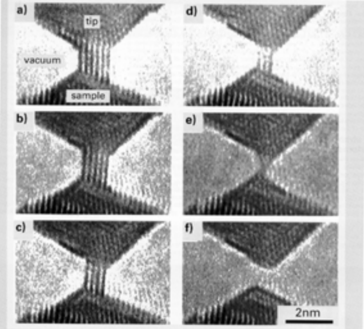
$$d = \lambda / 2n \sin\theta$$

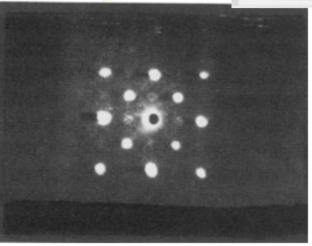




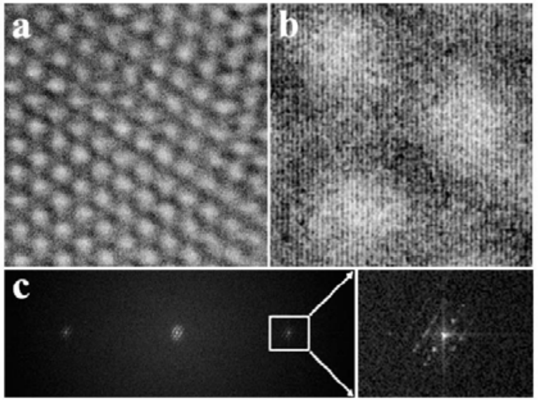
TEM综合能力

In situ

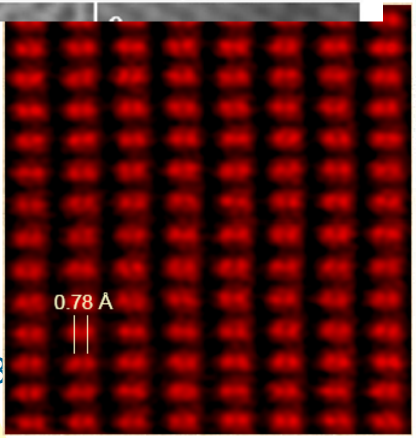




SAED



EH



HREM

2008

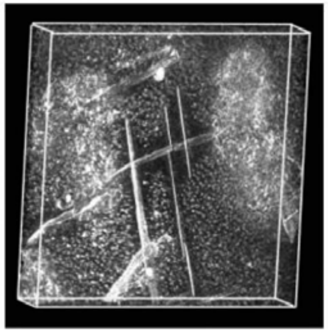
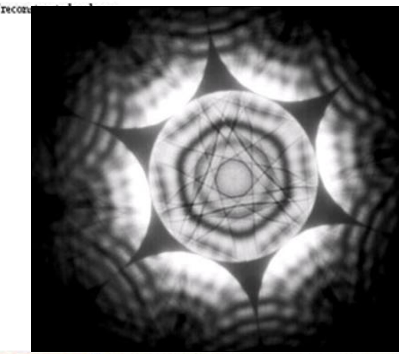


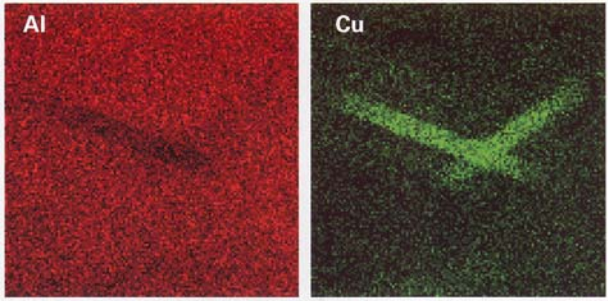
Fig. 3 : Voxel projection of recon

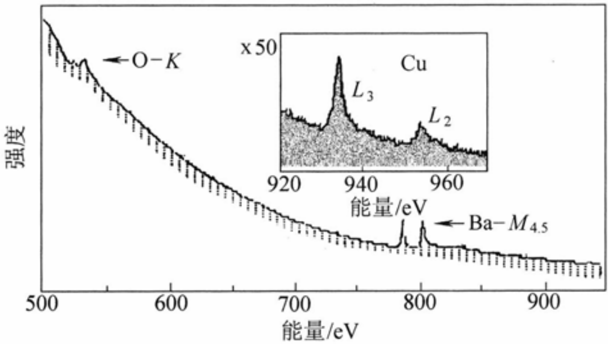
3D

CBED



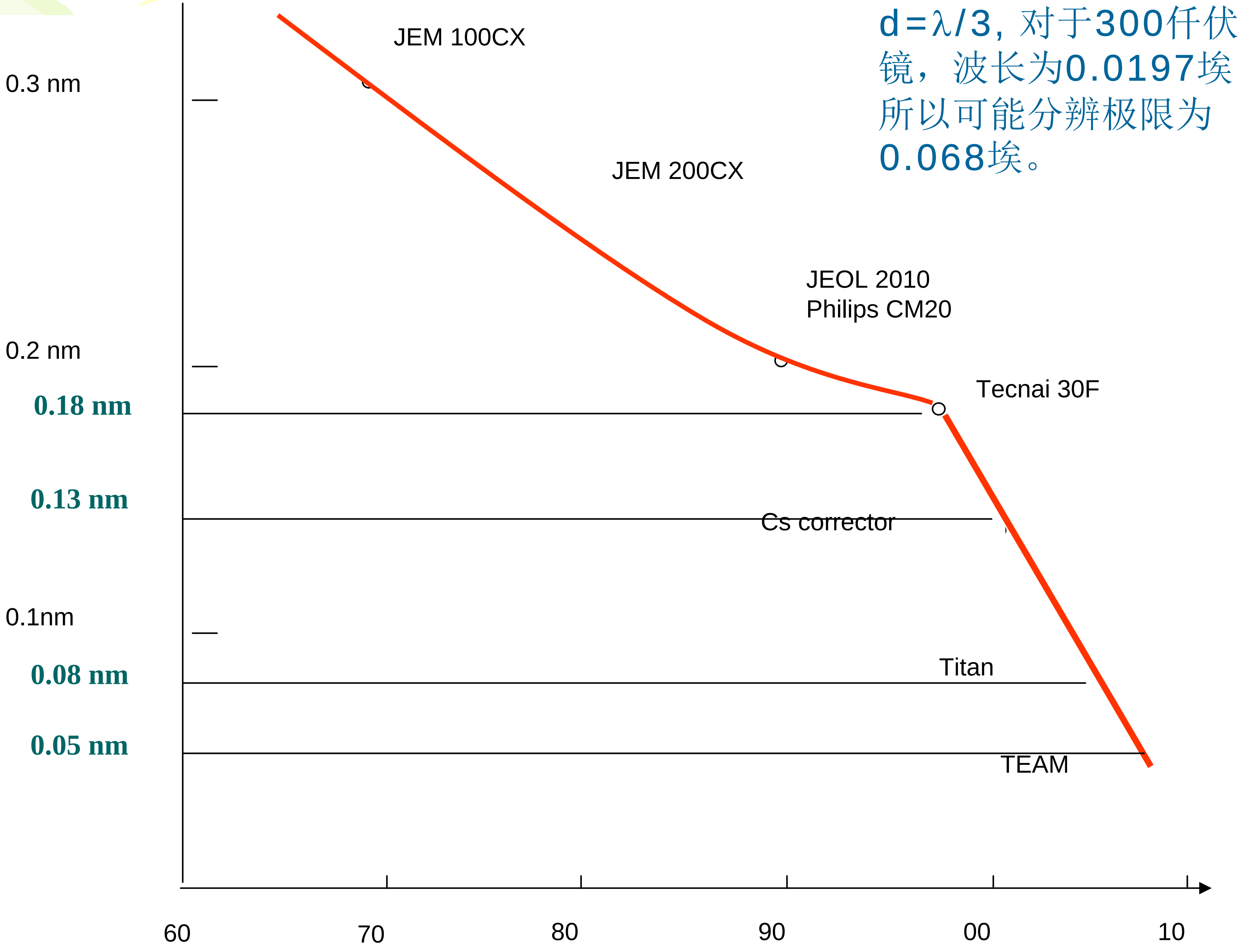
EDX





EELS

d=λ/3，对于300仟伏电镜，波长为0.0197埃，所以可能分辨极限为0.068埃。



50年来透镜电子显微镜分辨能力随时间的改善,近年突飞猛进

象差校正电镜渐趋成熟

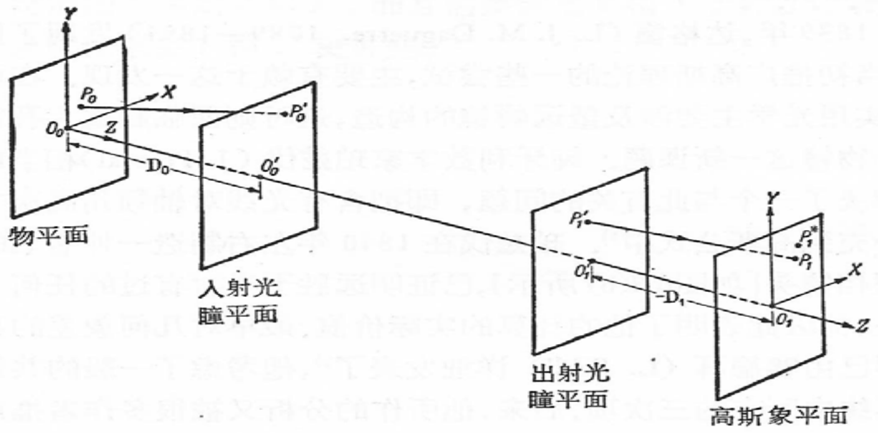
- M.Haider, H.Muller, S.Uhlemann, J.Zach, U.Loebau, and R.Hoeschen: “Prerequisites for a Cc/Cs-corrected ultrahigh-resolution TEM”, Ultramicroscopy 108 (2008) 167.
- O.L.Krivanek, G.J.Corbin, N.Dellby, B.F.Elson, R.J.Keyse, M.F.Murfitt, C.S.Own, Z.S.Szilagyi, J.W.Woodruff: “An EM for the aberration-corrected era”, Ultramicroscopy 108 (2008) 179.
- M.A.O’Keefe: “Seeing atoms with aberration-corrected sub-ÅngstrÖm EM”, Ultramicroscopy 108 (2008) 196.
- H.H.Rose: “Optics of high-performance EM”, Sci. Tech. Adv. Mat., 9 (2008) 014107.

提纲

- 1.　**象差及其测量**
- 1.1　象差
- 1.2　可数值化的实时测量象差
- 2.　**象差校正技术**
- 2.1　系列欠焦像
- 2.2　电子全息
- 2.3　象差校正器
- 3.　**由象差校正电镜拓展的研究**
- 3.1　提高分辨率
- 3.2　减少离位效应
- 3.3　可能看到轻元素
- 3.4　需要扣去非线性成象效应
- 3.5　走向原子柱分辨的成分分析
- 3.6　三维原子分辨STEM

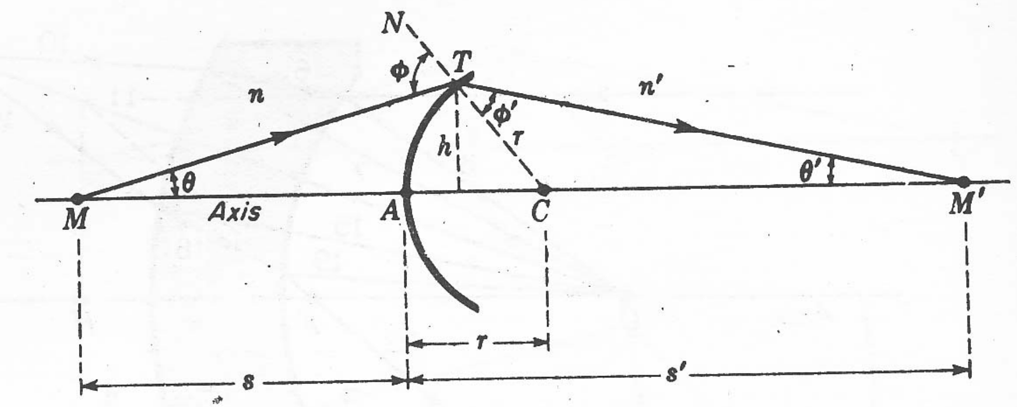
象差及其测量

线象差



- 光线经过光学系统后，一个物点被成像为一个像点。如果只考虑那些位于轴最近邻的点和光线，而忽略与轴的距离或光线与轴的夹角二者的平方项和更高次方项。由此得出的理论通常称高斯光学，或称理想成象。否则，就会出现象差。图中是一个旋转对称光学系统。如果P^*_1是P_0的高斯像，P_1是实际像，则矢量 $\overrightarrow{P_1^* P_1}$ 称为光线的象差，或简称线象差。下面讨论可以看出，线象差不仅局限在高斯像平面，还可以分解为纵向与横向的线象差。

几何线象差

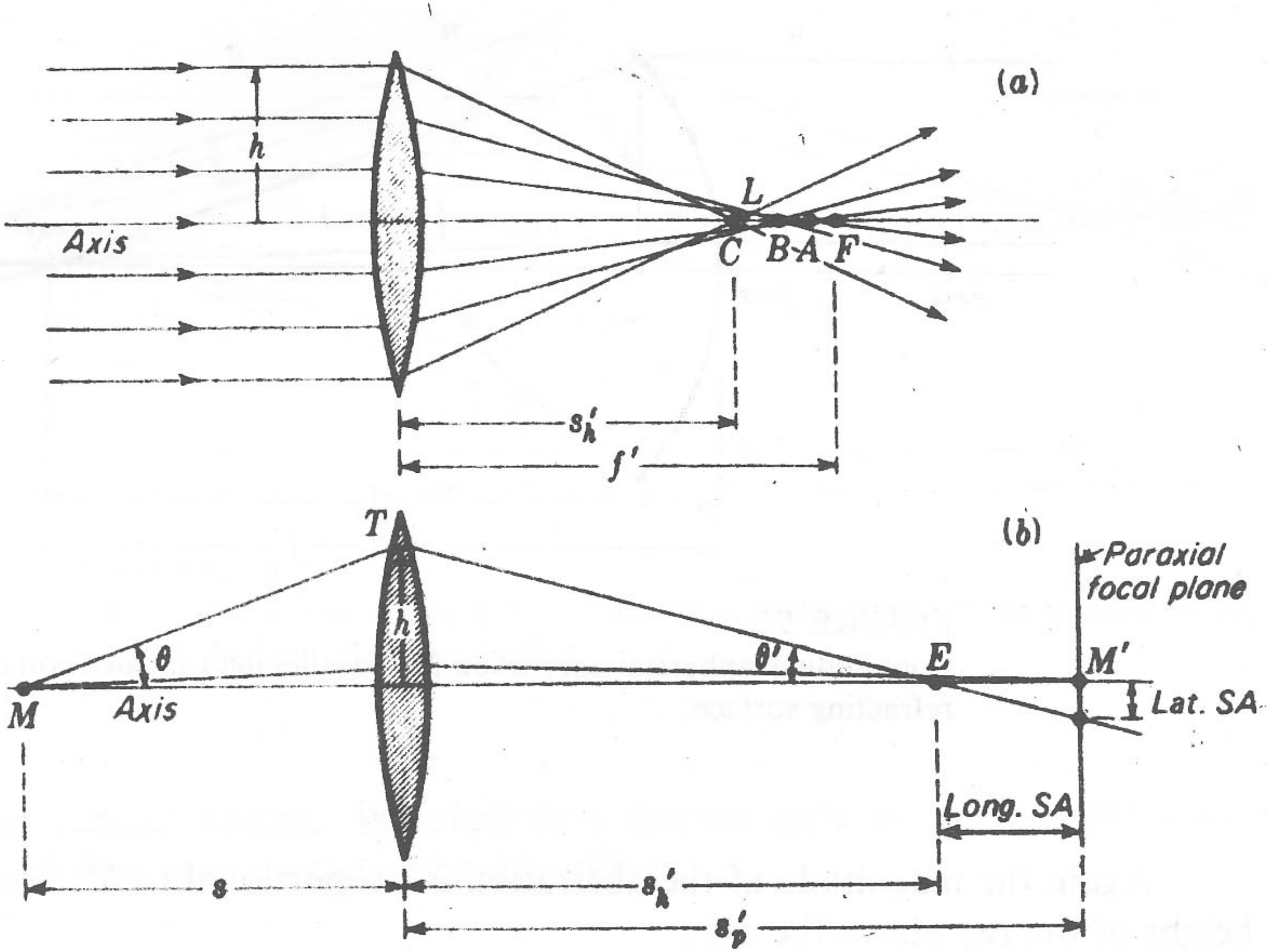


- 以光线从**n**媒质到达单球面的**n**′媒质后成像的情况为例，参看上图。从**M**点出发一斜入射光线（与光轴成θ角）与单球面交于**T**，在另一个介质到达光轴**M**′点，**TC**是球面半径**r**。角度的符号从轴反时针到光线为正，从球表面法线到光线反时针转为正，所以θ,ϕ,ϕ'为正，θ'为负。
- 从几何关系得到：△MTC中，$\phi=\theta+\angle TCM$；△TCM'中，$\phi'=\angle TCM-\theta'$。
- Snell 定律：$\sin\phi'/\sin\phi=n/n'$

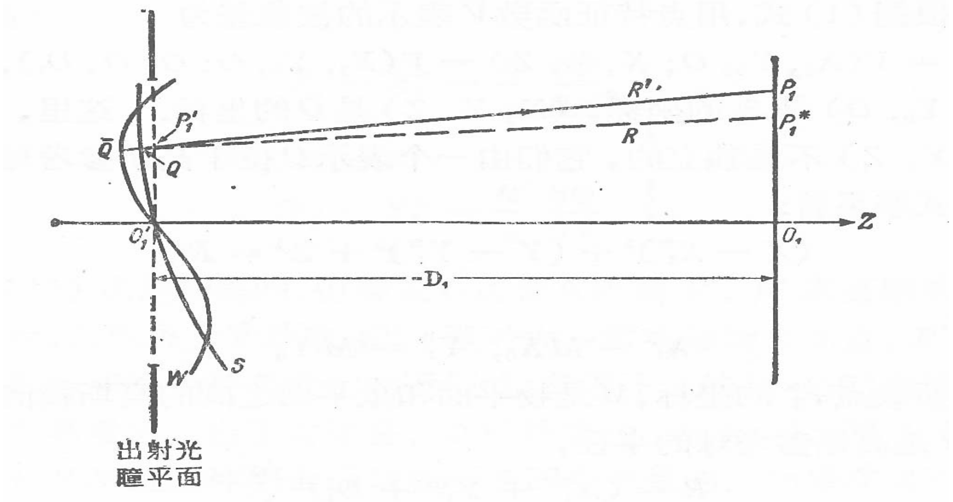
5种三级象差

- 从以上公式中，如果展开正弦函数 $\sin\theta = \theta - \frac{\theta^3}{3!} + \cdots$ 到第一项，即傍轴光线的情况，所得的一套公式便是高斯光学的公式 $\frac{n}{s} + \frac{n'}{s'} = \frac{n' - n}{r}$ 。如果用前两项展开式代入，则得到的公式与高斯光学公式的差别，有**5**项之多。这是由**L.Seidel**首先作出的[**L. Seidel. Astr. Nachr., 43(1856), No.1027,289, No.1028,305, No.1029,321.**]，称赛德尔和**(Seidel sums)**。每一项对应一种象差，分别是球差、彗差、象散、场曲、畸变。

薄透镜的球面象差


(a)
h
Axis
L
C
B
A
F
s_h'
f'
(b)
T
h
θ
θ'
M
Axis
E
M'
Paraxial focal plane
Lat. SA
Long. SA
s
s_h'
s_p'

波象差



- 由于 $\overline{Q}$ 与 O_1' 位于同一波阵面，所以 $[P_1\overline{Q}]=[P_1O_1']$，从而 Φ=[$P_1$Q]-[$P_1O'_1$] 就是两波阵面的光程差。
- **x_0,y_0,0是P_0**的坐标，X,Y,Z 是Q的坐标，由于对称性，Φ只是通过 X_0X+Y_0Y ,和 $x_0^2+y_0^2$, X^2+Y^2 这三种组合而依赖于这四个变量的。如果将Φ展开为相对于这四个坐标的幂级数，将只含偶次方项。
- (Max Born & Emil Wolf: << Principles of Optics>> (5th ed.) Pergamon Press, 1975. 中译本：《光学原理》，杨葭荪等译校。科学出版社，1978年。）

波象差的表达式

$$\Phi = c(x_0^2 + y_0^2) + \Phi^{(4)} + \Phi^{(6)} + \cdots$$

- 引入 $\gamma^2 = x_0^2 + y_0^2$ ，$\rho^2 = X^2 + Y^2$ ，$\kappa^2 = x_0 X + y_0 Y$
- 因为变量只以组合式的形式出现，Φ（4）必须具有下列形式：

$$\Phi^{(4)} = -\frac{1}{4}A\gamma^4 - \frac{1}{4}B\rho^4 - C\kappa^4 - \frac{1}{2}D\gamma^2\rho^2 + E\gamma^2\kappa^2 + F\rho^2\kappa^2$$

- 进一步的分析表明，$-\frac{1}{4}A\gamma^4$ 不应列入。因此最低级（四级）的波象差只有五种：**B-**球面象差，**C-**象散，**D-**场变曲，**E-**畸点，**F-**彗差。这就回归到线象差所定义的五种（三级）象差。

波象差在衍射空间表述

- 在电子显微学的文献中，习惯在物镜后焦面上描述象差。下面以欠焦与球差为例说明, $\chi(\vec{r})$, $\chi(\vec{g})$, $\chi(\theta)$ 在不同表象中的表示。
- 在物理空间，$\phi = c(x_0^2 + y_0^2) + \frac{1}{4}B\rho^4$ ，$\rho^2 = X^2 + Y^2$
- 在衍射空间，$\chi(\vec{g}) = \frac{1}{2}\Delta f \lambda^2 |\vec{g}|^2 + \frac{1}{4}C_s \lambda^4 |\vec{g}|^4$
- 在角度（倒易）空间，$\chi(\theta) = \frac{1}{2}\theta\tilde{\theta}C_1 + \frac{1}{4}(\theta\tilde{\theta})^2 C_3$

更高级象差受到重视

- 由于这类象差是由**sin**函数展开至角度的三级得到的，常称三级象差。依以类推，有五级、七级象差等等。但这些象差的代数表达式非常复杂，它的影响也显得不严重，而且由于应用的场合较窄，十分专门，所以常不为人知。随着象差校正电镜研究的深入，在消除（或减少）了三级象差之后，更高级象差的影响显露出来。

Seidel 7级象差函数

- 象差函数写到Seidel 7级是[M.Haider, H.Muller, S.Uhlemann, J.Zach, U.Loebau, and R.Hoeschen: Ultramicroscopy 108 (2008) 167.]

$$\chi(\theta)=\mathrm{Re}\left\{\begin{array}{l}\frac{1}{2}\theta\tilde{\theta}c_1+\frac{1}{2}\tilde{\theta}^2A_1+\frac{1}{3}\tilde{\theta}^3A_2+\theta^2\tilde{\theta}B_2\\+\frac{1}{4}(\theta\tilde{\theta})^2c_3+\frac{1}{4}\tilde{\theta}^4A_3+\theta^3\tilde{\theta}S_3+\frac{1}{5}\tilde{\theta}^5A_4\\+\theta^3\tilde{\theta}^2B_4+\theta^4\tilde{\theta}D_4+\frac{1}{6}(\theta\tilde{\theta})^3C_5+\frac{1}{6}\tilde{\theta}^6A_5\\+\theta^5\tilde{\theta}R_5+\theta^4\tilde{\theta}^2S_5+\frac{1}{7}\tilde{\theta}^7A_6+\theta^4\tilde{\theta}^3B_6\\+\theta^5\tilde{\theta}^2D_6+\theta^6\tilde{\theta}F_6+\frac{1}{8}(\theta\tilde{\theta})^4C_7\\+\frac{1}{8}\tilde{\theta}^8A_7+\theta^7\tilde{\theta}G_7+\theta^6\tilde{\theta}^2R_7+\theta^5\tilde{\theta}^3S_7\end{array}\right\}$$

象差系数含义

- 欠焦C_1(nm) ;二重象散A_1(nm) ;三重象散A_2(nm) ;二级彗差B_2（nm）;三级球差C_3,C_s(μm) ;
- 四重象散A_3(μm);三级星象差S_3(μm);五重象散A_4(μm);四级彗差B_4(μm);四级三瓣象差D_4(μm);
- 五级球差C_5(mm);六重象散A_5（mm）;五级玫瑰花结R_5(mm);五级星象差S_5(mm);七重象散A_6(mm);
- 六级彗差B_6（mm）;六级三瓣象差D_6(mm);六级五角象差F_6（mm）;七级球差C_7（mm）。

初级象差容限条件

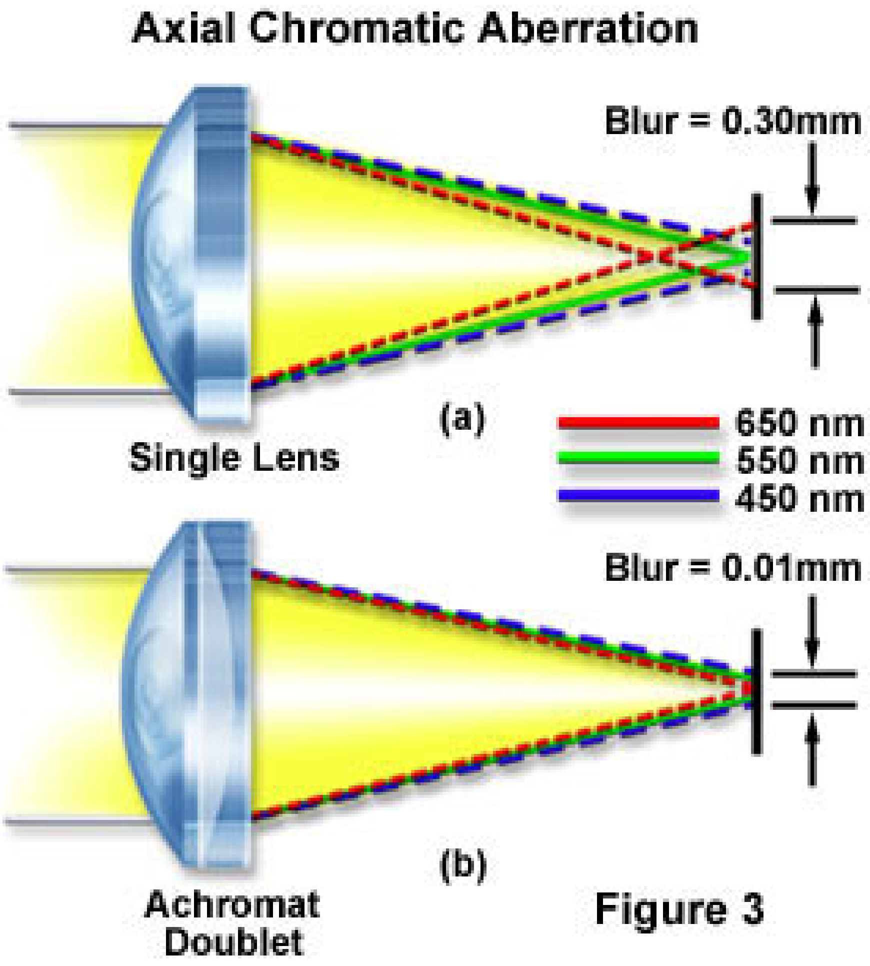
- 以上的象差效应基本上不考虑象的强度问题。
- 当存在象差时，衍射象中最大强度小于具有相同孔径和焦距的无象差系中的高斯象点处的强度。
- 瑞利首先证明[**Lord Rayleigh: Phil. Mag., (5)8 (1879), 463.**]，初级球面象差导致波阵面偏离不到**1/4**波长时，其强度减弱不到**20%**，光的这种损失通常是可以容许的。其后一些作者研究表明，当其它象差存在时，若波阵面形变小于**1/4**波长，则象的质量同样不受严重影响。

电子显微镜与光仪器的光学质量对比

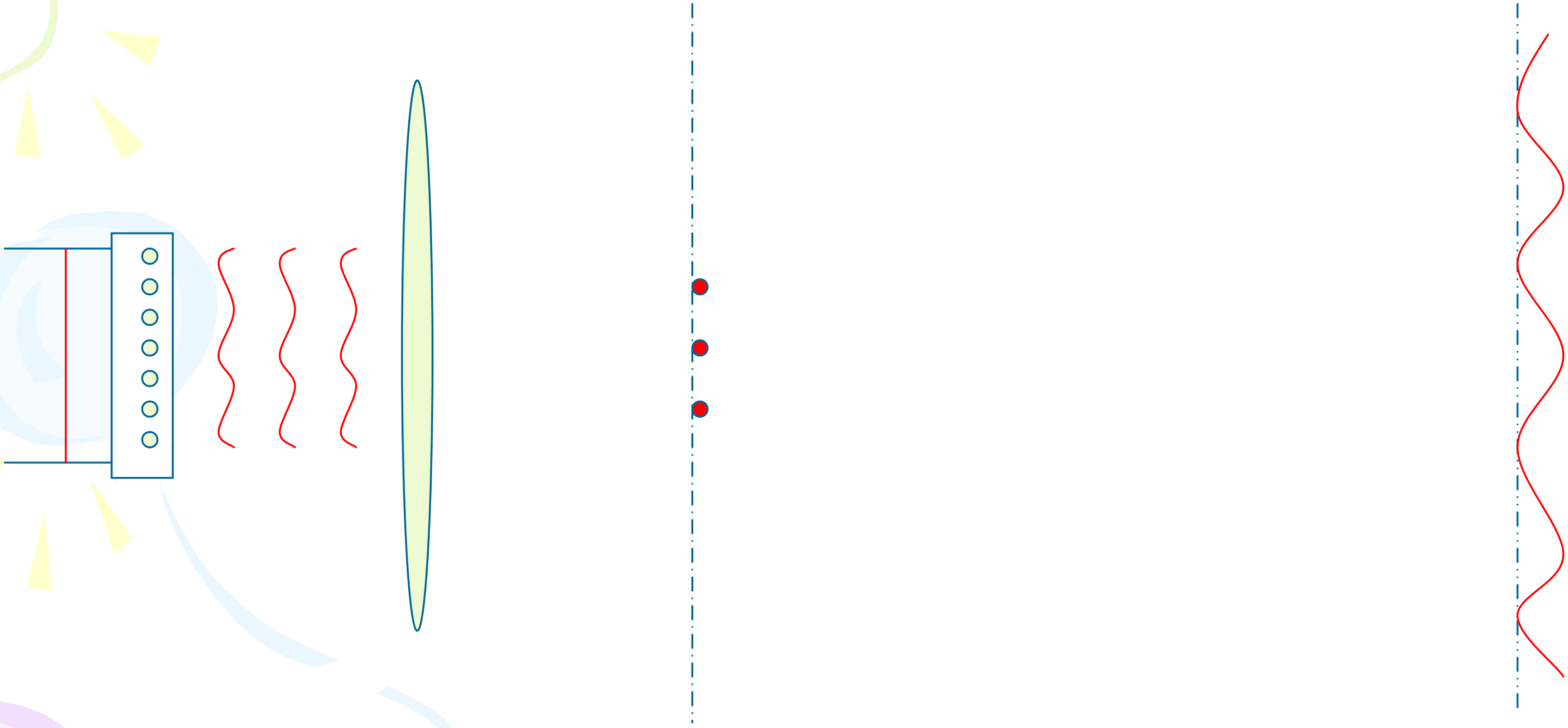
- 长期以来，由于电子透镜的象差校正进展迟缓，而光学仪器的象差校正似乎已臻完善。所以有人将电镜的光学质量堪比啤酒杯底那样粗糙（有一点放大镜作用）。
- 按照天文望远镜的标准，质量指标为入射光瞳尺寸与波阵面容限畸变之比。可见光的1/4波长取100nm。对地面镜子来说，质量指标约为0.3m/100nm=3×10^6。对于校正好的哈勃望远镜，这个数字为2.5m/100nm=2.5×10^7。
- 对于VG HB501 STEM，物镜光阑大小为40μm，电子波的λ/4约1pm，则40μm/1pm=4×10^7;对于象差校正的STEM，物镜光阑可放大至100μm，则100μm/1pm=1×10^8，这比哈勃望远镜好1.6-4倍。
- 电子透镜象差校正所以步履维艰，不是因为电镜的质量糟糕，而是它已经很不错，要进一步改进的确很难。(**O.L.Krivanek, P.D.Nellist, N.Dellby, M.F.Murfitt, and Z.Szilagyi: Ultramicroscopy 96 (2003) 229.**)

色差

- 如果考虑波的非单色性，在光学系统中，由于折射率不是一个物质常数，而随颜色（波长）而定。所以光经过一个折射面，就会分解为一组波长各不相同的光线，它们将沿稍微不同的路径传播。结果，象将会模糊，这是色差的影响。
- 电子显微镜的色差来自多方面，首先电子枪发出的电子有多色性，其次电子经过样品后波长也会改变，最后，电子透镜的励磁电流也有不稳定成分。



象差在电子显微镜中的作用



Sample

Lens

Diffraction Pattern

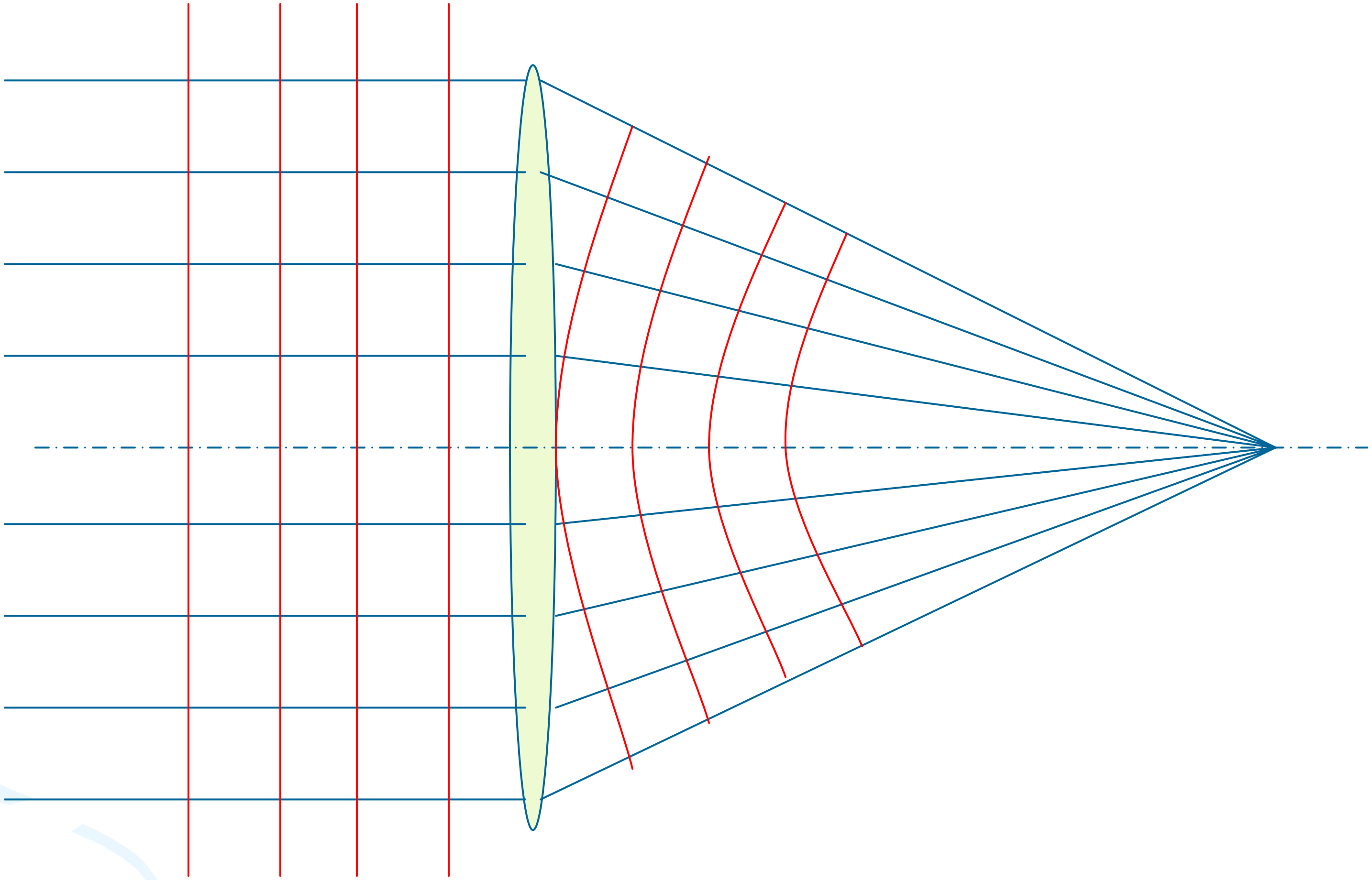
Image

Plane

Modified by sample

Modified by lens

Image reconstruction



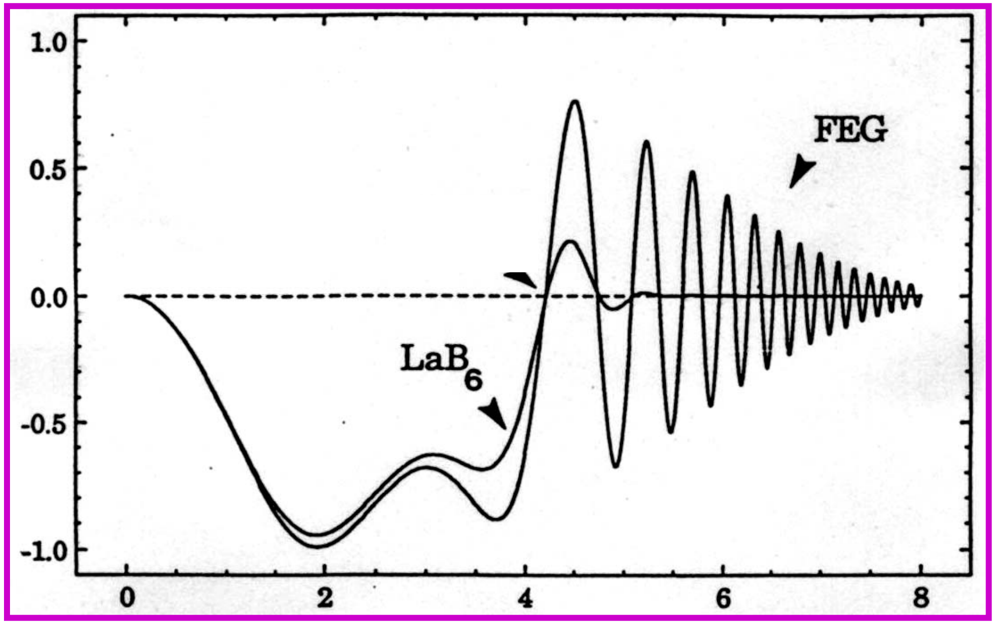
透镜是个相位变换器

O.Scherzer 提出透镜引入象差的相位表达式(J.Appl. Phys. 20,20, 1949)

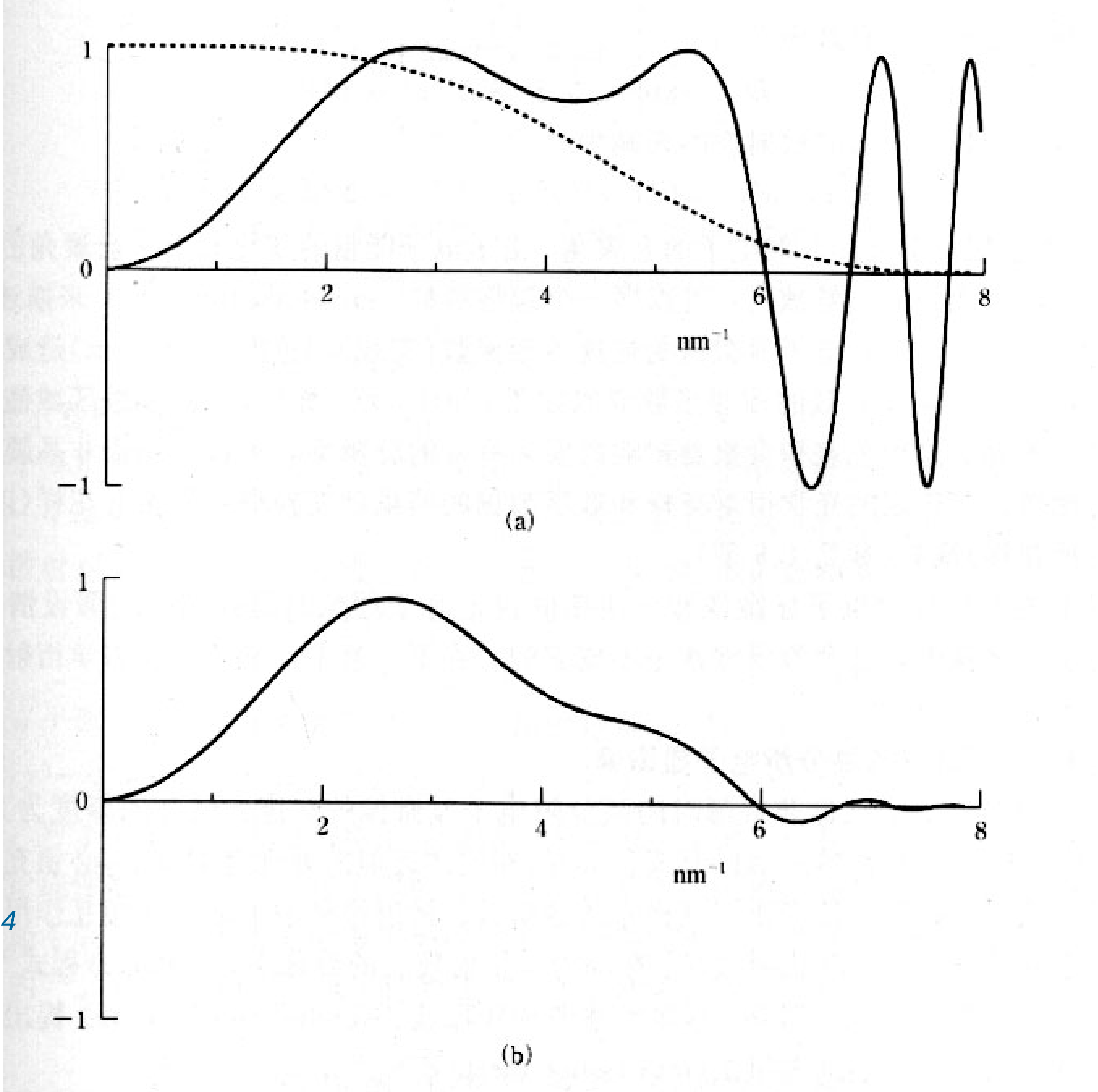
- $\chi=\pi[0.5C_s\lambda^3(u^2+v^2)^2+\Delta f\lambda(u^2+v^2)]$
  - C_s—物镜球差系数
  - λ——电子束波长
  - Δf—物镜欠焦值
  - u, v—衍射空间中动量矢（或晶体的倒易矢）在笛卡儿坐标的指数
- 在电子显微镜中，球差系数相对固定，调节物镜欠焦值有可能使物镜的相位影响减至最小

对于弱相位体,透镜象差函数对成象的影响可归结为在物镜后焦面上乘上一个以象差函数为宗量的正弦函数

$$I(g) \sim |A(g)|^2 |E(g)|^2 |\sin \chi(g)|^2 |Q_p(g)|^2$$



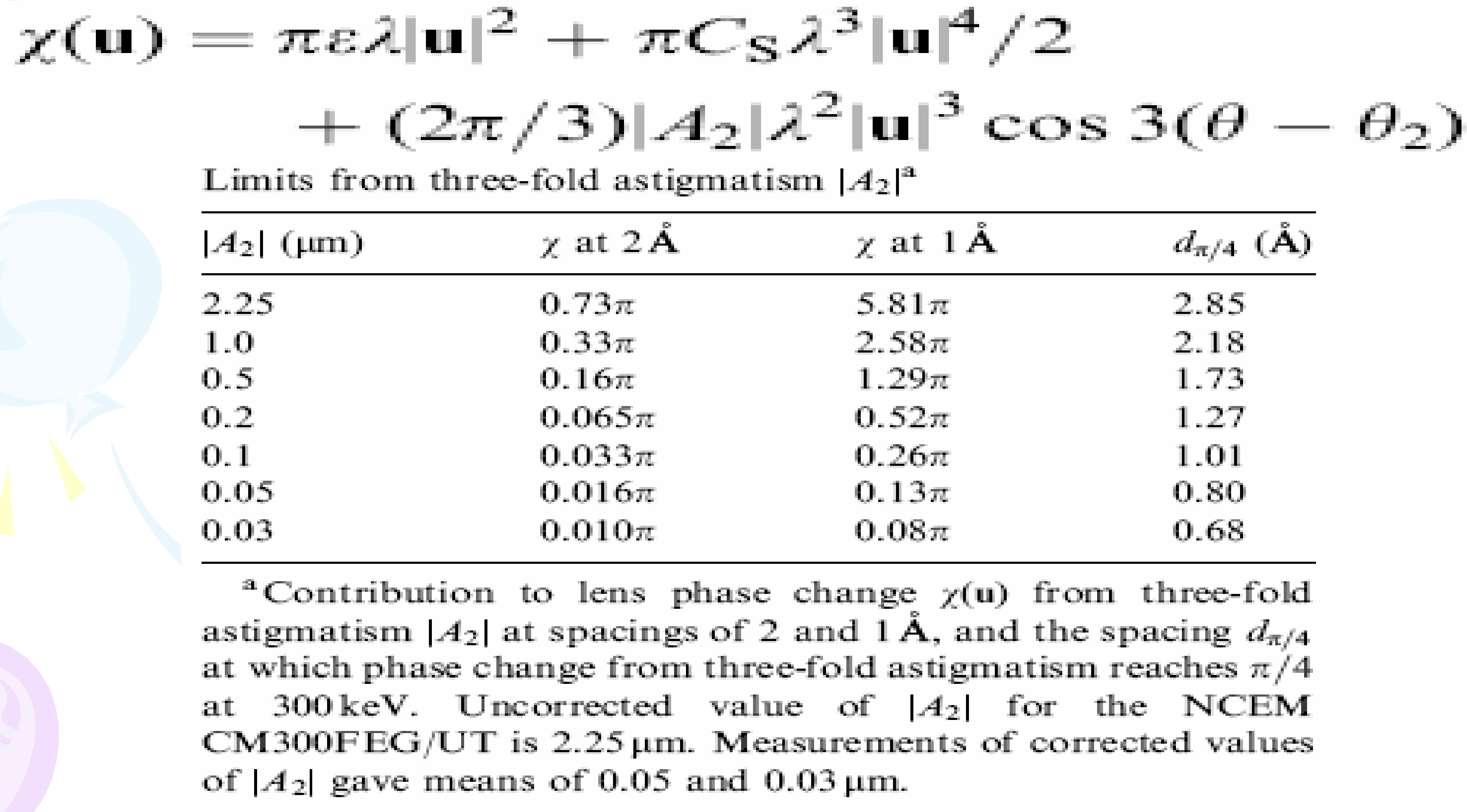
物镜衬度传递函数及电子束色差与束发散度的影响



目前仅考虑到欠焦与球差的影响

$d_s = 0.67\,C_s^{1/4}\lambda^{3/4}$

高级象差示例—三重象散A_2



$$\chi(\mathbf{u}) = \pi\varepsilon\lambda|\mathbf{u}|^2 + \pi C_S\lambda^3|\mathbf{u}|^4/2 + (2\pi/3)|A_2|\lambda^2|\mathbf{u}|^3\cos 3(\theta - \theta_2)$$

Limits from three-fold astigmatism $|A_2|$[a]

$\|A_2\|$ (μm)	χ at 2 Å	χ at 1 Å	$d_{\pi/4}$ (Å)
2.25	0.73π	5.81π	2.85
1.0	0.33π	2.58π	2.18
0.5	0.16π	1.29π	1.73
0.2	0.065π	0.52π	1.27
0.1	0.033π	0.26π	1.01
0.05	0.016π	0.13π	0.80
0.03	0.010π	0.08π	0.68

[a] Contribution to lens phase change $\chi(\mathbf{u})$ from three-fold astigmatism $|A_2|$ at spacings of 2 and 1 Å, and the spacing $d_{\pi/4}$ at which phase change from three-fold astigmatism reaches $\pi/4$ at 300 keV. Uncorrected value of $|A_2|$ for the NCEM CM300FEG/UT is 2.25 μm. Measurements of corrected values of $|A_2|$ gave means of 0.05 and 0.03 μm.

三重象散对金刚石[110]像的影响

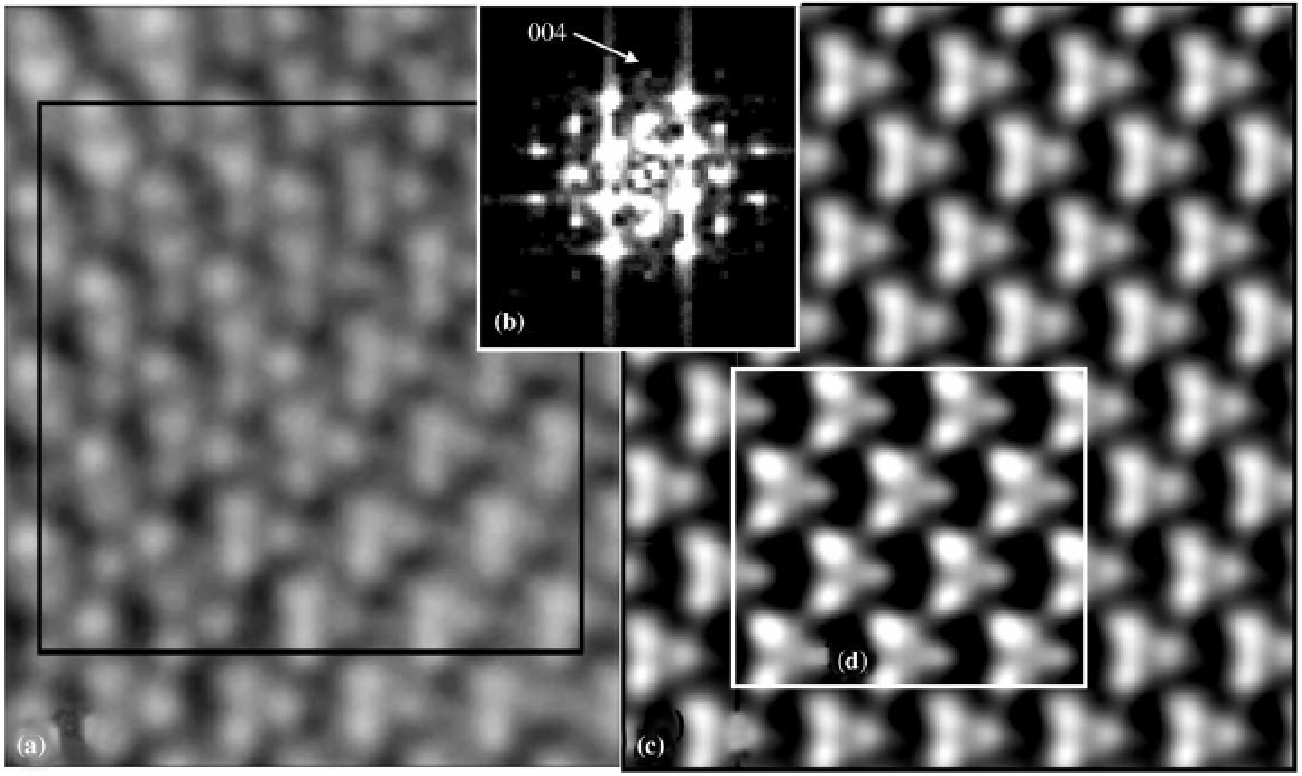


Fig. 8. (a) Experimental OÅM image of CVD diamond before correction of three-fold astigmatism. (b) Diffractogram shows specimen orientation is [1 1 0], with strong 1 1 1 and 113 spots, weak 220 and 331 spots, and very weak 004's (arrowed). (c) Averaging (p1 in Crisp™) shows white spots separated by approximately $|\mathbf{a}|_{\mathrm{diamond}}/4$, but with extra spots producing triangular white clusters. (d) Images simulated from diamond [1 1 0] match best at $|A_2| = 2.25\,\mu\mathrm{m}$.

校正A_2

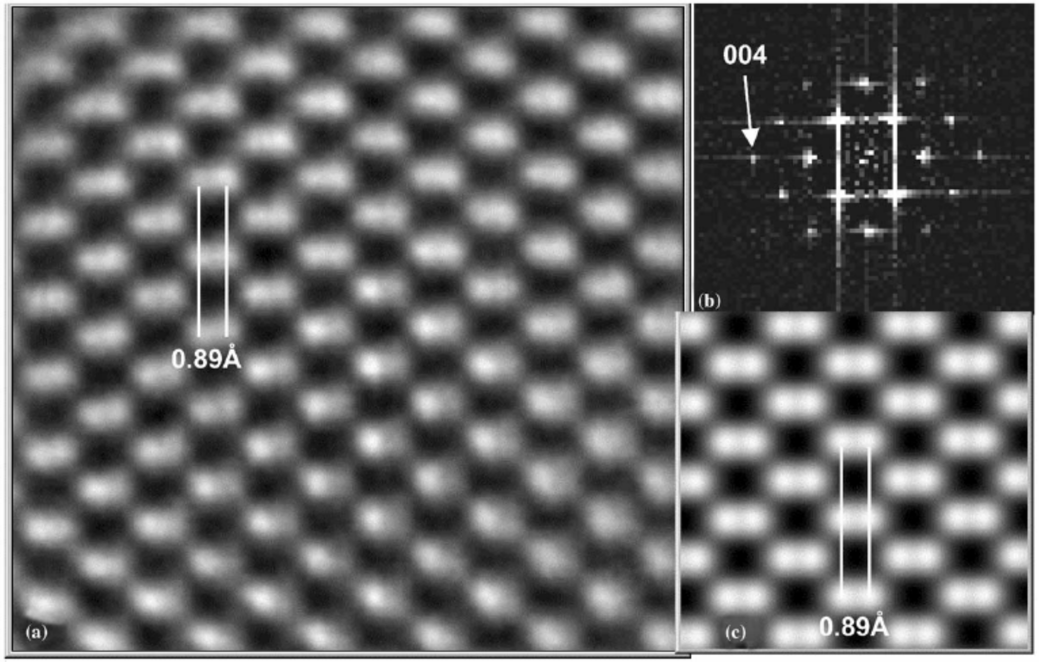


Fig. 10. (a) Experimental OÅM image of CVD diamond in [1 1 0] orientation after correction of three-fold astigmatism to below 0.05 μm. (b) Diffractogram shows a strong 0 0 4 presence (arrowed) producing "dumbbell" images with 0.89 Å spacing (marked) in the experimental and (c) averaged images.

M.A. O'Keefe et al., Ultramicroscopy 89 (2001) 215–241

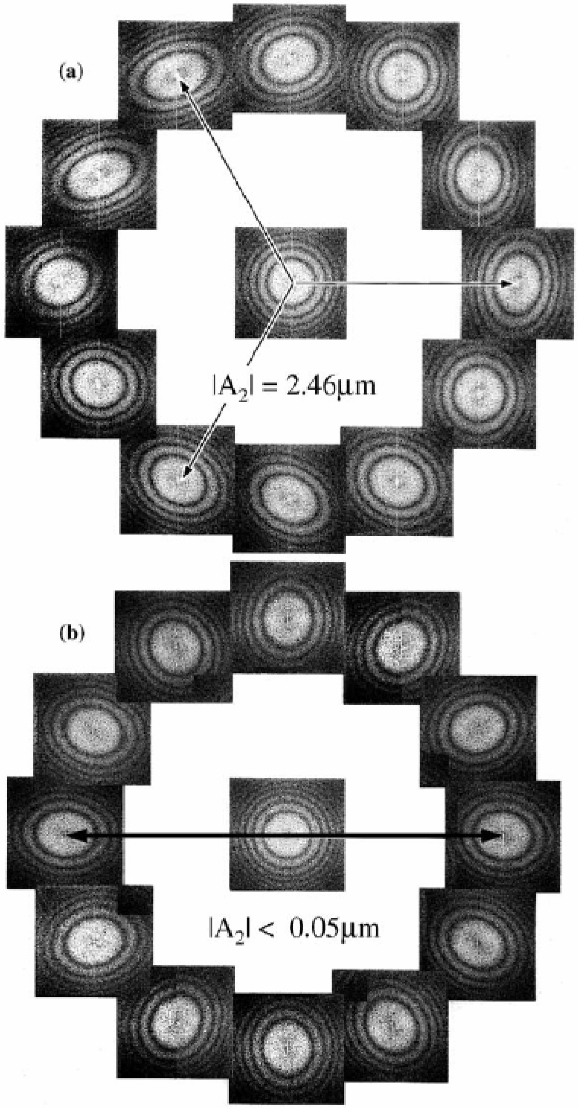
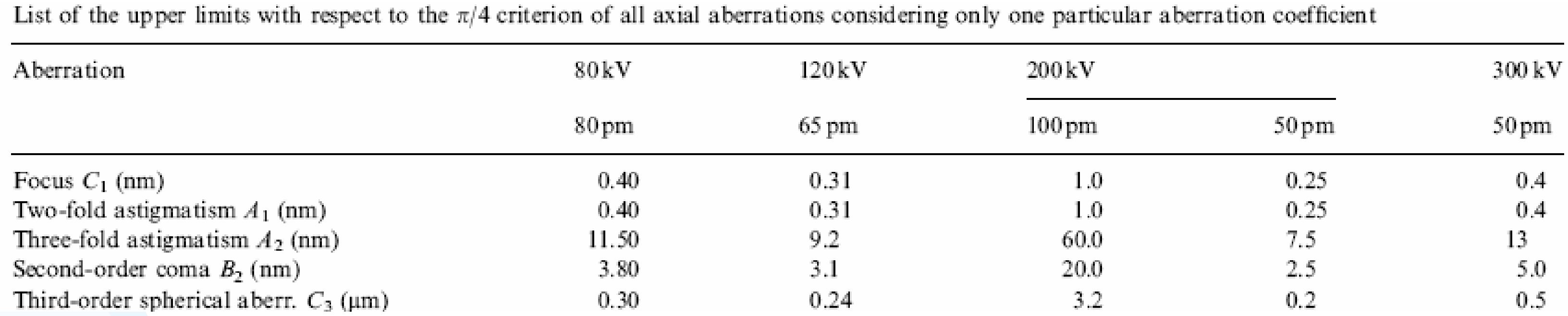


Fig. 9. OÅM "clock" tilt series of diffractograms from a thin amorphous carbon specimen. (a) Strong three-fold astigmatism measured at $|A_2| = 2.46\,\mu m$ before correction shows distinct three-fold character (arrowed). (b) Corrected series measured at 0.05 μm shows all ellipses pointing to the tilt origin.

$d_{A_2} = 1/|\mathbf{u}|_{A_2} = (8A_2\lambda^2/3)^{1/3}$

$A_2 = 3/8u^3\lambda^2$

可数值化的实时测量象差



List of the upper limits with respect to the $\pi/4$ criterion of all axial aberrations considering only one particular aberration coefficient

Aberration	80 kV	120 kV	200 kV		300 kV
	80 pm	65 pm	100 pm	50 pm	50 pm
Focus C_1 (nm)	0.40	0.31	1.0	0.25	0.4
Two-fold astigmatism A_1 (nm)	0.40	0.31	1.0	0.25	0.4
Three-fold astigmatism A_2 (nm)	11.50	9.2	60.0	7.5	13
Second-order coma B_2 (nm)	3.80	3.1	20.0	2.5	5.0
Third-order spherical aberr. C_3 (μm)	0.30	0.24	3.2	0.2	0.5

- 单项象差调节要求较高，考虑到象差部分的互补性而作的多重调节也很复杂。这一切自然要用电脑帮助完成，并且要有适当的可数值化的实时测量象差的办法。

M. Haider, H. Muller, S. Uhlemann, J. Zach, U. Loebau, R. Hoeschen:Ultramicroscopy 108 (2008) 167–178

电子显微像的衍射图与物镜衬度传递函数

$$I(g) \sim |A(g)|^2 |E(g)|^2 |\sin \chi(g)|^2 |Q_p(g)|^2$$

- 其中前两项是物镜光阑和源不相干性形成的衰减包络，样品投影势对无定物而言是均匀的，所以只余下物镜象差的衬度传递函数这一项。**sin**函数的宽通带形成中心部的亮区，而后各通带依次形成明亮相间的园环。
- 全部亮区最外延部分对应着衰减包络的截止点，对应着物镜的信息极限。

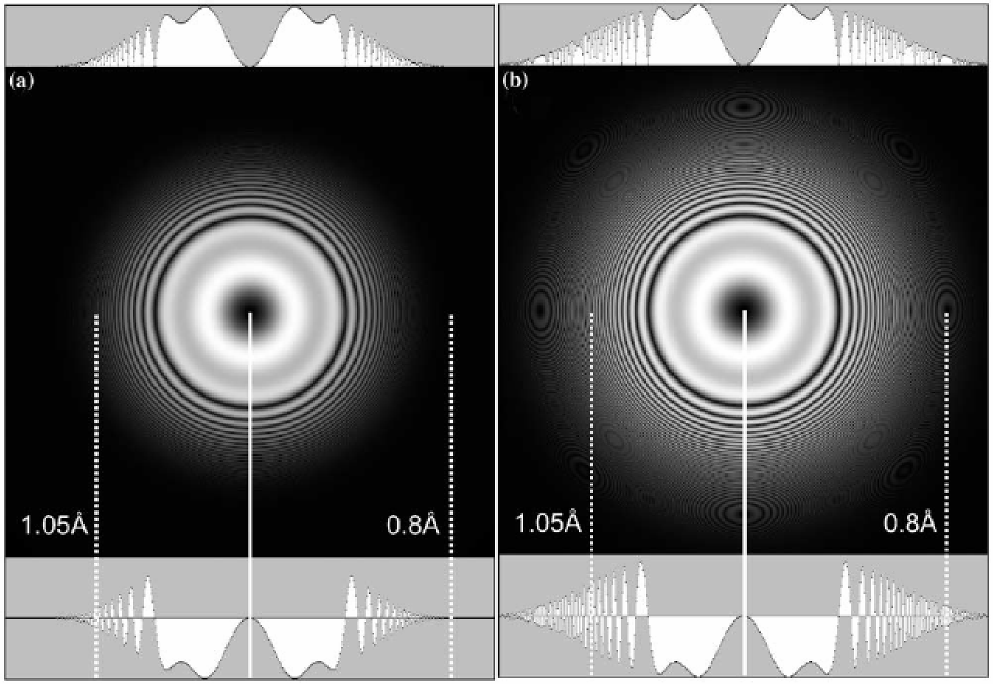
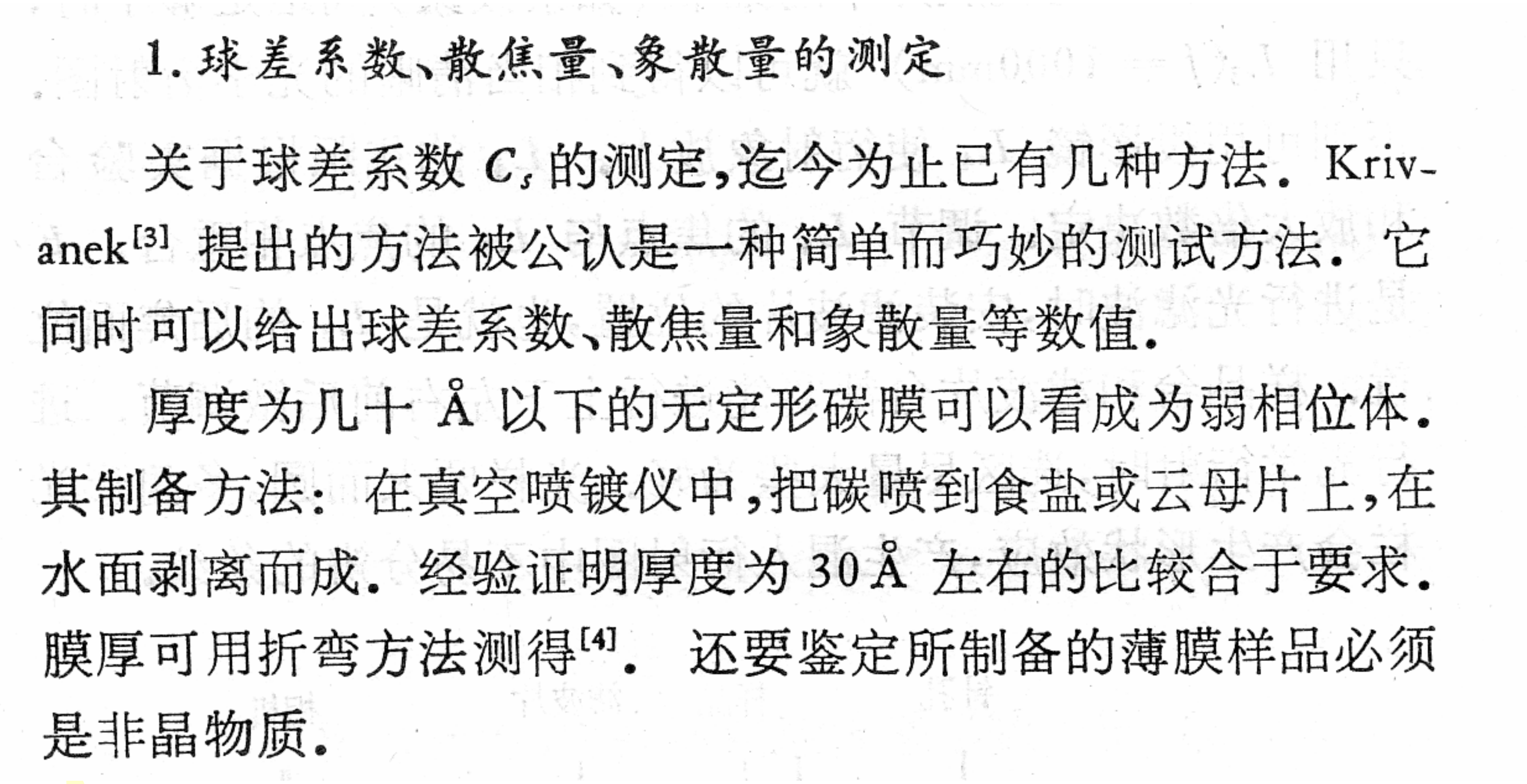


Fig. 6. CTFs (lower) and diffractograms (1-D top and 2-D center) computed for (a) standard CM300FEG spread of focus of 35.5 Å [30] and (b) OÅM value of 20 Å. Information limits of 1.05 and 0.80 Å are marked. Computed for zero beam convergence at Scherzer defocus. ("Ghosts" in the circular 2-D diffractograms are aliasing from sub-sampling of the fine rings.)

M.A. O'Keefe et al., Ultramicroscopy 89 (2001) 215–241

从无定形膜的衍射图测量像差

- 下述内容取自《高分辨电子显微学》234-236页。



1. 球差系数、散焦量、象散量的测定

关于球差系数 C_s 的测定，迄今为止已有几种方法．Krivanek[3] 提出的方法被公认是一种简单而巧妙的测试方法．它同时可以给出球差系数、散焦量和象散量等数值．

厚度为几十 Å 以下的无定形碳膜可以看成为弱相位体．其制备方法：在真空喷镀仪中，把碳喷到食盐或云母片上，在水面剥离而成．经验证明厚度为 30 Å 左右的比较合于要求．膜厚可用折弯方法测得[4]．还要鉴定所制备的薄膜样品必须是非晶物质．

将无定形碳膜的电子显微象作为样品放在光学变换仪的样品台上。在衍射透镜背焦面上，强度分布如(6.6)式所示。

因此

当

$$\chi(u)=n\pi/2\left(\begin{array}{l}n\ \text{为奇数}\cdots\cdots\text{最大衬度}\\ n\ \text{为偶数}\cdots\cdots\text{最小衬度}\end{array}\right)\tag{6.8}$$

碳膜电子显微象的光学衍射图，如图 6.2 所示，呈明暗相间的同心环形状。亮环的空间频率与 $n=2m+1$ 对应；暗环的空间频率与 $n=2m$ 对应。中心亮斑是(6.6)式中的 $\delta(u,v)$ 而成的强衬度区。由(6.7)式可知，这个衍射图的明暗是球差系数和散焦量的函数。(6.8)式的条件可改写为

$$C_s\lambda^3u^2+2\Delta f\lambda=\frac{n}{u^2}\tag{6.9}$$

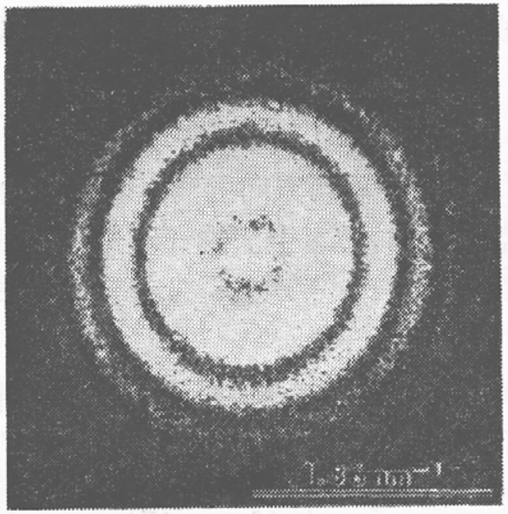


图 6.2 无定形碳膜电子显微象的光学衍射图

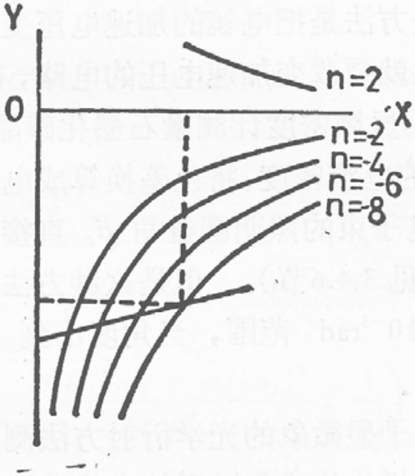


图 6.3 由图 6.2 求解 C_s 及 Δf

如果设 $u^2 = X$，上式可写成联立方程形式

$$\begin{cases} Y = (C_s\lambda^3)X + 2\Delta f\lambda & (6.10) \\ Y = n/X & (6.11) \end{cases}$$

从 X 的一次式和双曲线的交点能求出暗环的空间频率。

反之,从图 6.2 的光学衍射图求得明暗环的空间频率，画在图 6.3 上,连接成直线,则直线的斜率是 $C_s\lambda^3$，截距为 $2\Delta f\lambda$. 即

$$C_s = 斜率/\lambda^3 \tag{6.12}$$

$$\Delta f = 截距/2\lambda \tag{6.13}$$

为了准确,在图 6.2 的不同方向上测量明暗环的半径，并换算成所对应的空间频率,重复上面的计算过程，得到一系列 C_s 和 Δf，再求它们的算术平均值，就得到我们所要测定的 C_s 和 Δf.

从一张图各方向的 Δf 值中，取椭圆的长轴与短轴方向的 Δf 值,可以得到象散量

$$C_a = |\Delta f_{\parallel} - \Delta f_{\perp}| \tag{6.14}$$

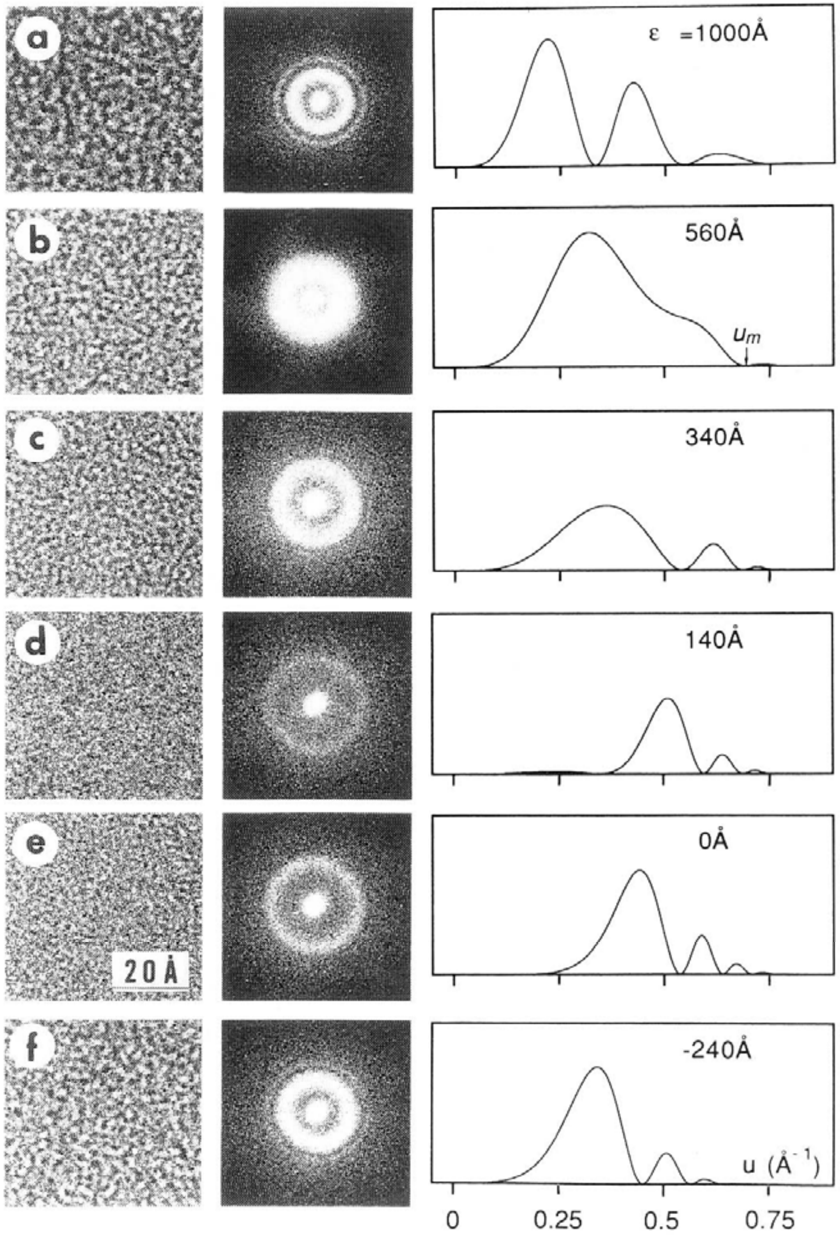
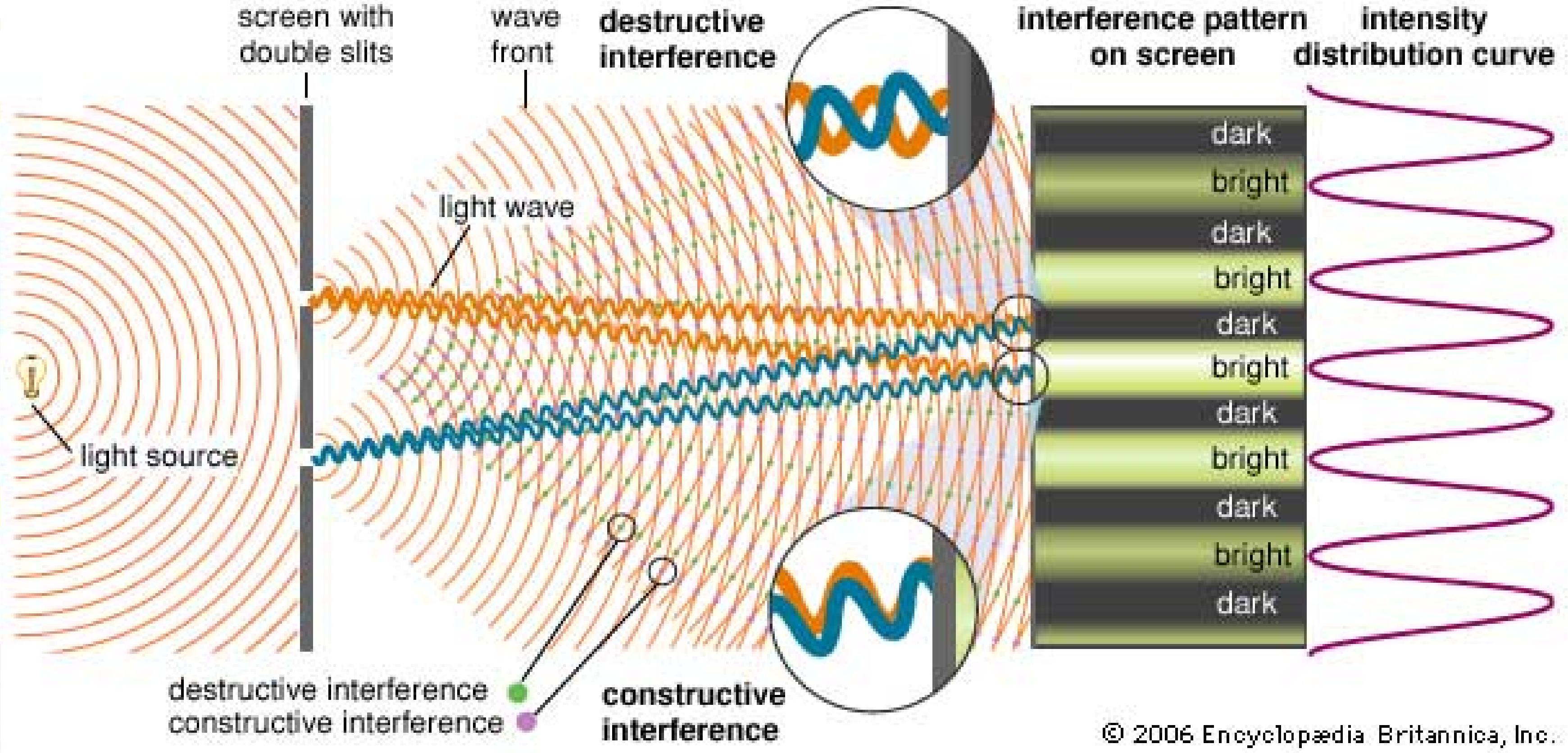


Fig. 8.23. Through-focus images of a Ge amorphous film and the corresponding optical diffraction patterns. The calculated intensities are also shown. The images are taken at $\varepsilon = 1000$ Å (underfocus) (a), 560 Å (b), 340 Å (c), 140 Å (d), 0 Å (Gaussian focus) (e) and -240 Å (overfocus) (f), respectively. $u_m = 0.69$ Å^{-1}, $E = 800$ kV, $C_s = 2.2$ mm and $\Delta = 100$ Å.

S.Horiuchi:<< Fundamentals of HRTEM>>, North-Holland, 1994, p.223

从杨氏条纹延伸的最外沿可以测定电子显微镜的信息分辨极限

杨氏干涉条纹



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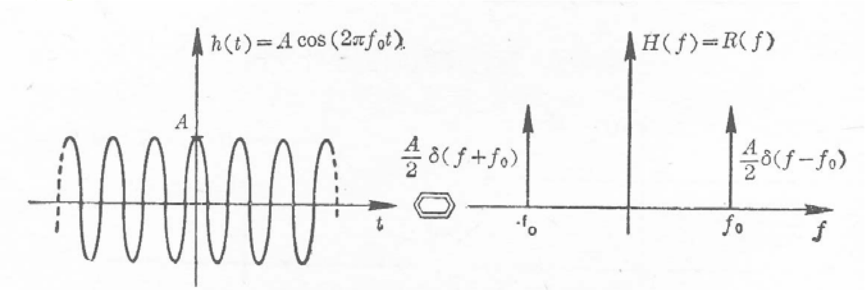
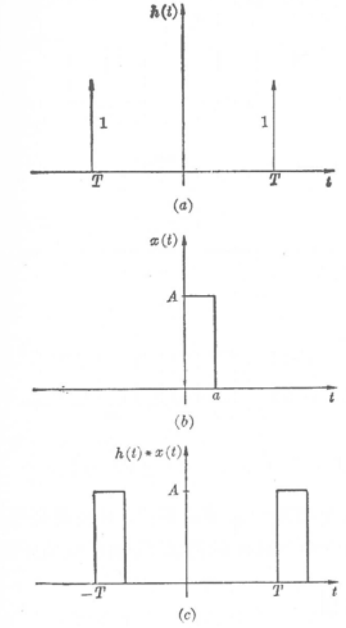
任意形状图像位移后重叠的衍射图

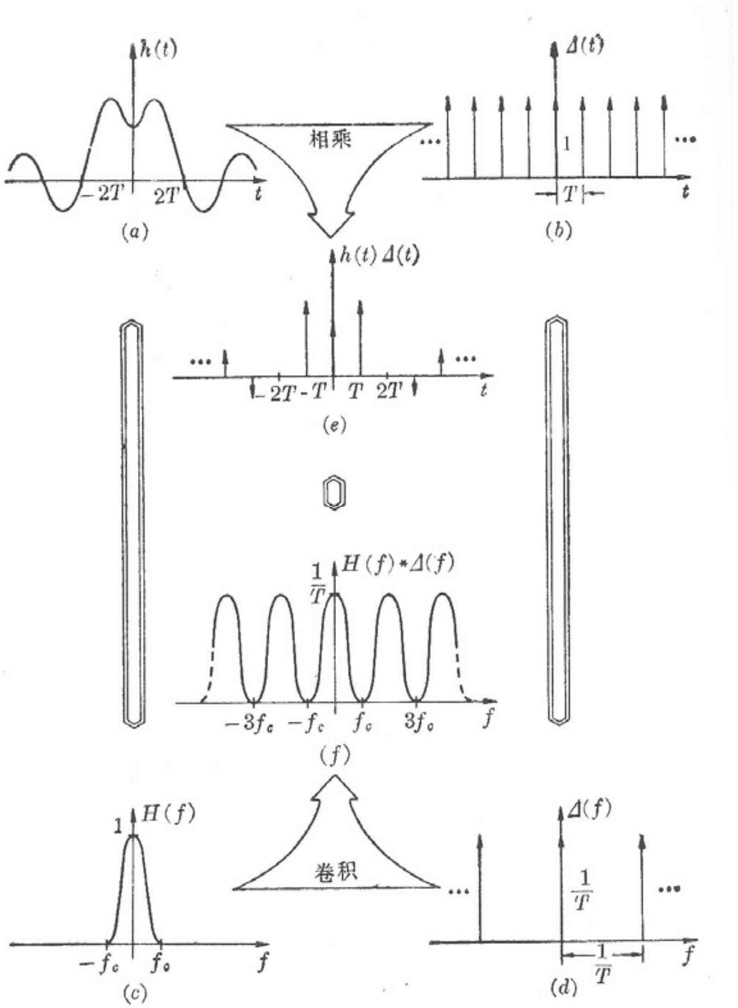


余弦函数与δ函数付利叶变换对。可作为杨氏干涉条纹的数学描述

狭缝被复杂形状的物函数取代效果是两者的卷积



E.O.Brigham: 《The fast Fourier transform》中译本：《快速富里叶变换》，柳群译，上海科学技术出版社，**1979**年。

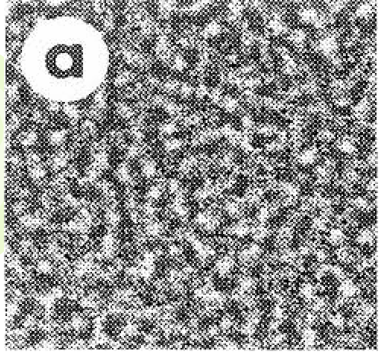


卷积定理的示意图

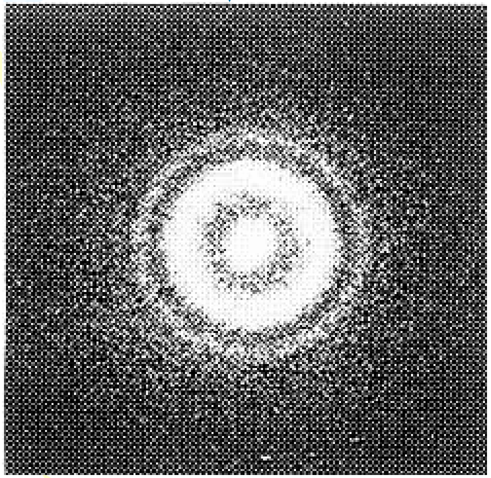
从杨氏条纹延伸的最外沿可以测定电子显微镜的信息分辨极限

- 如果显微像是一张由同视场、同放大倍数、仅平移少许的两幅像叠合而成，则其衍射图一如由两个相同物函数、但移开一段距离形成的衍射效应。这是前面所述的非δ函数形成杨氏干涉条纹的情况。即单一显微像与两个δ函数卷积（叠合的电子显微像）的付利叶变换（叠合像衍射图）是它们各自付利叶变换的乘积。这就是说，这时 **$Q_p=Q'_p(g)Y(g)$**，**Q'_p**是单一电子显微像的投影势的付利叶变换（衍射图），**Y**是两δ函数的杨氏干涉条纹（源自两显微像叠合时存在的光程差）。但它们都受**A**、**E**、**sinχ**函数的调制。从而从杨氏条纹延伸的最外沿可以测定电子显微镜的信息分辨极限。

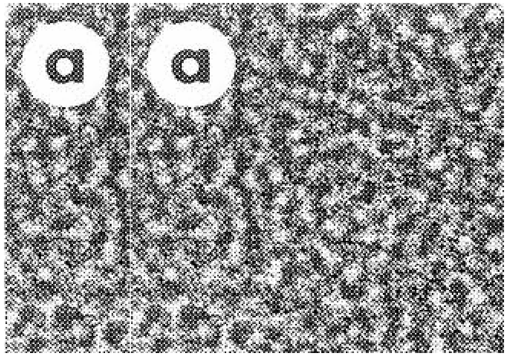
$$I(g)\sim\left|A(g)\right|^2\left|E(g)\right|^2\left|\sin\chi(g)\right|^2\left|Q_p(g)\right|^2$$


a

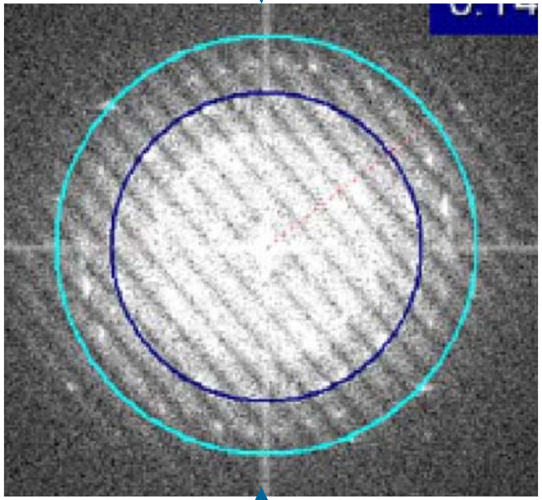
ℱ



⊕

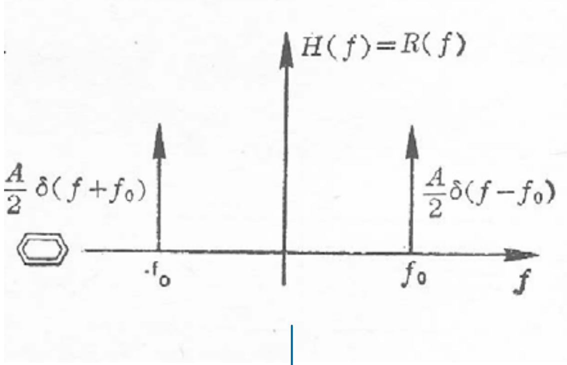

a
a

ℱ

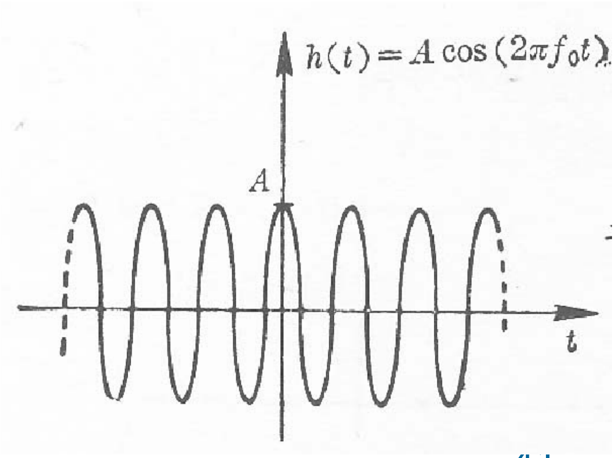


×

A-C TEM


$H(f)=R(f)$
$\frac{A}{2}\delta(f+f_0)$
$\frac{A}{2}\delta(f-f_0)$
$-f_0$
f_0
f

ℱ


$h(t)=A\cos(2\pi f_0 t)$
A
t

常规、球差校正、再加单色器电镜的信息分辨极限

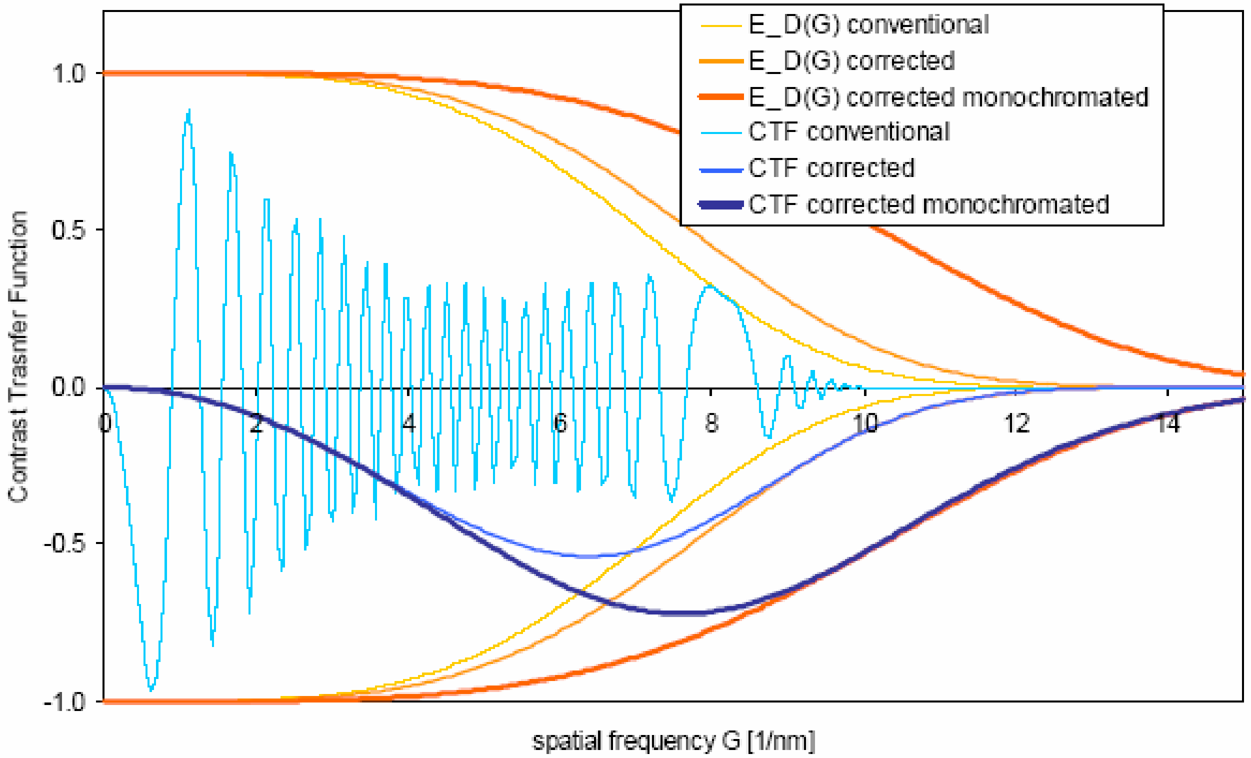


Fig. 1. Typical temporal coherence-damping envelopes $E_D(G)$ and contrast transfer functions (CTF) for a conventional microscope, for a Cs corrected microscope, and for a Cs corrected and monochromated microscope. A large defocus of −500 nm has been used for the conventional CTF in order to boost the CTF at 8 nm^{-1}. The Cs corrected CTFs have been calculated for a defocus of only −3 nm. The CTFs without monochromation have half convergence angles of 0.2 mrad. The CTF with monochromation has a half convergence angle 2 mrad. The Cs corrected CTFs hardly depend on the half convergence angle.

B. Freitag,S. Kujawa,P.M. Mul,J. Ringnalda,P.C. Tiemeijer:Ultramicroscopy 102 (2005) 209–214

杨氏干涉条纹显示单色器效果

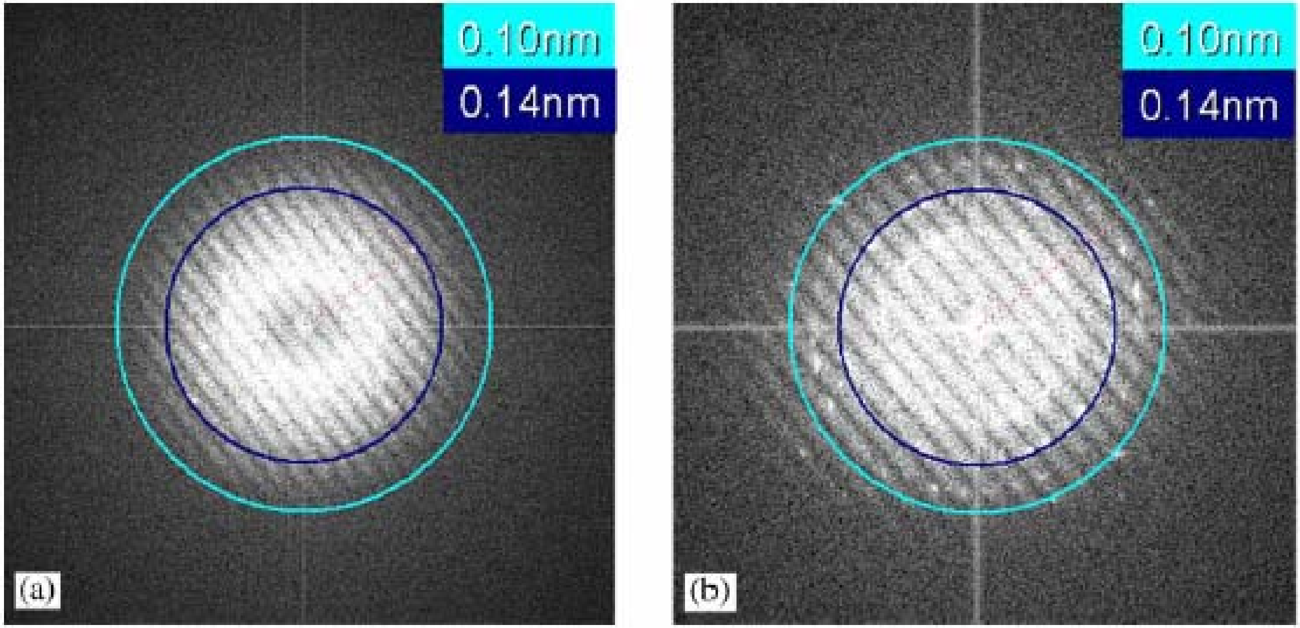


Fig. 2. Two Young fringe images of an amorphous tungsten film, showing the improvement of information limit obtained by the monochromator: (a) monochromator off ($\Delta E = 0.55\,\mathrm{eV}$) and Cs corrector on ($\mathrm{Cs} = -3\,\mu\mathrm{m}$), (b) monochromator on ($\Delta E < 0.15\,\mathrm{eV}$) and Cs corrector on ($\mathrm{Cs} = -3\,\mu\mathrm{m}$). The dots in the right image are lattice reflections from small gold particles in the tungsten film used for calibration. The light blue circle shows the 0.10 nm frequency. The dark blue circle shows the 0.14 nm frequency. The Young fringes show that, without monochromator, the information limit is a little worse than 0.1 nm. With monochromator, the information limit is well below 0.1 nm. The images were taken with 0.3 nA beam current on the CCD, 1 s exposure time, and 0.2 mrad half convergence angle (a) or 2 mrad half convergence angle (b).

B. Freitag,S. Kujawa,P.M. Mul,J. Ringnalda,P.C. Tiemeijer:Ultramicroscopy 102 (2005) 209–214

单一衍射图可测量欠焦、象散、球差等

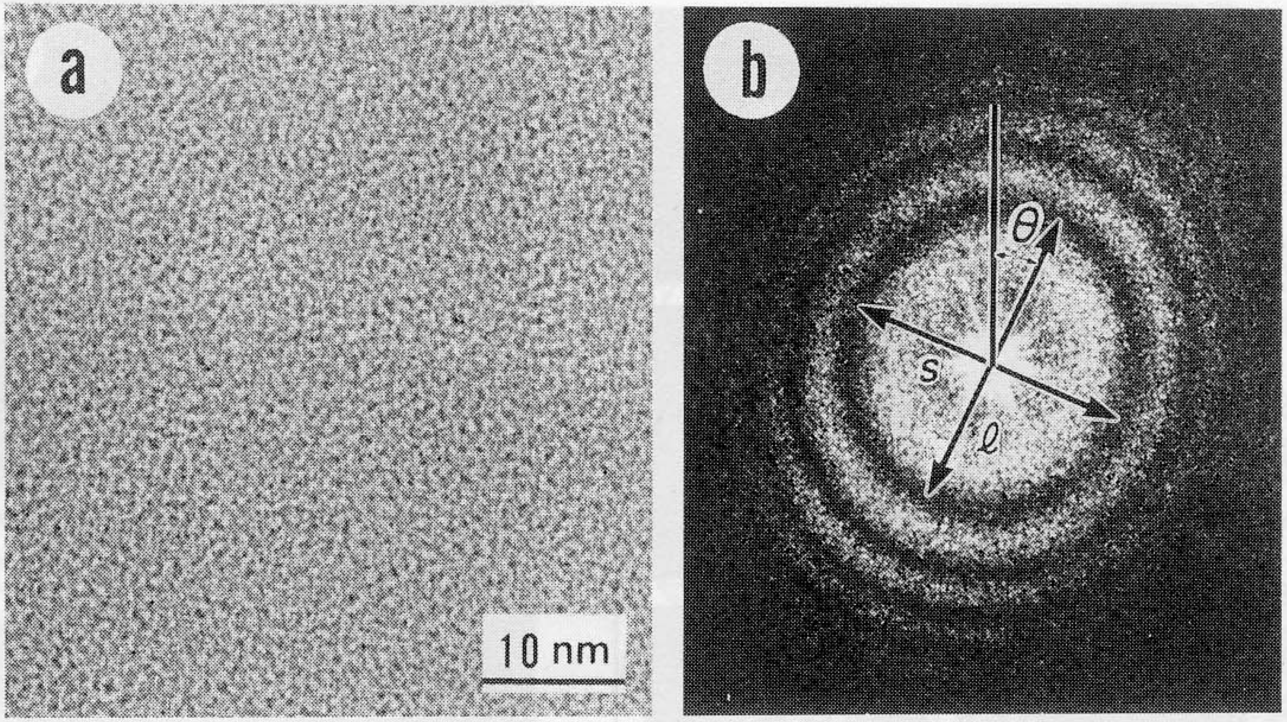


Fig. 8.24. (a) Granular structure of an amorphous C film. (b) Optical diffraction pattern, whose rings are slightly ellipsoidal, showing the existence of residual astigmatism.

S.Horiuchi:<<Fundamentals of HRTEM>>, North-Holland, 1994, p.224.

测量象差的衍射图列

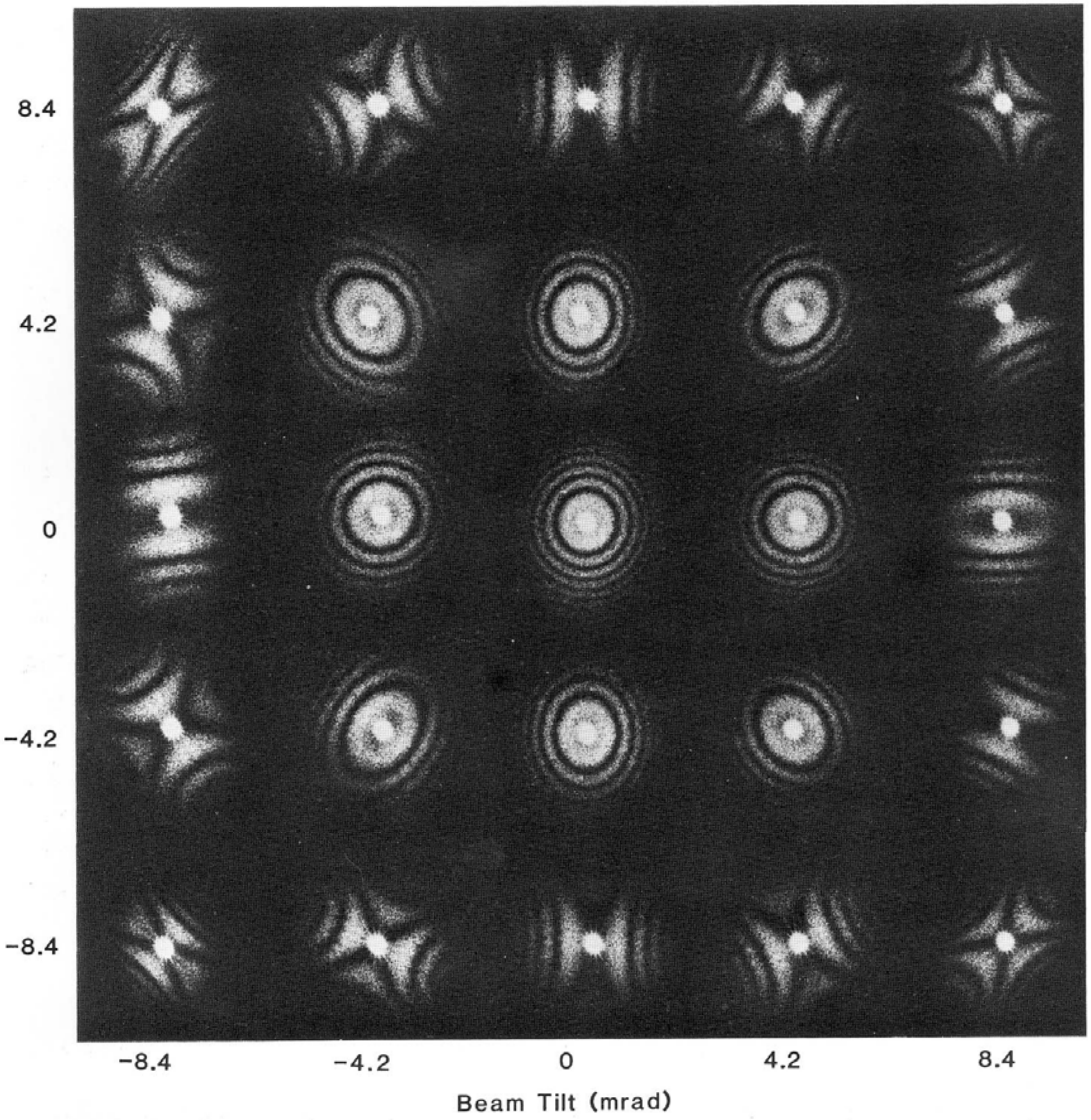


FIGURE 12.8 Diffractograms showing the effect of the tilt of the incident beam on the contrast transfer. Intentional beam tilt is proportional to the distance of the diffractogram from the center of the tableau. Micrographs were taken on the Siemens 102 at 125 kV.

O.L.Krivanek: Chapter 12 <<HRTEM>>, Editors: P.R.Buseck, J.M.Cowley, L. Eyring. Oxford Univ. Press, 1988, pp 546.

考虑高级象差的衍射图列

- 实际的高分辨电子显微术和象差校正电镜测量象差要求更高。束倾斜 τ 的引入，使的表达式复杂化，同时也使欠焦及象散的表达式复杂化。
- **S.Uhlemann**等［**S.Uhlemann & M.Haider: Ultramicroscopy 72 (1998) 119**］给出欠焦（Δ**f**＝**C1**）和象散**(A1)**与束倾斜相关联的表达式:

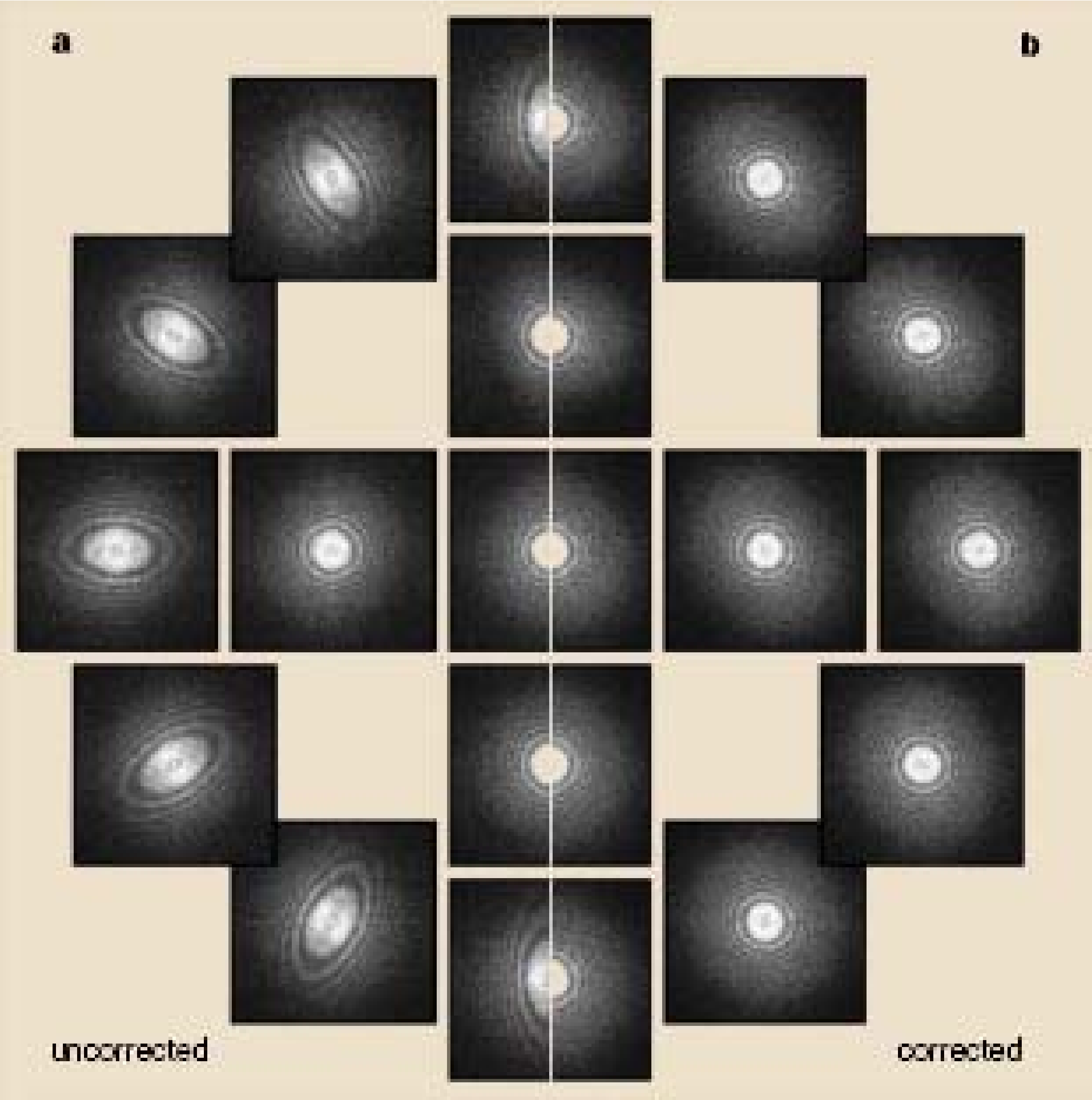
$$C_1(\tau) = C_1(0) + 4\,\mathrm{Re}\{\tau B_2\} + 2\tau\tilde{\tau}C_3 + 6\,\mathrm{Re}\{\tau^2 S_3\} + 12\,\mathrm{Re}\{\tau^2\tilde{\tau}B_4\} + 8\,\mathrm{Re}\{\tau^3 D_4\} + 3(\tau\tilde{\tau}^2)C_5 + \cdots$$

$$A_1(\tau) = A_1(0) + 2\tau\tilde{B}_2 + 2\tilde{\tau}A_2 + \tau^{e}C_3 + 6\tau\tilde{\tau}\tilde{S}_3 + 3\tau^2 A_3 + 2\tau^2 B_4$$

$$+ 6\tau^2\tilde{\tau}B_4 + 12\tau\tilde{\tau}^2 D_4 + 4\tau^3 A_4 + 2\tau^3\tilde{\tau}C_5 + 5\tau^4 A_5 + \cdots$$

高级象差值的测量

- 式中**A,B…**的象差含义已如前述，并且它们是束对中时的量值。如果我们在系列的τ值记录衍射图，并测量相应的**C1**及**A1**，则一套衍射图从上述公式中两个方程将给出有关象差系数的充盈的解。进一步用最小二乘法数据处理得到各高级象差的值。
- 得到这些值后，返馈给电镜的计算机，控制有关多极透镜组的参数，从而校正象差。

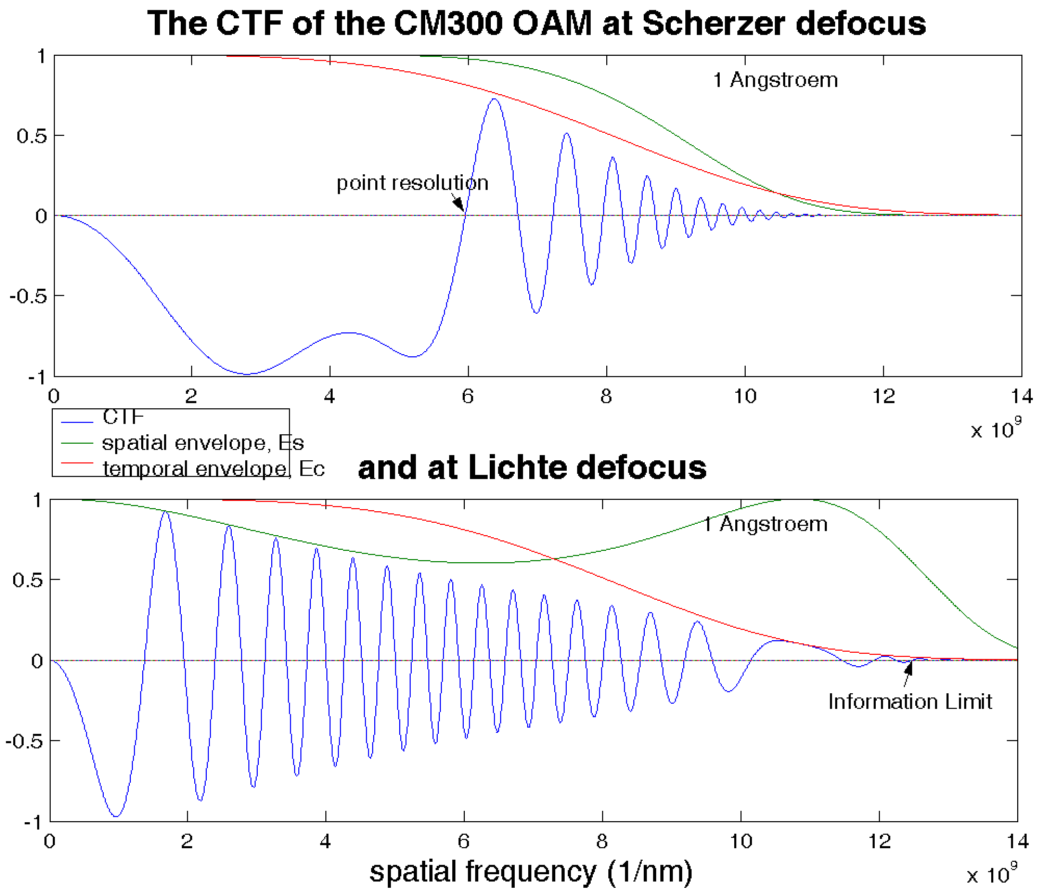


利用无定形膜在已知倾角时记录下来的衍射图测量并调节象差。左半部是象差未校正的情况，在倾斜时衍射图呈椭园形；右半部是象差校正的情况，在各方位都看不到象差的影响。束倾斜角为**10.8毫弧度，M.Haider, S.Uhlemann, E.Schwan, H.Rose, B.Kabius and K.Urban : Nature, 392 (1998) 768.**

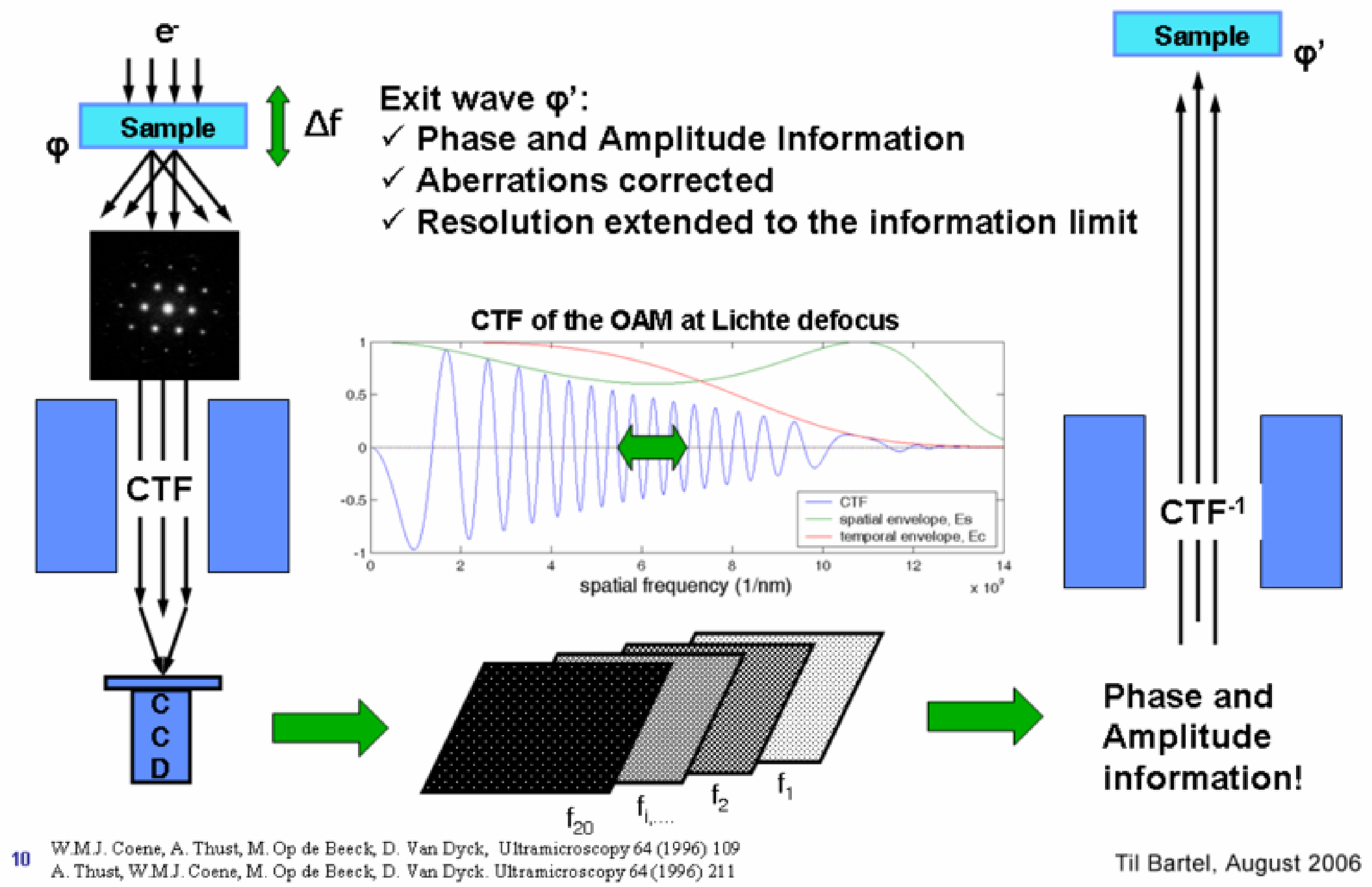
象差校正技术

系列欠焦
电子全息
象差校正器

充分利用点分辨与信息分辨之间的余量



利用系列欠焦重构出射波的策略



Exit wave φ':

- ✓ Phase and Amplitude Information
- ✓ Aberrations corrected
- ✓ Resolution extended to the information limit

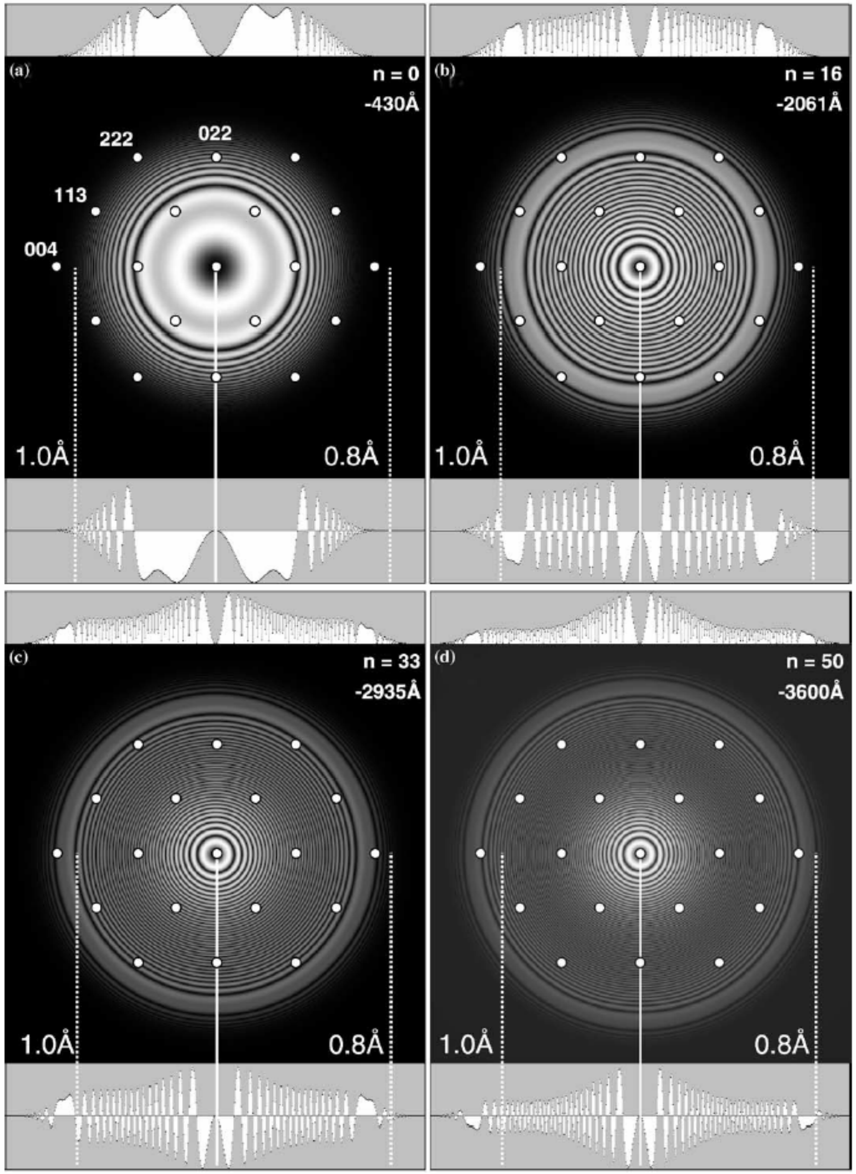
Phase and Amplitude information!

W.M.J. Coene, A. Thust, M. Op de Beeck, D. Van Dyck, Ultramicroscopy 64 (1996) 109
A. Thust, W.M.J. Coene, M. Op de Beeck, D. Van Dyck. Ultramicroscopy 64 (1996) 211

Til Bartel, August 2006

重构金刚石[110]像要（111），（220），（113），（400）等衍射波无畸变地传递

M.A. O’Keefe et al., Ultramicroscopy 89 (2001) 215–241



14. CTF (lower) and diffractograms (1-D top and 2-D center) computed for OÅM parameters. Diamond [1 1 0] diffraction spots marked on the 2-D diffractograms. Defocus and the number of zero-crossings before the main passband (n) are marked. (a) erzer defocus. (b) $n = 16$. (c) Lichte defocus for 0.8 Å. (d) $n = 50$ to reach the 0.8 Å OÅM information limit.

各衍射波在不同欠焦值传递权重不同，还要考虑部分相干性的影响

M.A. O’Keefe et al., Ultramicroscopy 89 (2001) 215–241

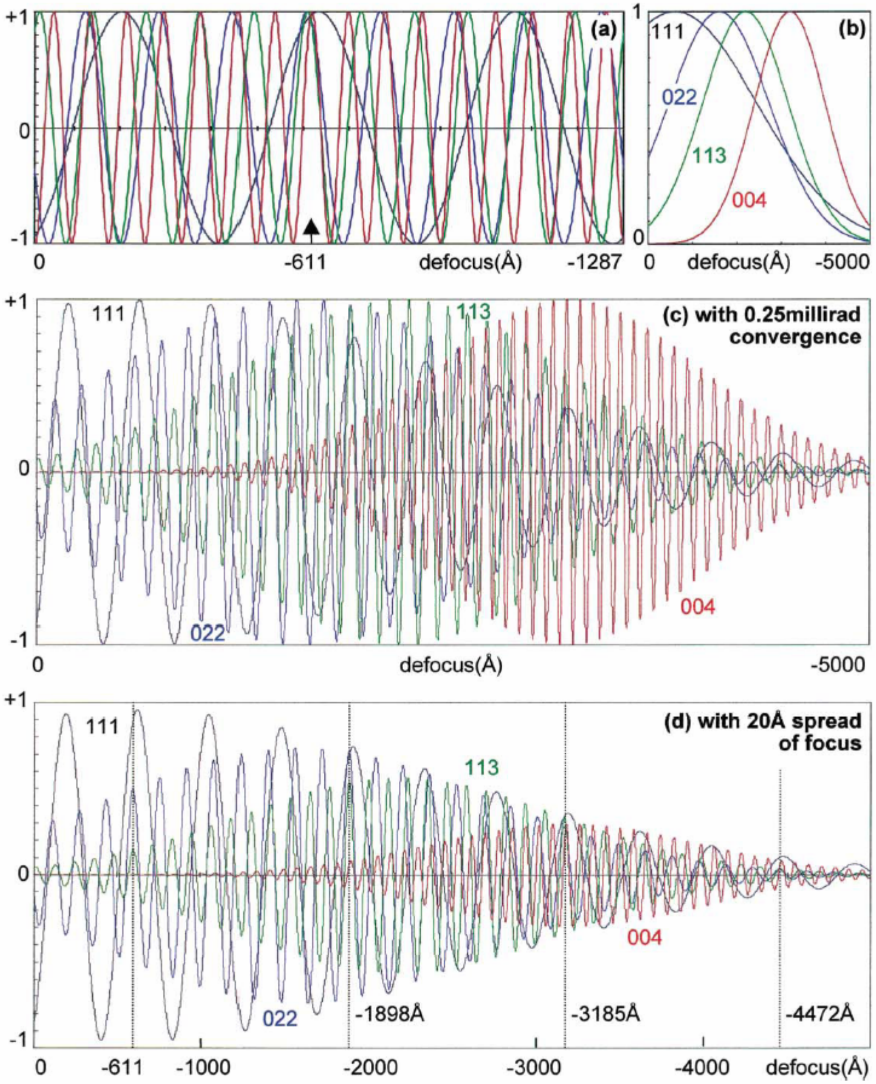
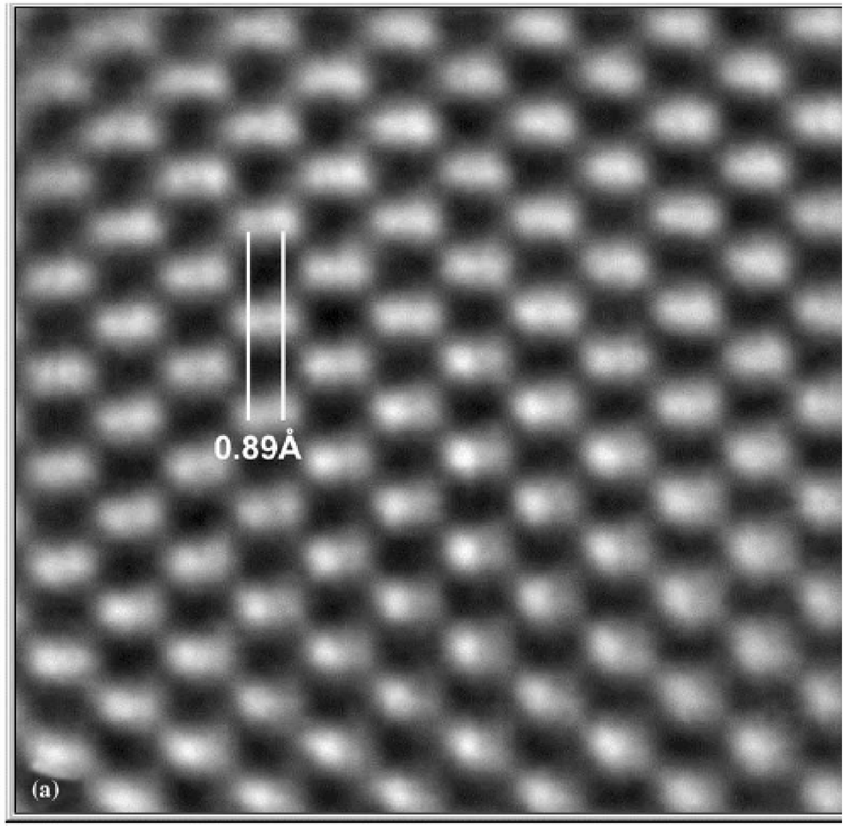


Fig. 12. Conditions for focal-series information retrieval for diamond. (a) Plot of sin $\chi(u)$ shows oscillatory transfer of diffracted-beam amplitudes with defocus over one Fourier period for the projected [1 1 0] diamond unit cell. Arrow at −611 **Å** defocus marks a fortuitous AFF condition. (b) Incident-beam convergence of 0.25 mrad defines four defocus ranges centered on each beam’s alpha-null defocus. (c) With convergence applied, oscillatory transfer is confined to four Gaussian packets with alpha-limits of $\pm\varepsilon_{\alpha}^{2\sigma}$ centered on each alpha-null defocus. (d) Inclusion of spread-of-focus reduces transfer for higher spatial frequencies.

校正A_2像（左）与出射波重构像（右）



M.A. O’Keefe et al., Ultramicroscopy 89 (2001) 215–241

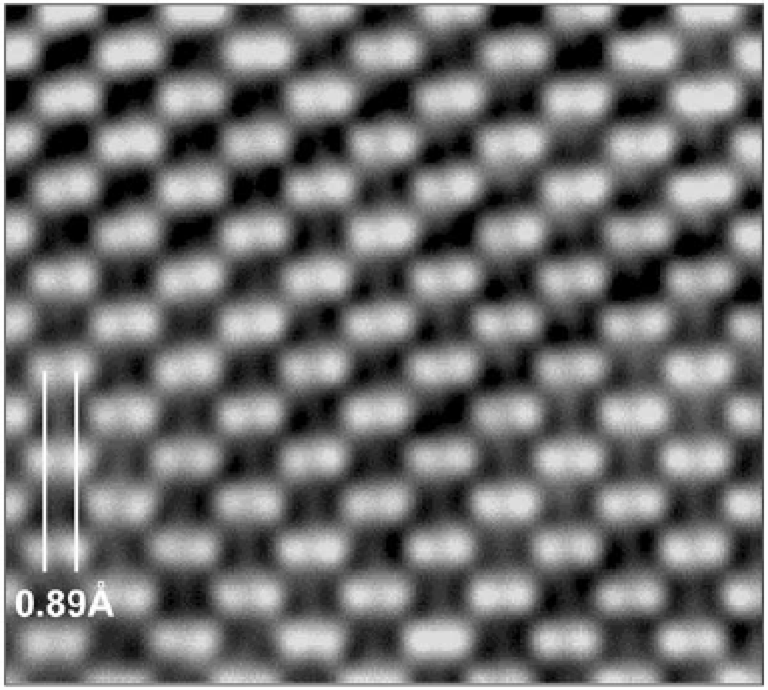


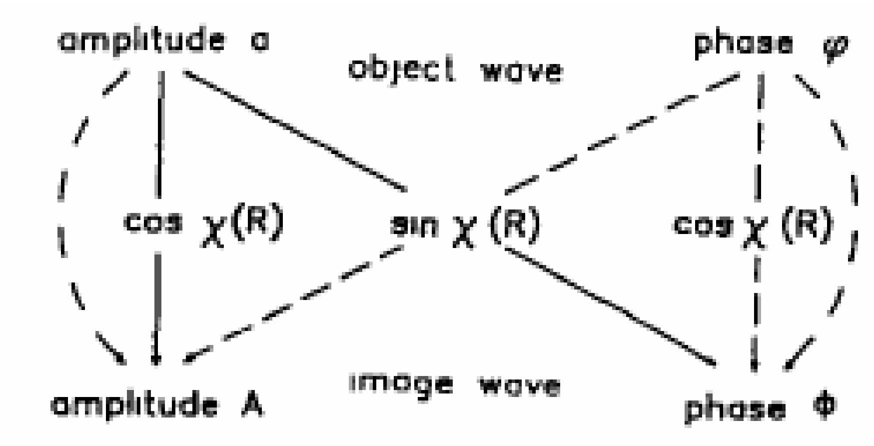
Fig. 15. Phase image of [1 1 0] diamond reconstructed from OÅM focal series using the Philips/Brite-Euram software shows 0.89 Å resolution (marked).

电子全息校正象差

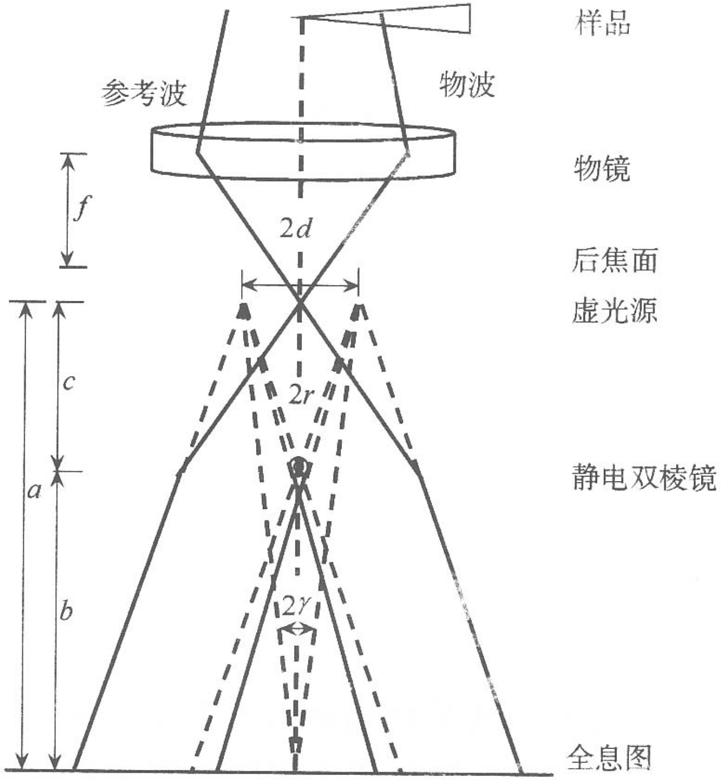
- Gabor上世纪四十年代提出用干涉波将电子波的振幅、相位同时纪录下来，进一步扣除电子透镜象差附加相位的影响，以提高像的质量。
- 当时电子源的相干性不好。上世纪六十年来，相干性极好的激光问世，光学全息术得到快速发展。
- 上世纪90年代，FEG出现大大改善电子源相干性，电子全息重新活跃起来。

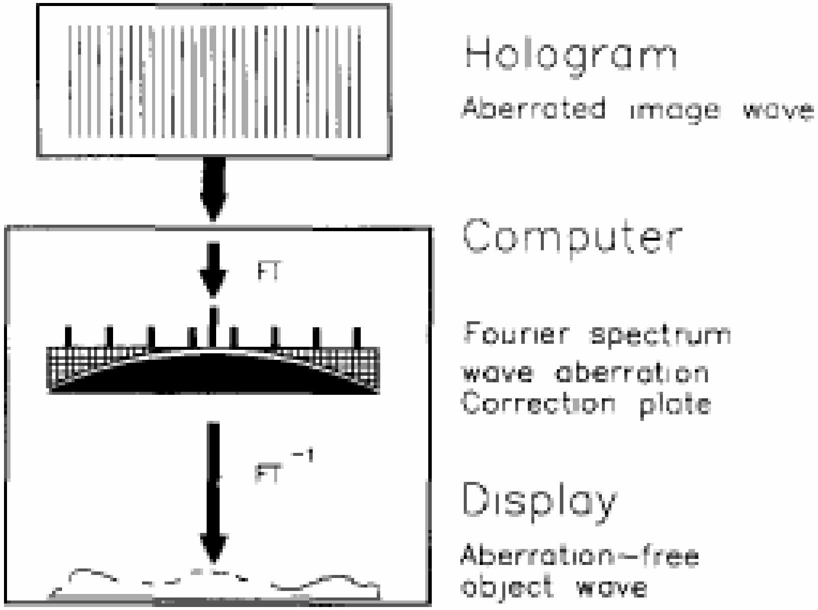
电子全息的策略

- 试样下表面出射波振幅部分由吸收项代表，相位部分由势投影代表：$q(x,y)=\exp\{-i\sigma\phi(x,y)-\mu(x,y)\}$,对于弱相位与弱吸收物体，展开得：$q(x,y)=1-i\sigma\phi(x,y)-\mu(x,y)$.
- 在物镜后焦面，考虑到象差函数影响：$Q(u,v)=[\delta(u,v)-M(u,v)-i\sigma\Phi(u,v)]\exp\{i\chi\}=\delta(u,v)-M(u,v)\cos\chi+\sigma\Phi(u,v)\sin\chi-i\{\sigma\Phi(u,v)\cos\chi\}$



电子全息几何光路及重构





采用双棱镜得到0.0083nm条纹

Ken Harada at al.,
Proceedings of 8APEM,
Kazakawa, Japan, pp 90.

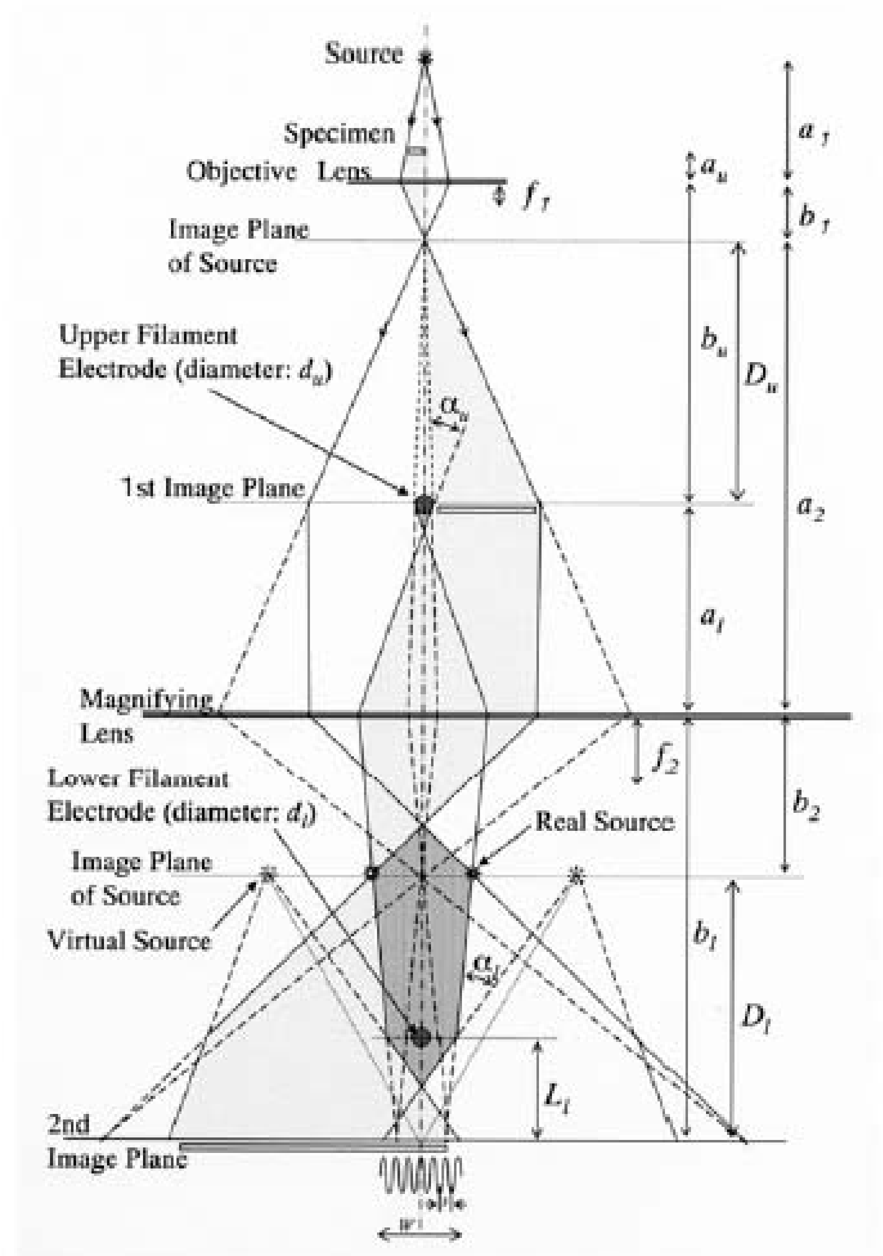
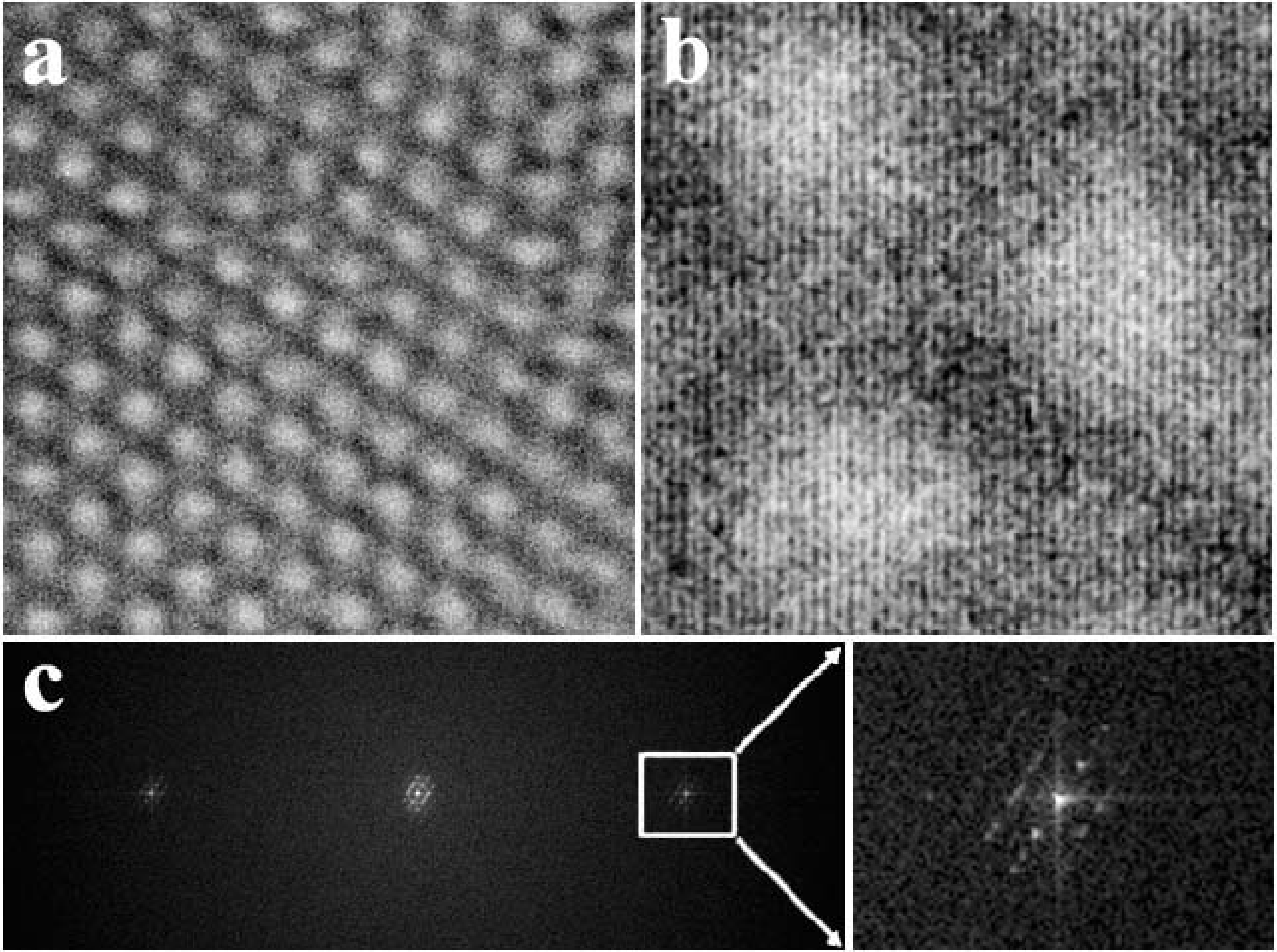


Figure 1 Optical set-up of double-biprism electron holography.

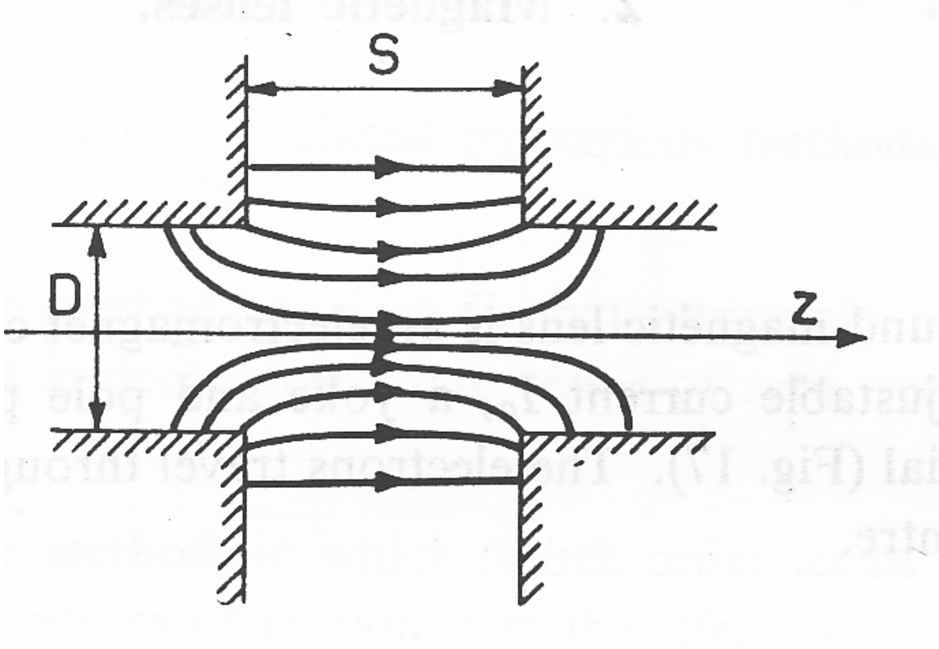


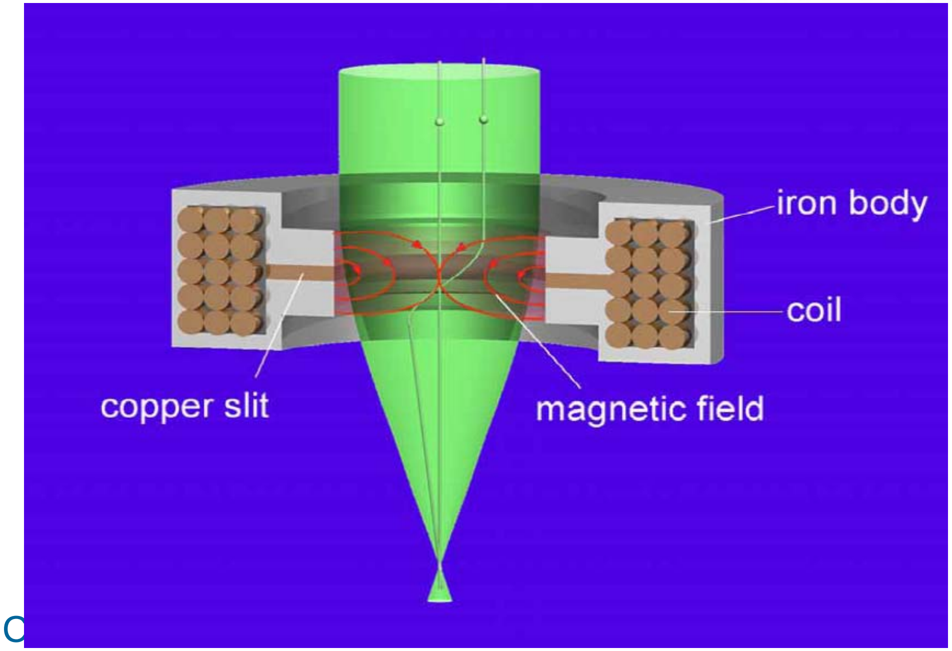
Ken Harada at al., Proceedings of 8APEM, Kazakawa, Japan, pp 100.

象差校正器

电子在电子透镜中的运动轨迹

- 在右图的磁电子透镜中，磁场强度大部分是平行于光轴的。按电子受力公式，$F=e\boldsymbol{v}\times\boldsymbol{B}$,在电子刚刚进入透镜时，磁场有径向分量，它使电子绕轴转。所产生的角速度将受轴向磁场施予的径向力，使电子总是朝向光轴弯折。





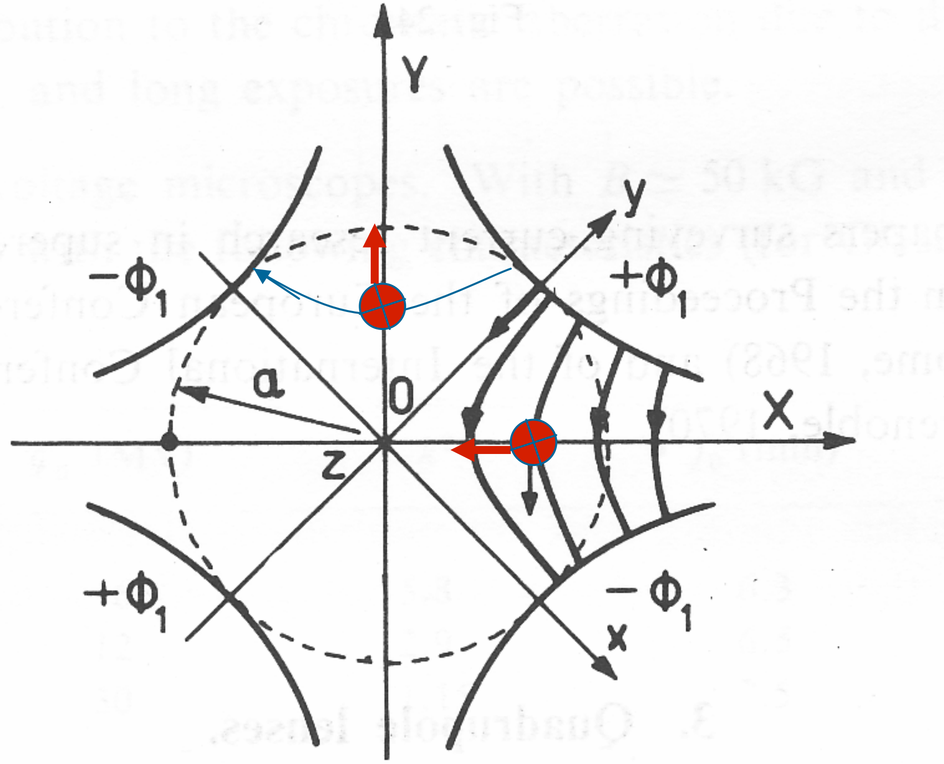
球（色）差校正的困难

- Scherzer在1936年指出:由于电子磁透镜的园对称性,球差不可校正。但在1948年他又指出,采用多极透镜可以校正象差。经过近半个世纪的努力,人们认识 到,由于多极透镜及相应伴随透镜的复杂安排,仅靠人工调节对中 是不可能的。

O.Scherzer, (1936) Z.Phys. 101, 23;
(1948) Optik 4, 258

四极透镜

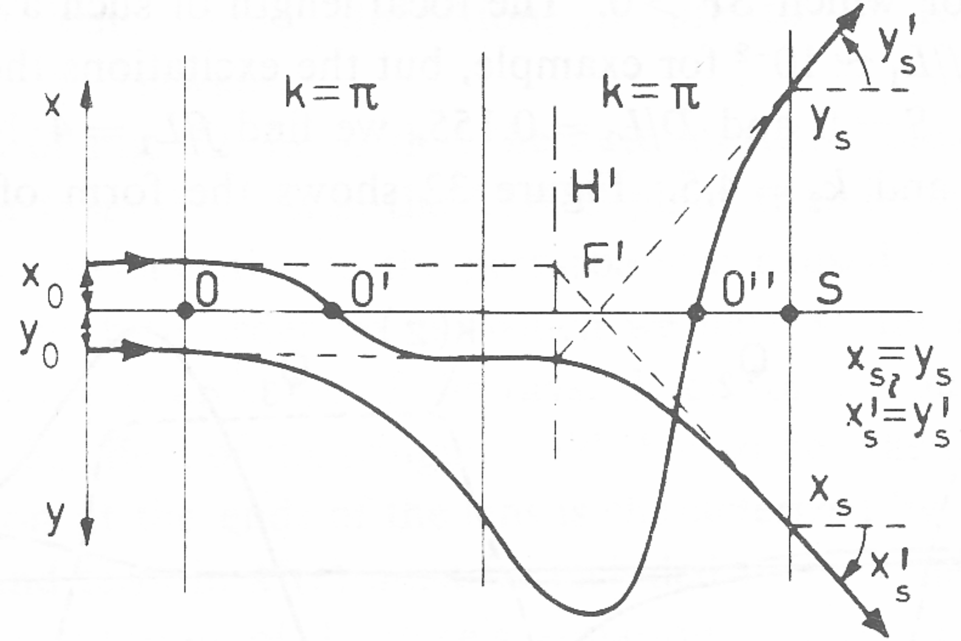
- 不像园透镜，四极透镜场分布是横向的（两端除外）。从定性分析就可以看出，如果电子从纸面朝里走去，则在OX平面受到向光轴弯折的力，光束是会聚的；而在OY平面则受到背向光轴的力，光束是发散的。这说明，有可能用这一点校正球差。



A.Septier: Chapter 2, in <<Electron Microscopy in Material Science>>, U.Valdre Edited, (1971) AP, p14-73.

四极透镜象差校正器

- 为了得到光学系统使所有方向的电子束轨迹都是会聚的（或都是发散的），需求两组四极透镜。使Q_1的会聚面C与Q_2的发散面D重合起来。通过调节透镜的激发k，并使两个四极透镜的激发同步相等，有可能得到如右图的轨迹图。
- 实际上这样简单的四极透镜组合不易得到园对称的线列。为此中间还要加一些用作传输和改善对称性的组件，如八极透镜、弱的园透镜等。



A.Septier: Chapter 2, in <<Electron Microscopy in Material Science>>, U.Valdre Edited, (1971) AP, p14-73.

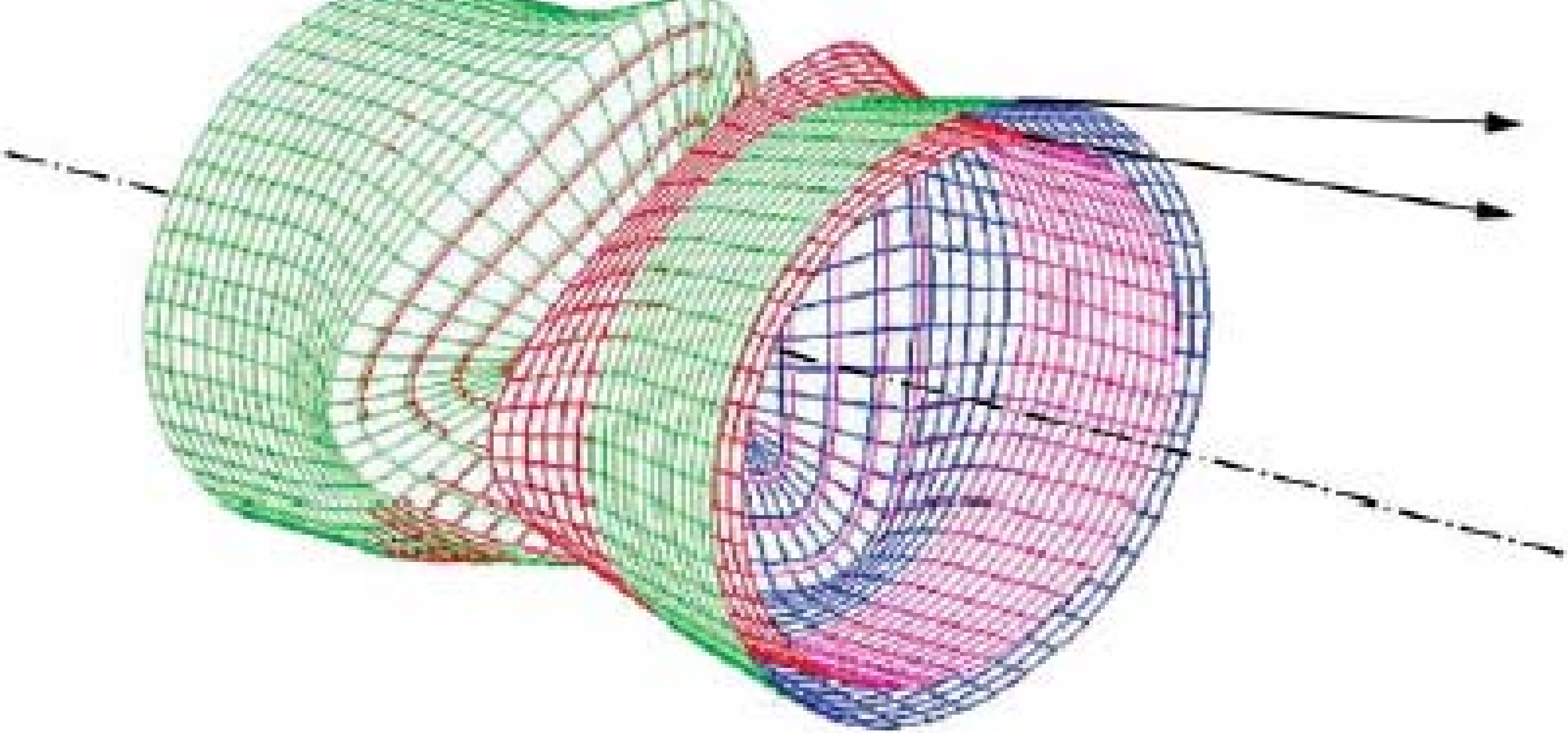
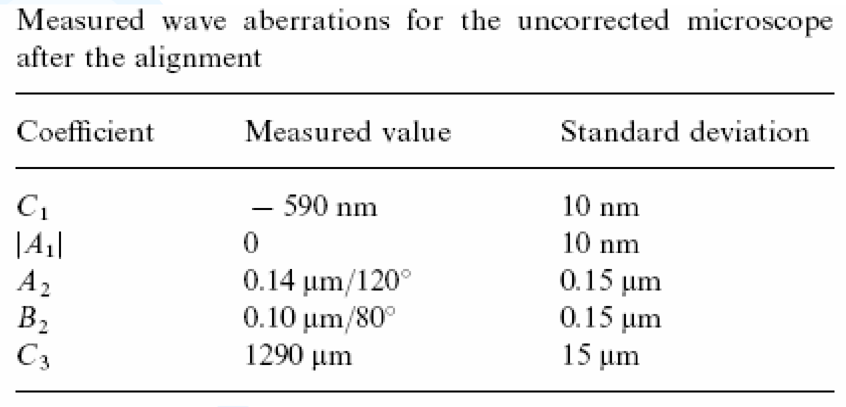


Figure 2 : Ray path through the hexapole Cs-corrector consisting of two hexapoles (rectangular boxes), which are separated by a telecentric round lens couple. It can be seen that the outer ray-path (green) is tilted away from the optical axis in order to compensate for the spherical aberration of the objective lens. Figure courtesy of Dr. S. Uhlemann, CEOS GmbH.

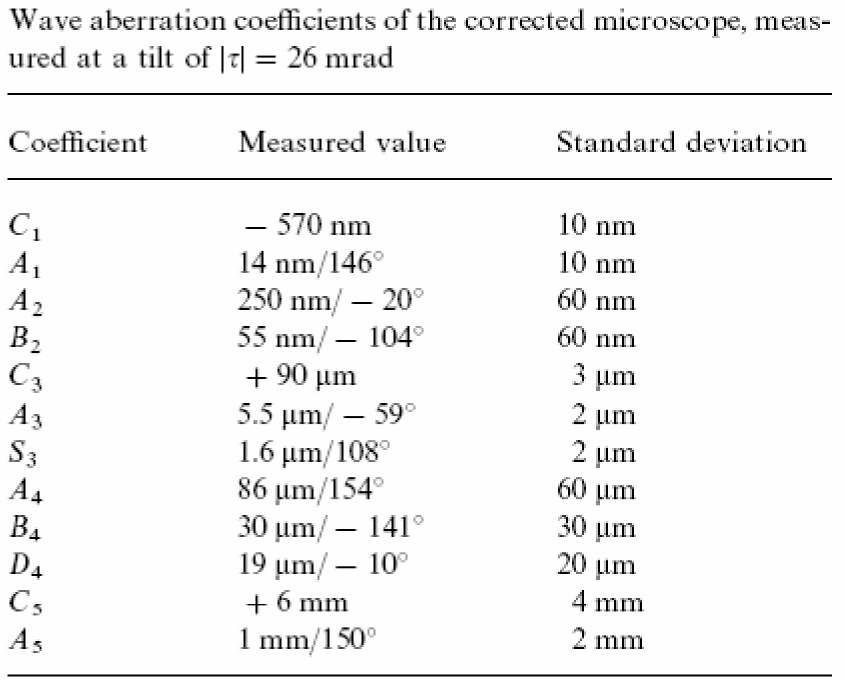
六极透镜用于TEM,1998年



Measured wave aberrations for the uncorrected microscope after the alignment

Coefficient	Measured value	Standard deviation
C_1	-590 nm	10 nm
$\|A_1\|$	0	10 nm
A_2	0.14 μm/120°	0.15 μm
B_2	0.10 μm/80°	0.15 μm
C_3	1290 μm	15 μm

S.Uhlemann & M.Haider: Ultramicroscopy 72 (1998) 119.



Wave aberration coefficients of the corrected microscope, measured at a tilt of $|\tau| = 26$ mrad

Coefficient	Measured value	Standard deviation
C_1	-570 nm	10 nm
A_1	14 nm/146°	10 nm
A_2	250 nm/-20°	60 nm
B_2	55 nm/-104°	60 nm
C_3	$+90$ μm	3 μm
A_3	5.5 μm/-59°	2 μm
S_3	1.6 μm/108°	2 μm
A_4	86 μm/154°	60 μm
B_4	30 μm/-141°	30 μm
D_4	19 μm/-10°	20 μm
C_5	$+6$ mm	4 mm
A_5	1 mm/150°	2 mm

四极透镜用于STEM, 2001年

N.Dellby, O.L.Krivanek, P.D.Nellist, P.E.Batson, and R.Lupini: J. of EM, 50(3) (2001) 177.

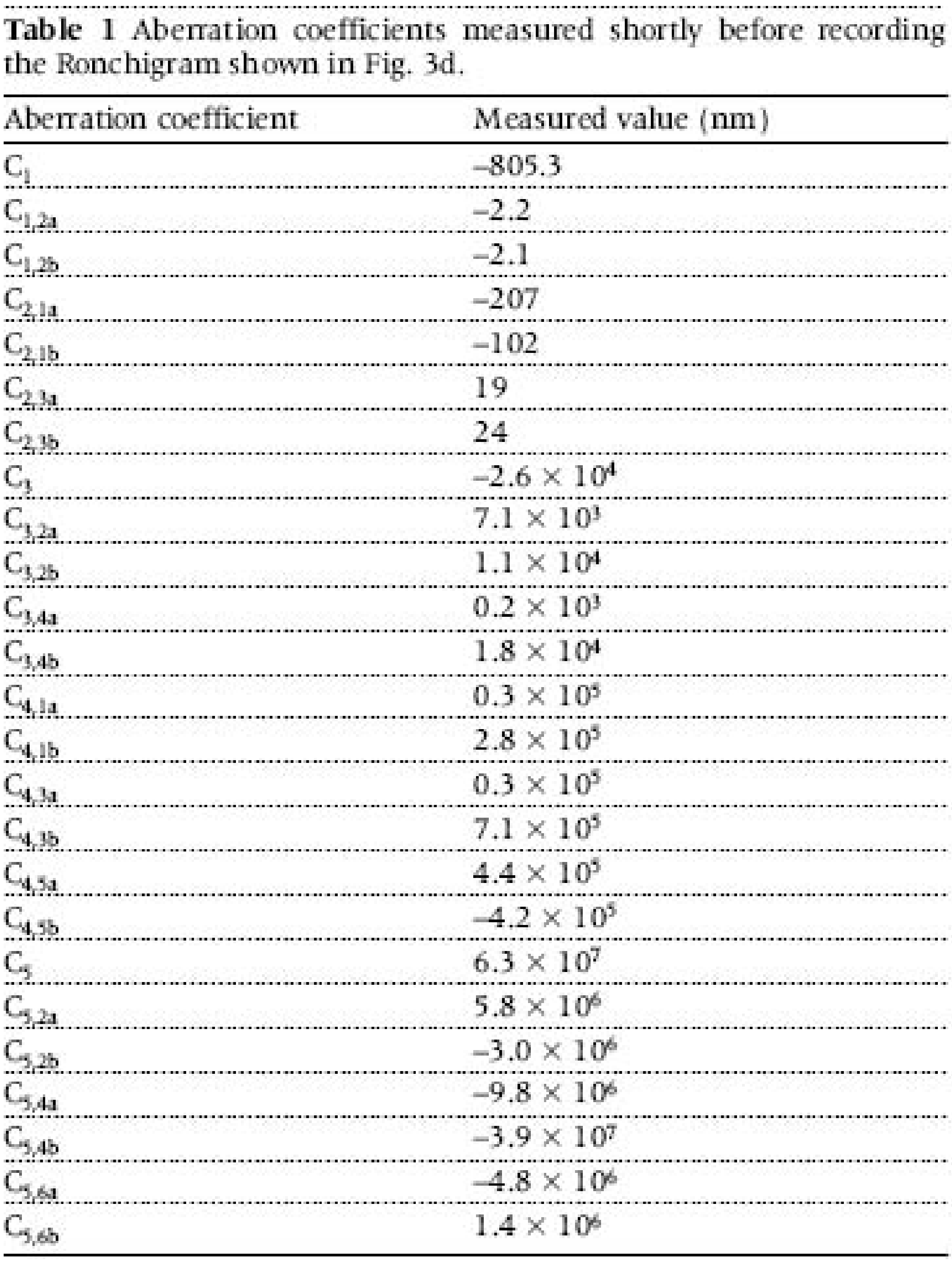
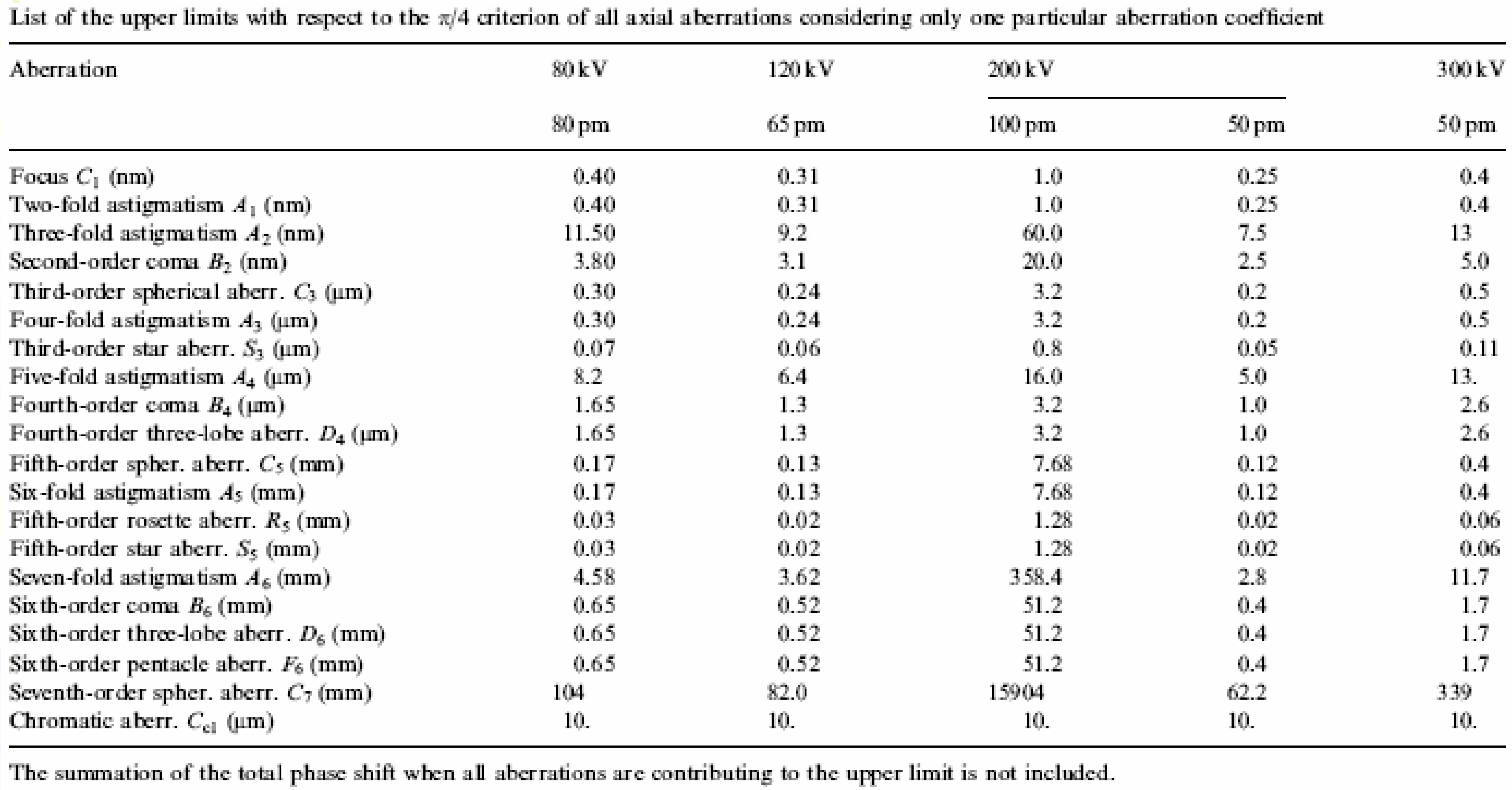


Table 1 Aberration coefficients measured shortly before recording the Ronchigram shown in Fig. 3d.

Aberration coefficient	Measured value (nm)
C_1	–805.3
$C_{1,2a}$	–2.2
$C_{1,2b}$	–2.1
$C_{2,1a}$	–207
$C_{2,1b}$	–102
$C_{2,3a}$	19
$C_{2,3b}$	24
C_3	-2.6×10^4
$C_{3,2a}$	7.1×10^3
$C_{3,2b}$	1.1×10^4
$C_{3,4a}$	0.2×10^3
$C_{3,4b}$	1.8×10^4
$C_{4,1a}$	0.3×10^5
$C_{4,1b}$	2.8×10^5
$C_{4,3a}$	0.3×10^5
$C_{4,3b}$	7.1×10^5
$C_{4,5a}$	4.4×10^5
$C_{4,5b}$	-4.2×10^5
C_5	6.3×10^7
$C_{5,2a}$	5.8×10^6
$C_{5,2b}$	-3.0×10^6
$C_{5,4a}$	-9.8×10^6
$C_{5,4b}$	-3.9×10^7
$C_{5,6a}$	-4.8×10^6
$C_{5,6b}$	1.4×10^6

对于π/4标准的像差校正起码要求，2008年



List of the upper limits with respect to the π/4 criterion of all axial aberrations considering only one particular aberration coefficient

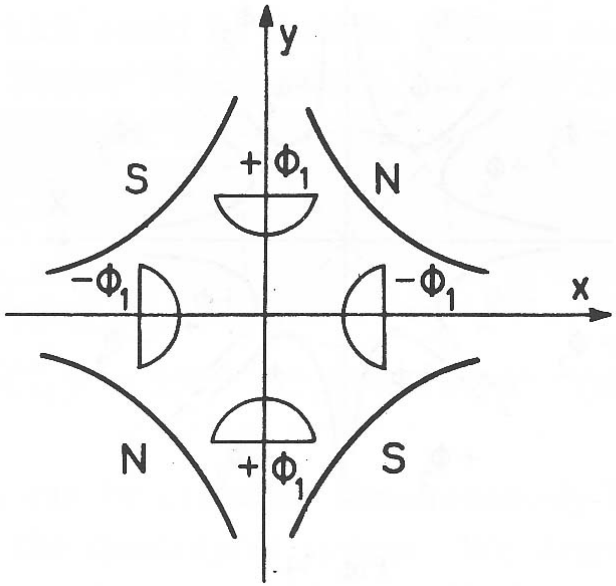
Aberration	80 kV	120 kV	200 kV		300 kV
	80 pm	65 pm	100 pm	50 pm	50 pm
Focus C_1 (nm)	0.40	0.31	1.0	0.25	0.4
Two-fold astigmatism A_1 (nm)	0.40	0.31	1.0	0.25	0.4
Three-fold astigmatism A_2 (nm)	11.50	9.2	60.0	7.5	13
Second-order coma B_2 (nm)	3.80	3.1	20.0	2.5	5.0
Third-order spherical aberr. C_3 (μm)	0.30	0.24	3.2	0.2	0.5
Four-fold astigmatism A_3 (μm)	0.30	0.24	3.2	0.2	0.5
Third-order star aberr. S_3 (μm)	0.07	0.06	0.8	0.05	0.11
Five-fold astigmatism A_4 (μm)	8.2	6.4	16.0	5.0	13.
Fourth-order coma B_4 (μm)	1.65	1.3	3.2	1.0	2.6
Fourth-order three-lobe aberr. D_4 (μm)	1.65	1.3	3.2	1.0	2.6
Fifth-order spher. aberr. C_5 (mm)	0.17	0.13	7.68	0.12	0.4
Six-fold astigmatism A_5 (mm)	0.17	0.13	7.68	0.12	0.4
Fifth-order rosette aberr. R_5 (mm)	0.03	0.02	1.28	0.02	0.06
Fifth-order star aberr. S_5 (mm)	0.03	0.02	1.28	0.02	0.06
Seven-fold astigmatism A_6 (mm)	4.58	3.62	358.4	2.8	11.7
Sixth-order coma B_6 (mm)	0.65	0.52	51.2	0.4	1.7
Sixth-order three-lobe aberr. D_6 (mm)	0.65	0.52	51.2	0.4	1.7
Sixth-order pentacle aberr. F_6 (mm)	0.65	0.52	51.2	0.4	1.7
Seventh-order spher. aberr. C_7 (mm)	104	82.0	15904	62.2	339
Chromatic aberr. C_{c1} (μm)	10.	10.	10.	10.	10.

The summation of the total phase shift when all aberrations are contributing to the upper limit is not included.

M. Haider, H. Muller, S. Uhlemann, J. Zach, U. Loebau, R. Hoeschen:Ultramicroscopy 108 (2008) 167–178

色差校正器

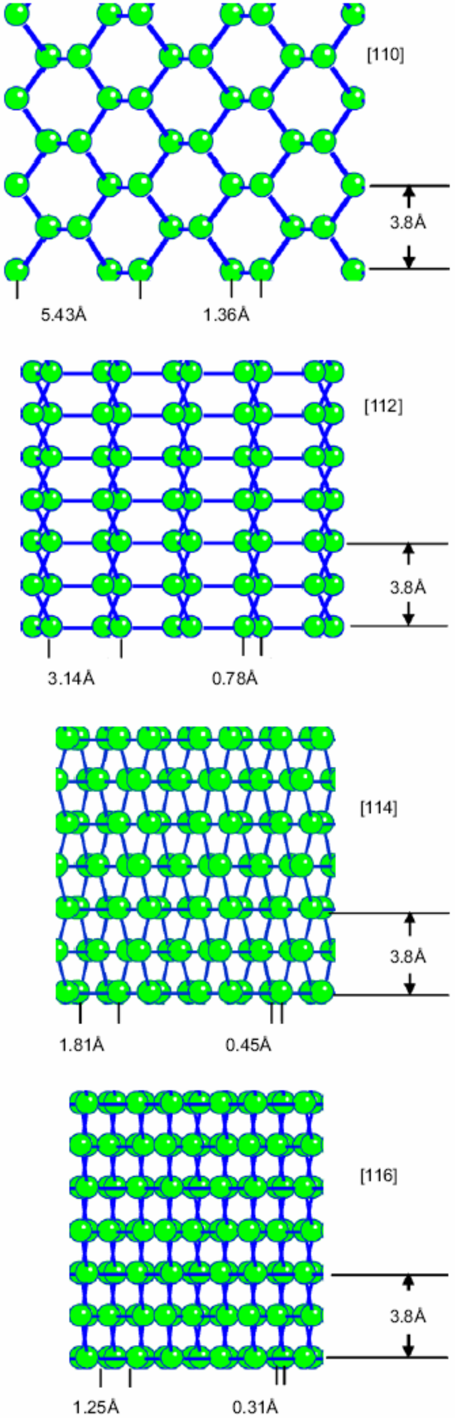
- 用静电透镜和磁透镜混合组成的四极透镜，在xoz平面，如果磁透镜使电子束会聚，静电透镜则使之发散。相互调节的结果可补偿由于色差带来的偏离；在yoz面也有类似的情况。
- 在低压SEM中已有商品
- 在TEM中据说也在实验室研制成功（Hieder讲演，2008-10-15）

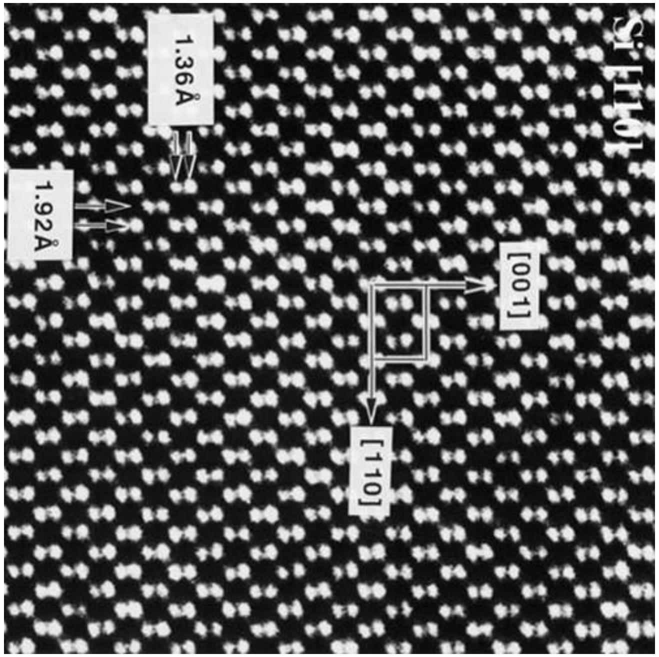


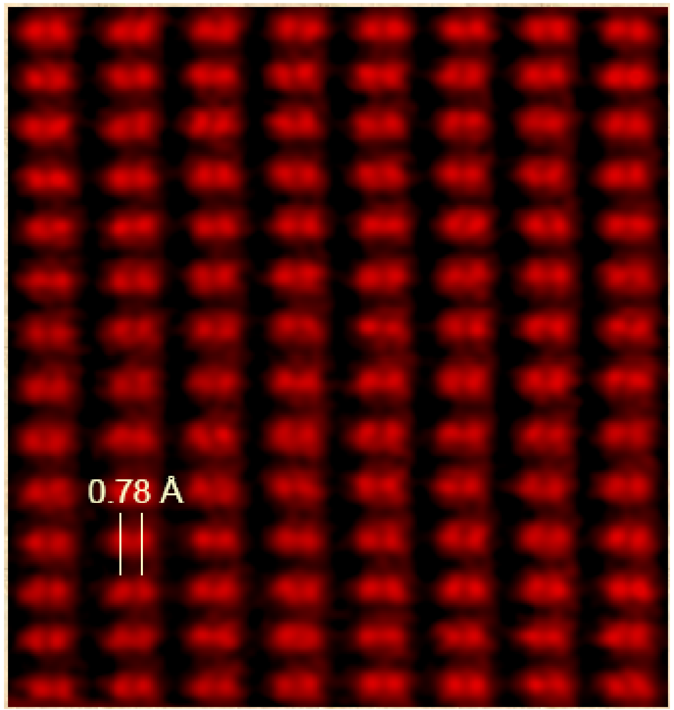
由象差校正电镜拓展的研究

提高分辨率

追求更高分辨的梦想





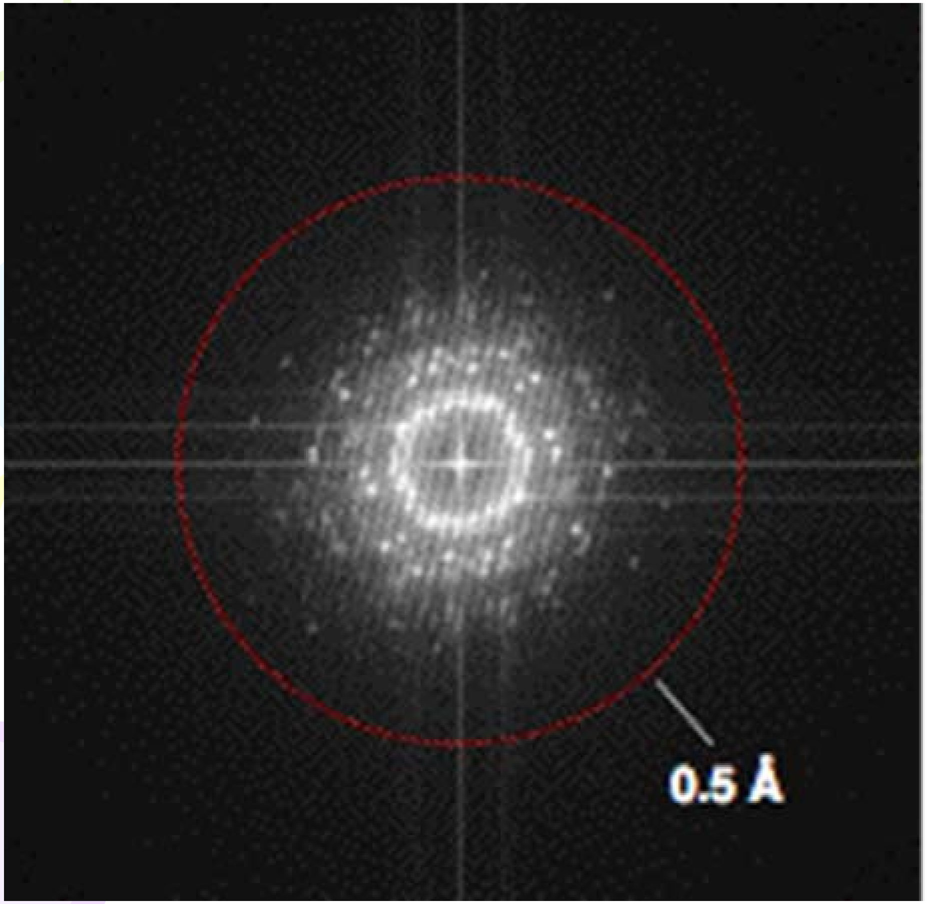


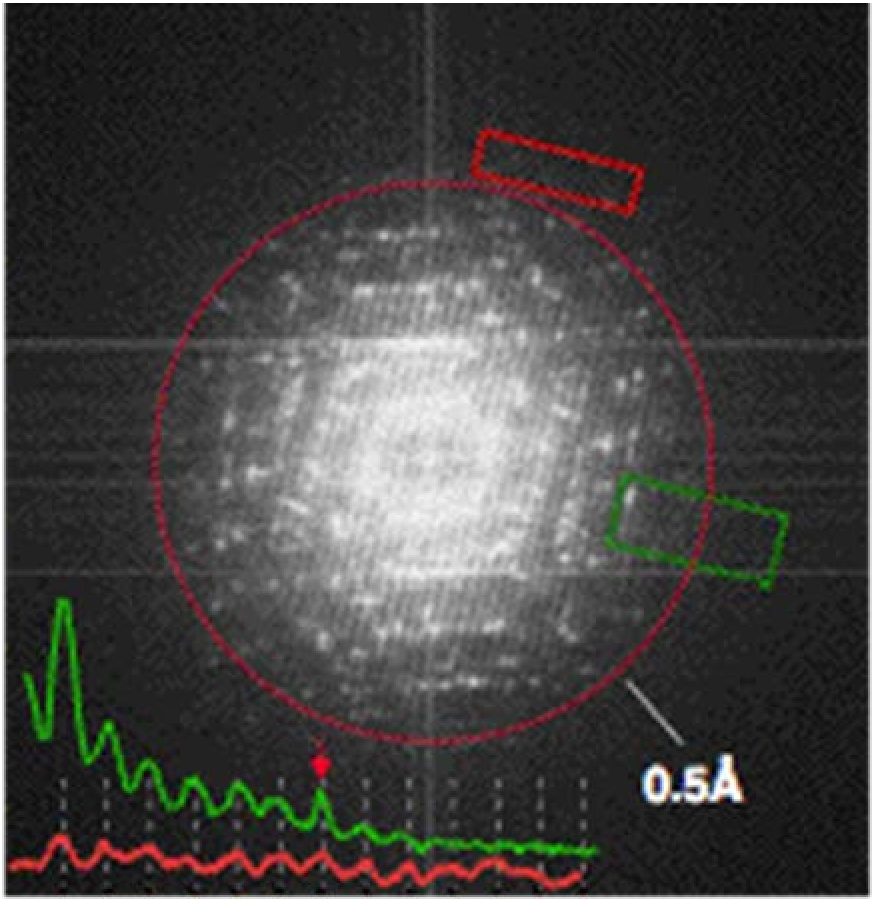
EM

P.D. Nellist et al., Science 305, (2004)1741.

2008/12/5

号称0.5埃分辨水平的杨氏干涉条纹

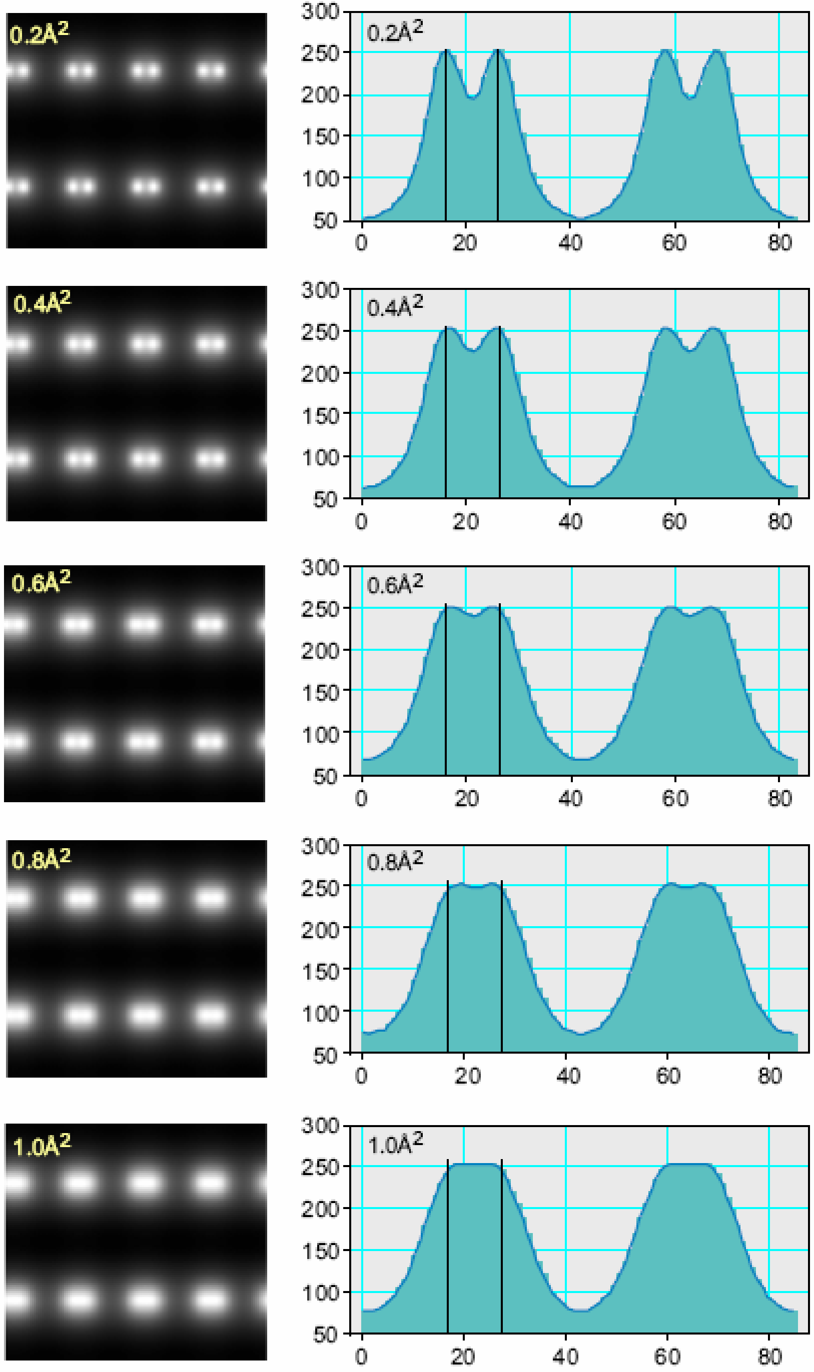




取自TEAM网站，（2008）

原子像

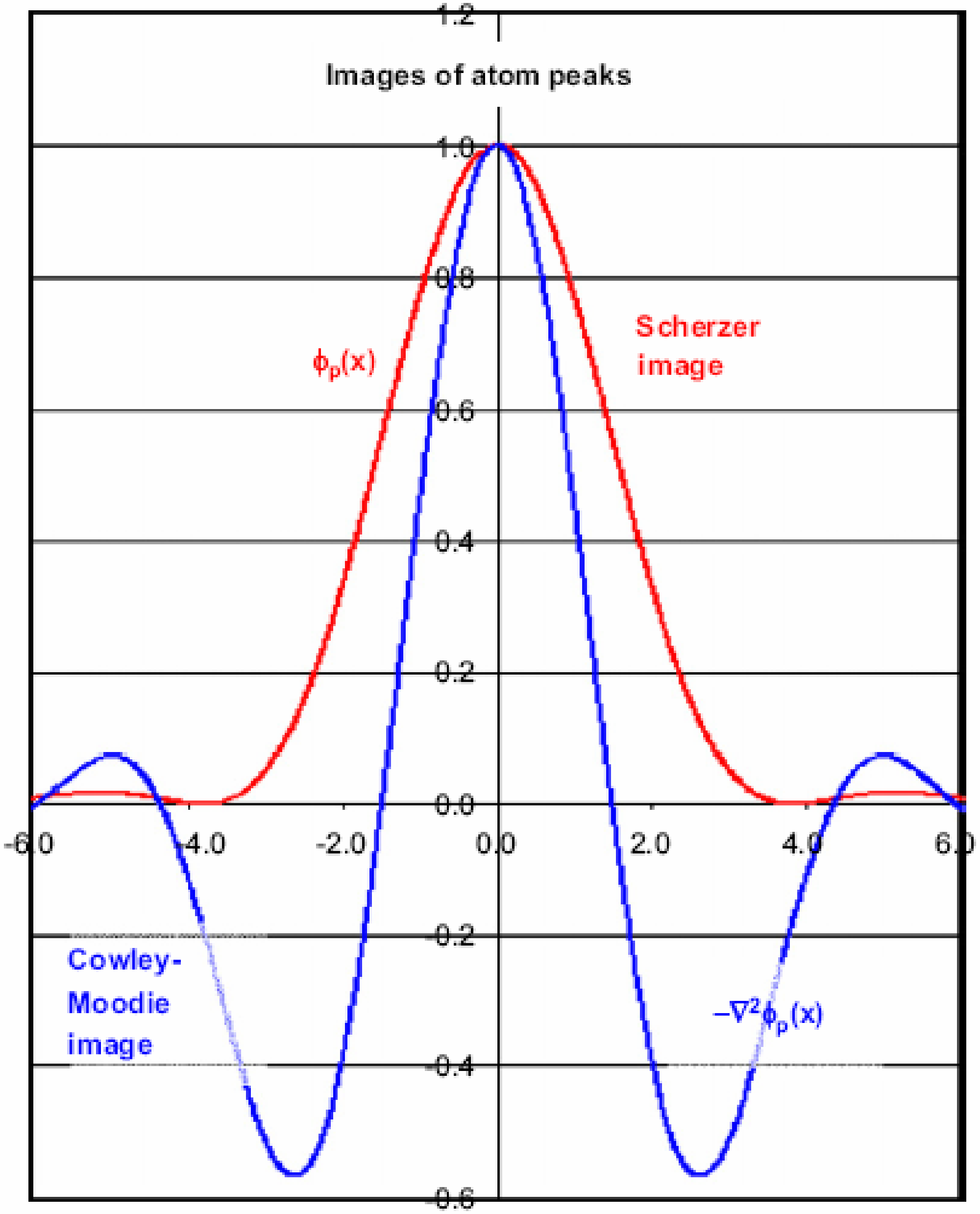
- 对于高分辨透射电子显微术而言，原子半径约在1埃左右，所以Scherzer像的分辨应在这个量级。如果象差校正电镜使分辨率提高到0.5埃，那么原子大小本身是不是也会成为妨碍成像的因素呢？以Si原子为例，按共价健半径为1.11 Å, 在［116］取向下，原子作为几何点的分隔为0.31 Å。但考虑原子热振动的Debye-Waller因子对硅来说是0.4668 Å^2,相应的1.11 Å的两个峰摆在0.31 Å两点上，由于热振动引致两峰重叠留下的峰之间的凹谷仅有强度差为12％左右，这不满足瑞利判据(M.A.O'Keefe: Ultramicroscopy 108 (2008)



投影电荷密度成像

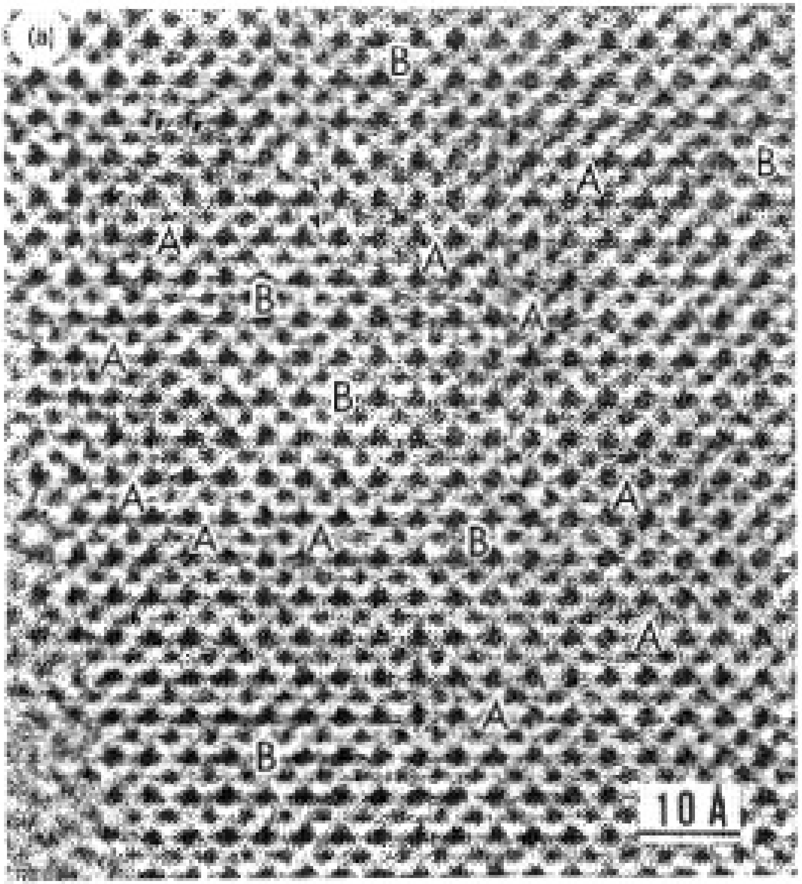
$$I = qq * \left[\frac{1-\sigma\lambda H\Delta f\nabla^2\phi_p(x)}{2\pi}\right]$$

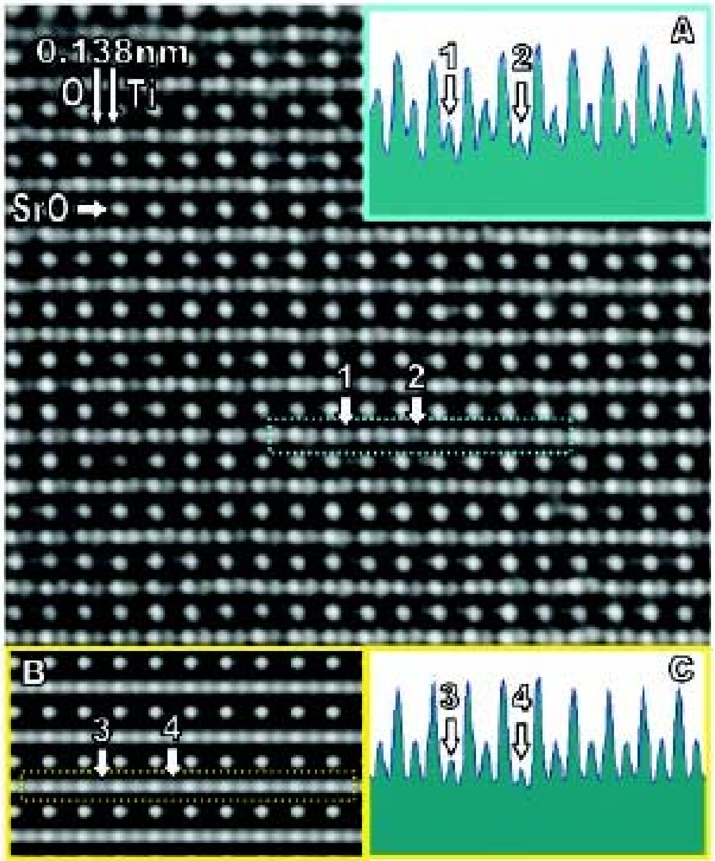
- 势场是静电产生，按泊松方程，势的二次微高是电荷密度的投影。衬度在Δf=0时为零，并随散焦符号面反转。而且在散焦是不大的前提下，衬度与离焦量成正比。图是投影势与其负的二次微商的比较[M.A.O’Keefe: Ultramicroscopy 108 (2008) 196]。显然，“电荷密度原子”要比“投影势原子”要小。但“电荷密度原子”的像有一个暗环相伴。



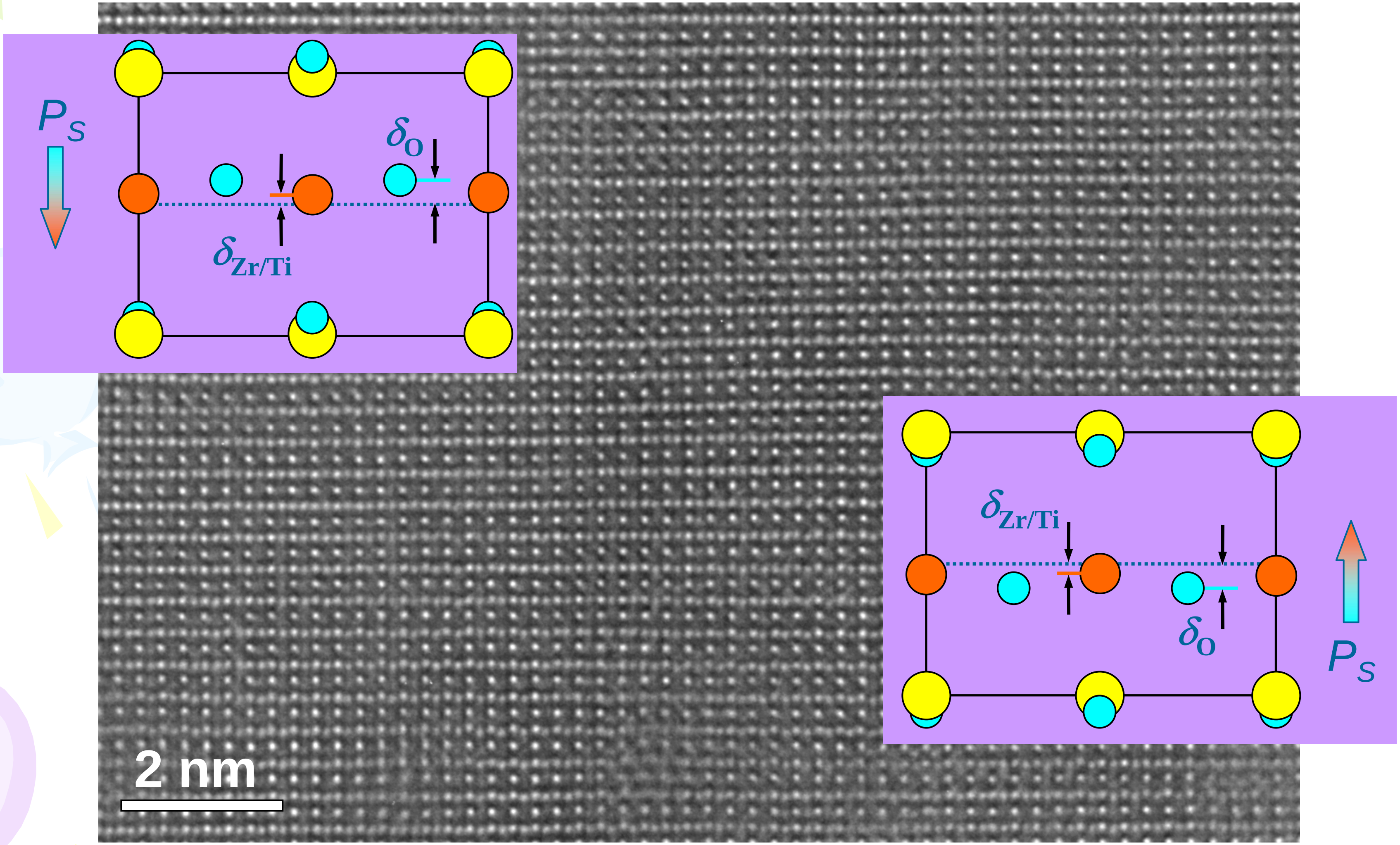
可能分辨轻元素

氧原子成像





直观观察化合物中轻原子一直是电子显微学中的难题。图左侧是**1994**年用分辨率为**1.1**埃的**1500**千伏超高压电镜观察高温超导体中氧原子像的图片**[S. Horiuchi, Y.Mastui and B.Okai: Jpn. J. Appl. Phys. 31 (1992) L59]**。大黑点对应金属原子位置，两大黑点之间有氧原子。但仅有少数地方能看到氧原子的影子，如图左上方黑箭头所示。右侧图则是球差校正电镜拍摄**ScTiO3(**与高温超导体同属钙钛矿结构**)**的氧原子像。这里金属原子和氧原子都成象为白亮点。由白箭头指示的氧原子位置清晰可见 **[C.L.Jia et al., Science 299 (2003) 870]**



P_S
δ_O
$\delta_{Zr/Ti}$
$\delta_{Zr/Ti}$
δ_O
P_S
2 nm

利用负球差成象有利于增强轻原子衬度：正球差（左）；负球差（右）

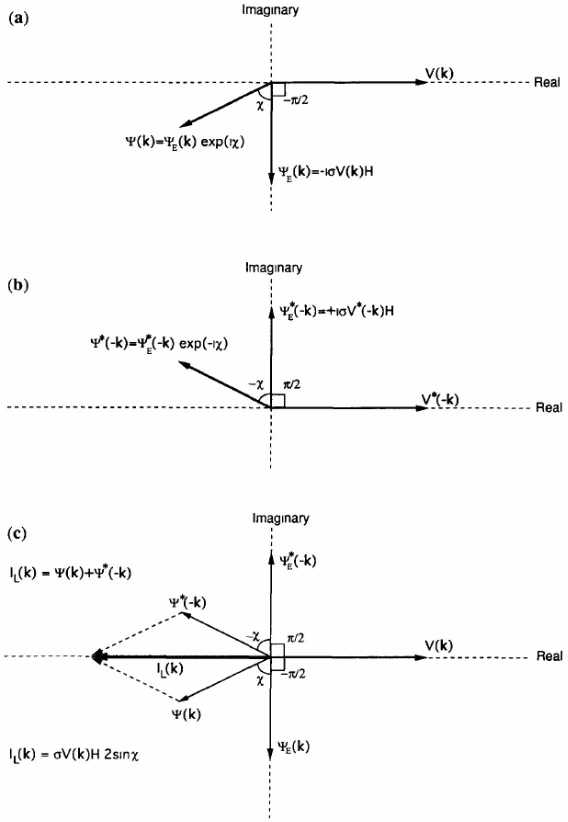
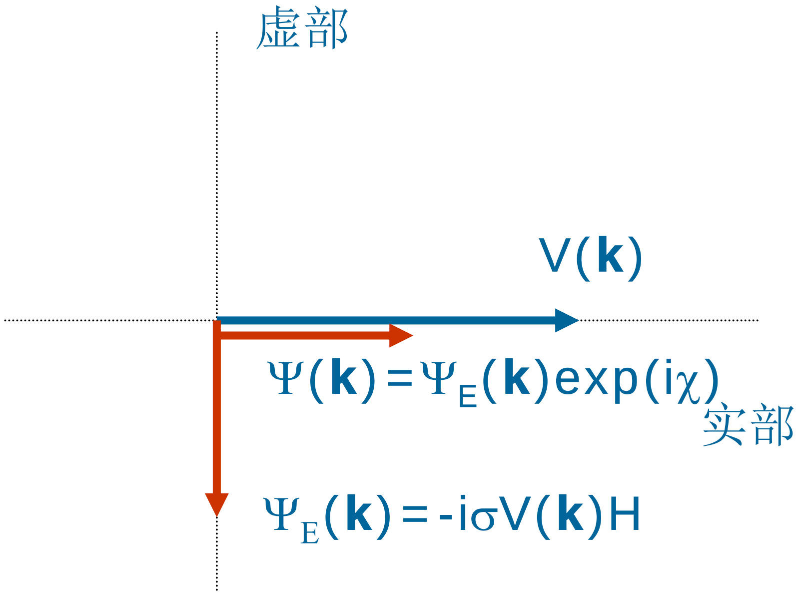


Fig 2 Argand diagrams showing the action of sin $\chi(\boldsymbol{k})$ under WPO conditions (a) Formation of the kth image amplitude component $\Psi(\boldsymbol{k})$ The specimen potential component $V(\boldsymbol{k})$ gives rise to an exit-surface diffracted beam $\Psi_E(\boldsymbol{k})$ at a phase difference of $-\pi/2$ from $V(\boldsymbol{k})$ Passage through the objective lens rotates the phase of $\Psi_E(\boldsymbol{k})$ through an angle of $\chi(\boldsymbol{k})$ to form $\Psi(\boldsymbol{k})$ (b) Formation of the second amplitude component contributing to the kth image intensity component (c) Summation of the two amplitude components to produce the intensity component $I_L(\boldsymbol{k})$, which lies along the negative extension of the original $V(\boldsymbol{k})$ and has an amplitude (length) proportional to 2 sin $\chi(\boldsymbol{k})$



虚部

$V(\mathbf{k})$

$\Psi(\mathbf{k})=\Psi_E(\mathbf{k})\exp(i\chi)$

实部

$\Psi_E(\mathbf{k})=-i\sigma V(\mathbf{k})H$

M.O’Keefe: UltraM, 47(1992) 282

在有内标的单胞内测量原子位置精确到 +/-6pm

$YBa_2Cu_3O_{7-\delta}$单胞及投影

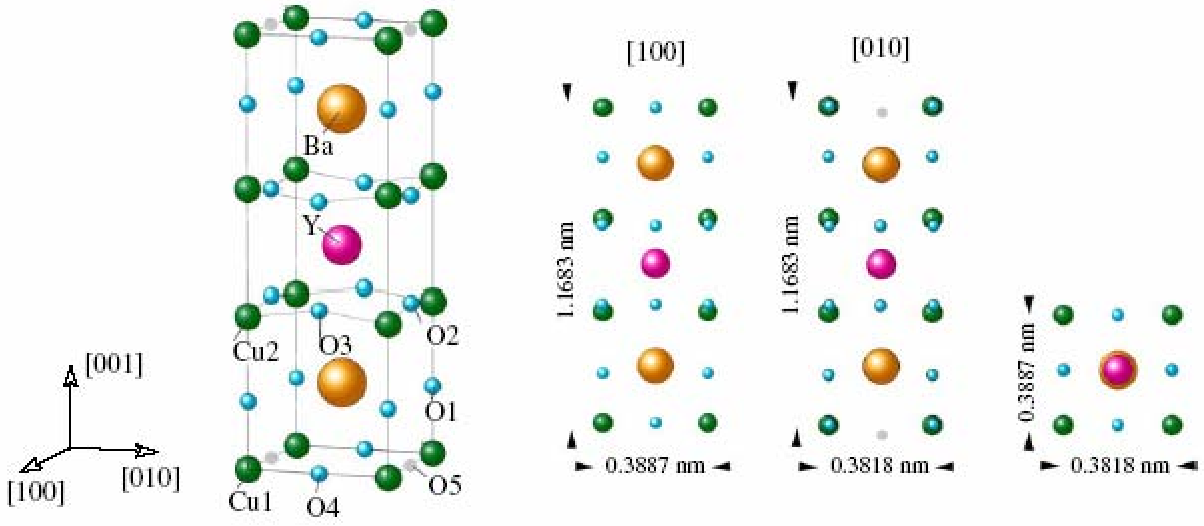


Fig. 2. The unit cell of orthorhombic $YBa_2Cu_3O_{7-\delta}$ with oxygen deficiency δ close to zero. Oxygen atoms are ordered occupying the O4 sites along the [0 1 0] axis. Projections of the orthorhombic unit cell along the [1 0 0], [0 1 0] and [0 0 1] direction are shown to the right. Room temperature unit cell dimensions are indicated.

90°孪晶

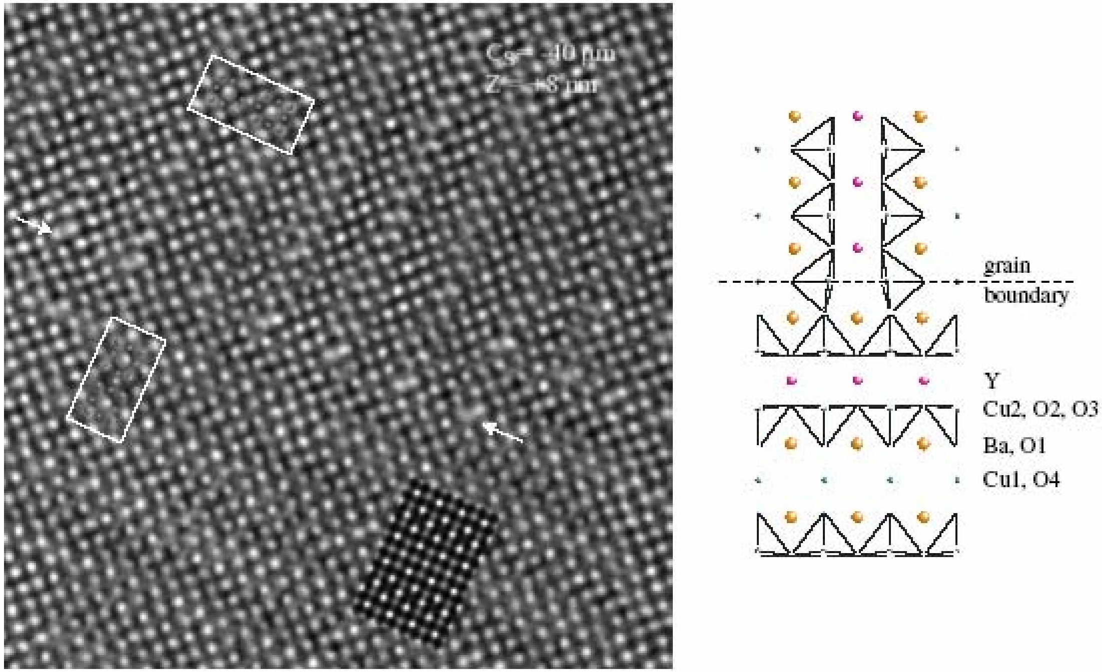


Fig. 1. Experimental high-resolution image of a 90° [1 0 0] tilt grain boundary in $YBa_2Cu_3O_{7-\delta}$. The image is taken along the [1 0 0] zone axis. Arrows mark a step-free part of the grain boundary. A projection of a unit cell of $YBa_2Cu_3O_{7-\delta}$ in [1 0 0] direction is indicated in the boxed region (see also the structure projections in Fig. 2). A corresponding simulated image is shown as inset in the lower right part of the high-resolution image. The geometric structure of a repeat cell of the grain boundary structure is given to the right. Polygons point out the square pyramidal oxygen coordination of the plane copper Cu2.

L. Houben, A. Thust, K. Urban: Ultramicroscopy 106 (2006) 200–214

用20张欠焦系列像重构的出射波函数：振幅（左），相位（右）

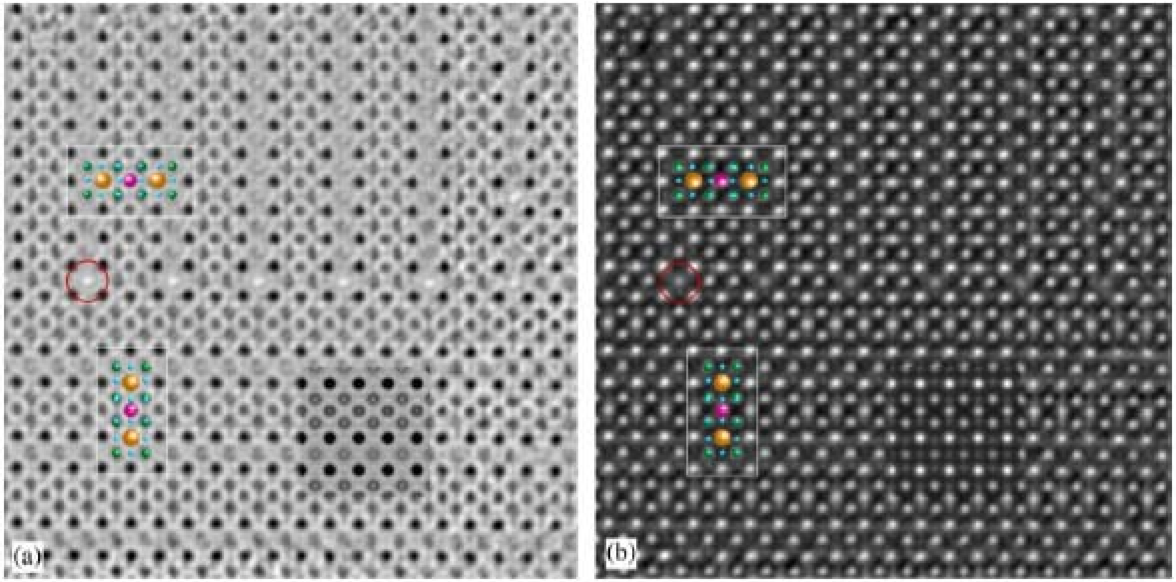


Fig. 6. Magnified region of the exit-plane wave function showing the grain boundary structure averaged parallel to the boundary over five repeat cells. (a) Amplitude image and (b) phase image. Unit cell projections along the [1 0 0] axis are shown in the boxed regions. The insets at the lower right display simulated exit-plane wave data. The circle highlights a Cu1 site of deviating contrast in the grain boundary plane.

L. Houben, A. Thust, K. Urban: Ultramicroscopy 106 (2006) 200–214

从像点位置反推孪晶界上下金属原子位置。误差据称可达+/-6pm

L. Houben, A. Thust, K. Urban: Ultramicroscopy 106 (2006) 200–214

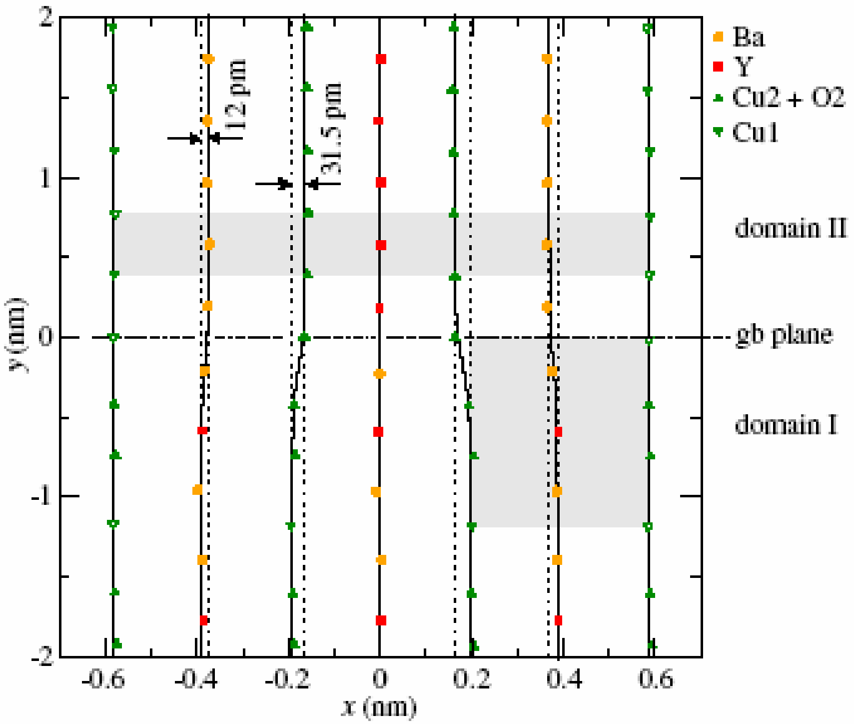
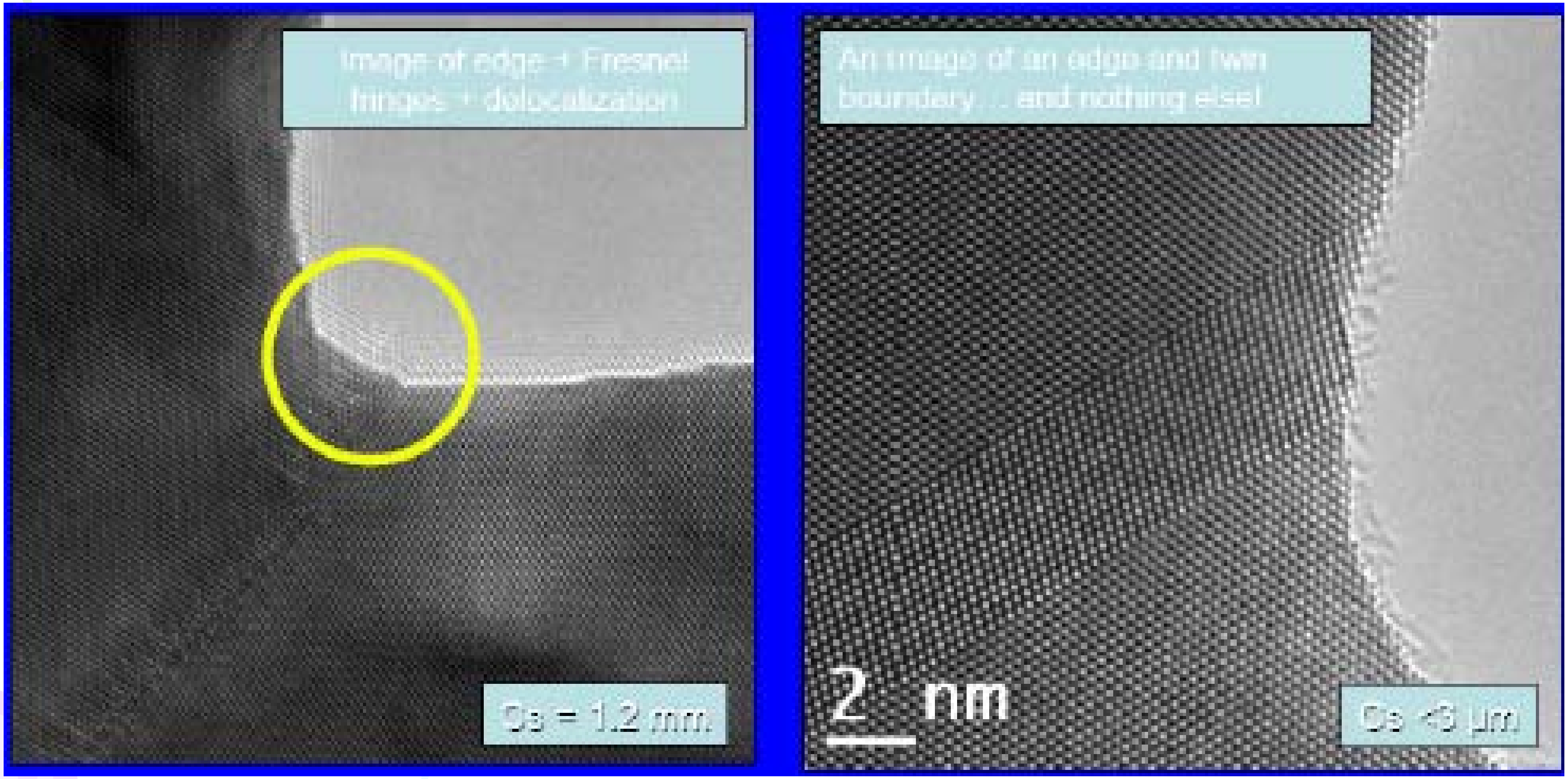


Fig. 8. Phase peak positions measured by a two-dimensional Gaussian fit for a single repeat cell of the periodic grain boundary. Peak positions for Ba, Cu1, Cu2+O2 and Y-columns are indicated. Solid lines point out the bending of lattice planes across the grain boundary. The aspect ratio is blown up in order to uncover the bending of lattice planes. Elementary unit cells are indicated as the gray shaded rectangles. Dotted lines represent the prolongation of lattice planes from one domain into the other. The symbol size in *x*-direction matches the 2σ radius of ±6 pm for the statistical error in the distance between two individual peaks.

减少离位效应

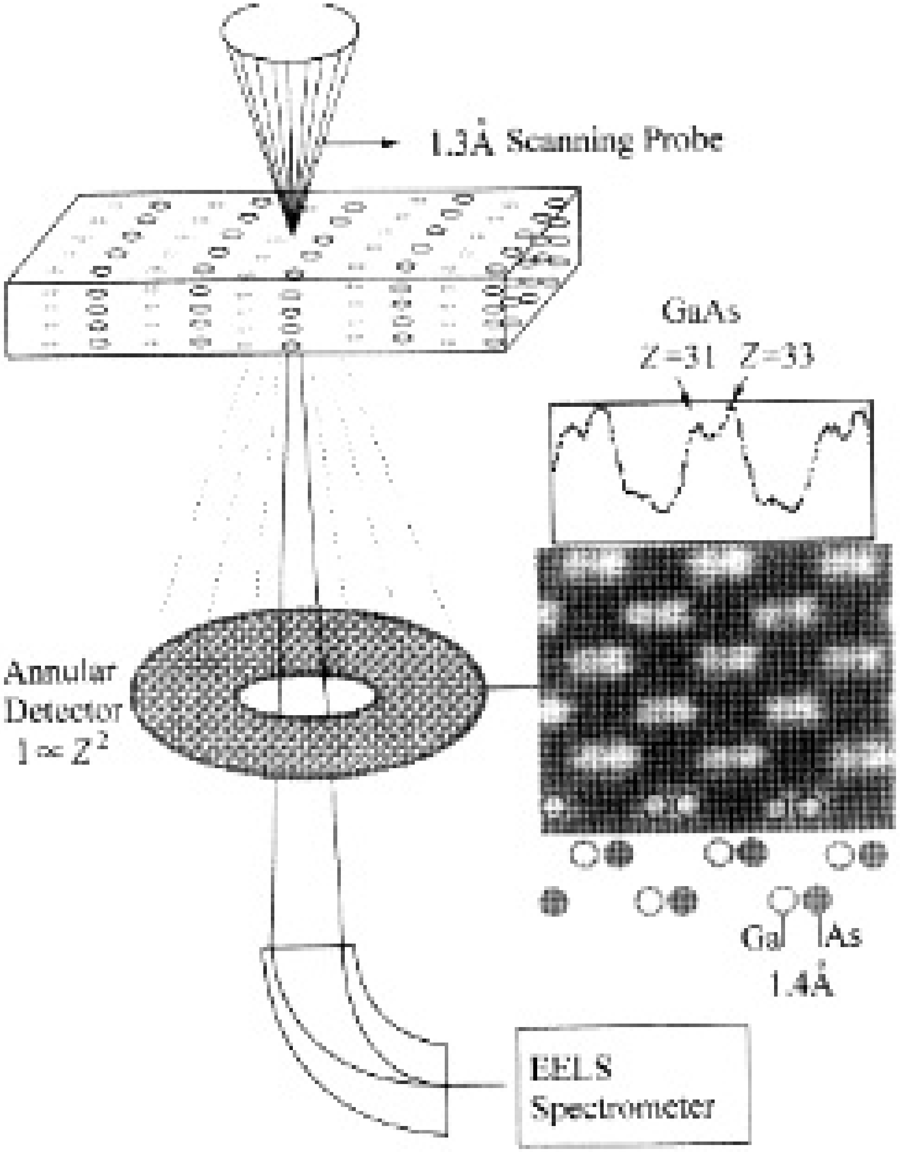
更清晰的图像



在象差未校正前，金孪晶在膜边及孪晶界显示严重离位效应；而在校正象差后，图像变得清晰许多 **B. Freitag, S.Kujawa, P.M.Mul, J.Ringnalda, P.C.Tiemeijer: Ultramicroscopy 102 (2005) 209.**

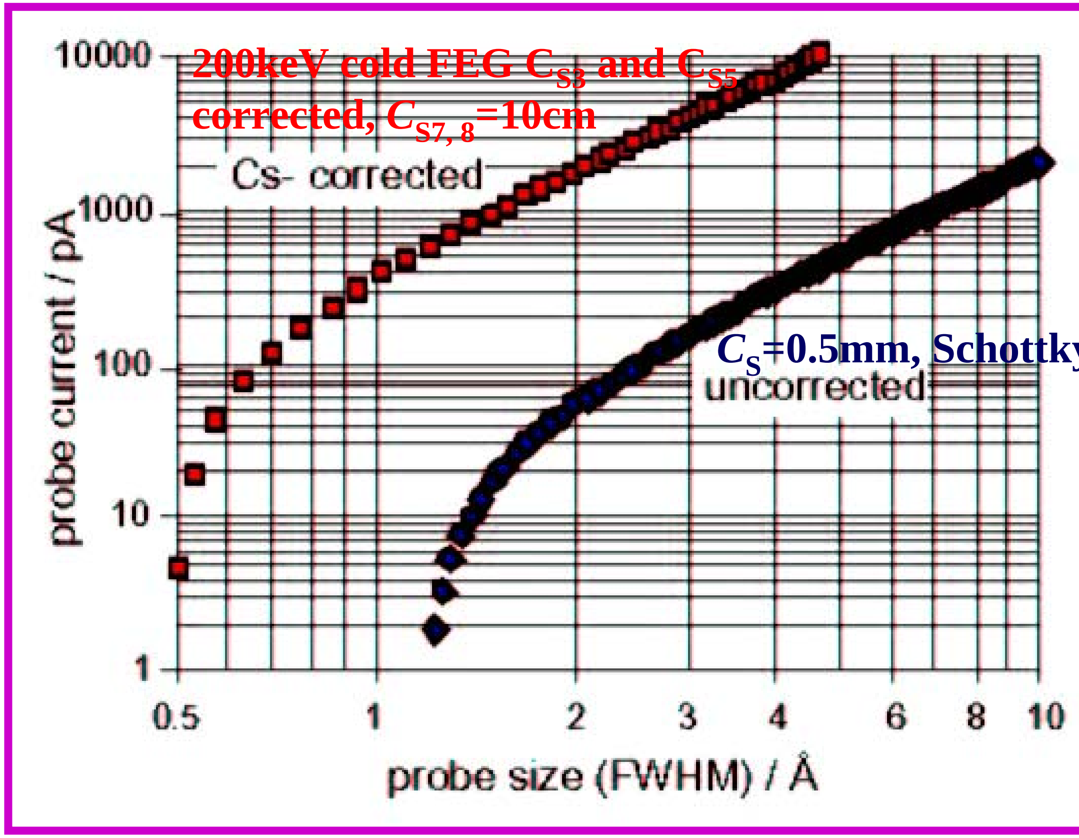
走向原子柱分辨的成分分析

扫描透射电子显微术--STEM



Increasing beam current

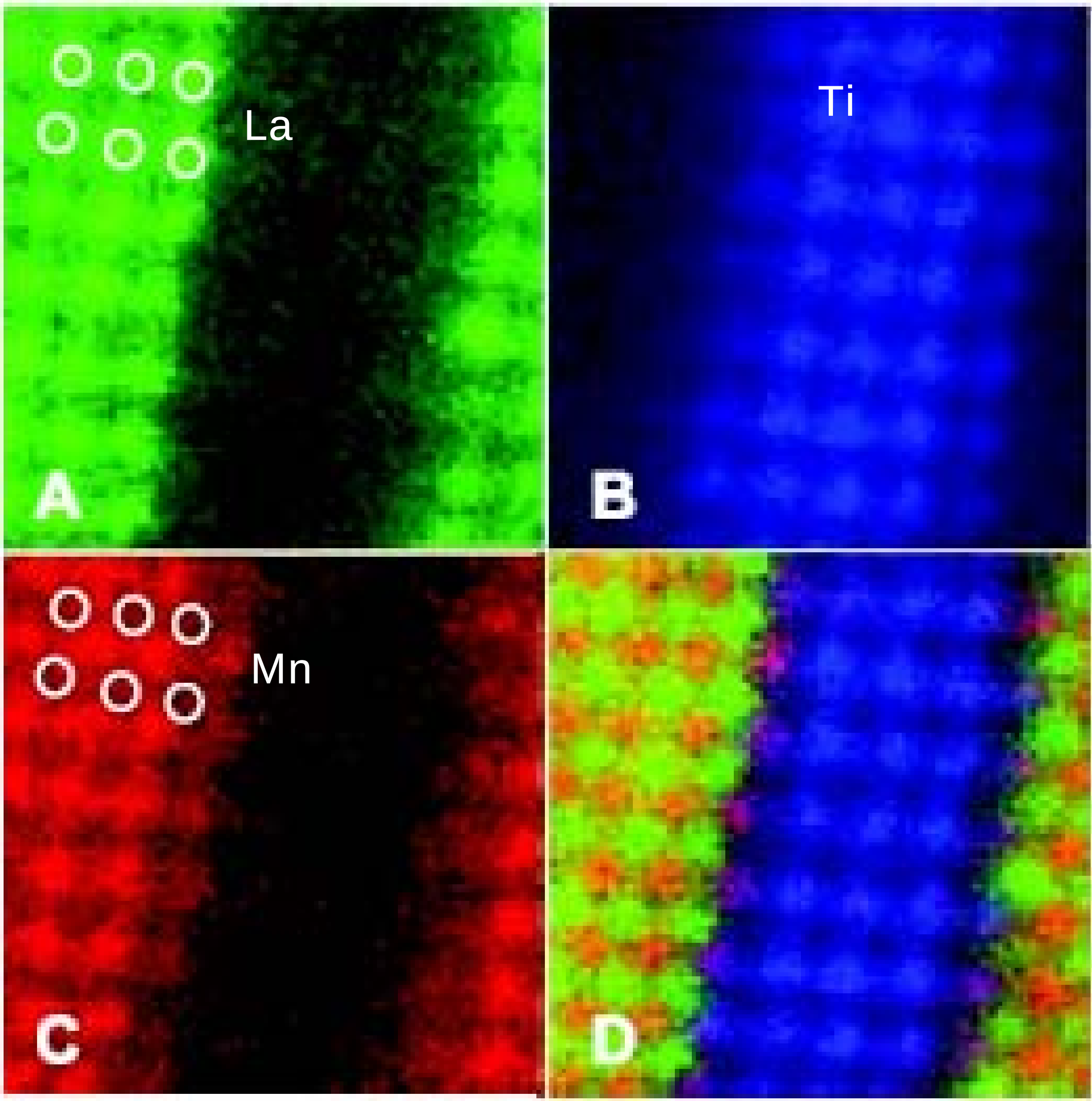
- For 0.1-0.2 nm beam size, beam current increases 1-2 order.
- It is benefit to EELS analysis with atomic resolution.
- Improve electron lithography.
- Easier radiation damage.



从选择电子能量损失谱得出的原子尺度的成份化学成像

- 在一般电子显微镜中，用选择电子能量损失谱所成的成分化学像的分辨不优于1纳米。这是由于要将束形成小于1nm，不仅需要象差校正，而且要使这么小束斑下有足够大的束流，困难很大。Nion公司研制的校正三级象差的STEM，使束流增加4~6倍。无象差校正STEM的束形成光阑半角为10 mrad，三级象差校正器使之加倍，因此对于同样光源束流增加4倍。五级象差校正器使半角再加倍，因此束流增加16倍。电子枪用冷场发射枪取代Schottky热发射枪，又可得到近10倍的收益。再加上相应的样品之后光学系统的改进保证收集更大散射角的信号，这一切使得束流达0.78 nA。

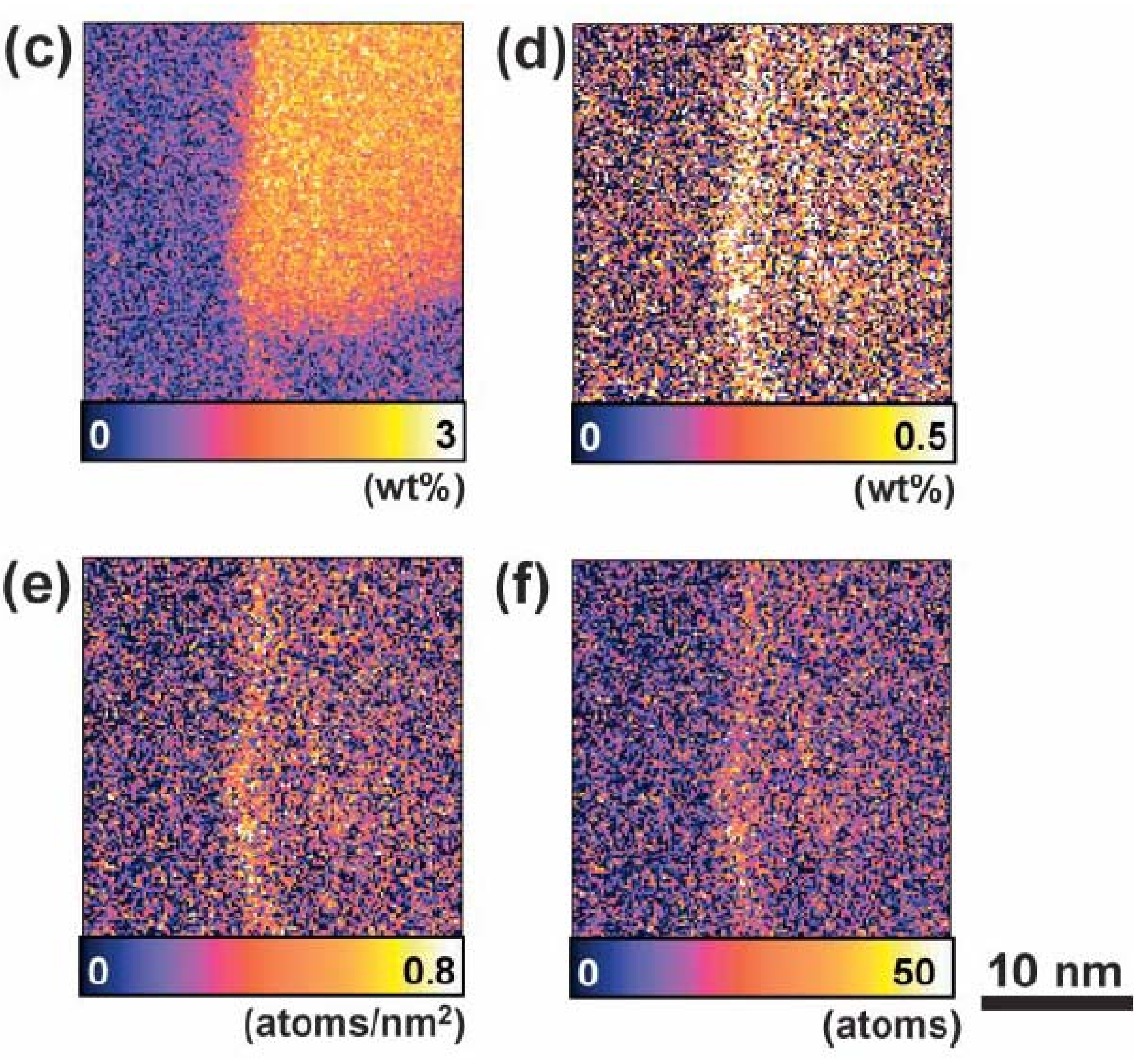
- **$La_{0.7}Sr_{0.3}MnO_3$/SrTiO_3**多层膜截面的电子能量损失谱元素选择成像。图边长为**3.1nm**。（**A**）是**La M**边成像，白圈标出**La**原子位置。（**C**）是**Mn**的**L**边成像，亮点对应**Mn**原子柱，图上白圈标出**La**原子，可见**La**、**Mn**原子位置是分开了的，距离为**1.9 Å**。图（**B**）是**Ti**的**L**边成像。图（**D**）是全成像，红、绿、兰分别对应**Mn**、**La**和**Ti**原子像[D.A.Muller, L.F.Kourkoutis, M.Murfitt, J.H.Song, H.Y.Hwang, J.Silcox, N.Dellby, and O.L.Krivanek: Science 319 (2008) 1073]



走向原子柱分辨的X射线分析

- 束形成象差校正STEM减小入射束大小又保持高束流的能力使得原子柱分辨的X射线分析也逐渐成为可能。在美国Lehigh大学专门为提供最佳X射线微分析性能而设计的VG HB603 STEM（300KeV，冷场发射枪，～1.0nA束流，1.5nm束斑，Be窗口，样品台真空<10-7Pa，Cs校正：Cs=-0.16nm; C5=500nm，等等），得到约1nm分辨水平X射线谱像

- 某Ni基合金晶界上Nb，Zr偏析的XEDX谱像。(c)是Nb的分布图。图下方的灰度图表示重量百分比的表示。(d)是Zr在晶界的分布， (e)则是对Zr按面积表示其密度；（f）是对Zr按厚度内有多少原子表示其密度 [M. Watanabe, D.W. Ackland, A. Burrows, C.J. Kiely, D.B. Williams, O.L. Krivanek, N. Dellby, M.F. Murfitt, and Z. Szilagyi: Microsc Microanal. 12, (2006) 515]



三维STEM

焦点附近的三维光分布状态

- 考虑会聚球面波在园孔的衍射，a是半径，f是焦距，张角$\theta=a/f$；引入的无量纲变量u，v见图标注。焦平面上强度分布$I(v)=[2J_1(v)/v]^2 I_0$, 这是园孔夫琅和费衍射的爱里公式。
- 轴上的强度分布，$I(u)=[\sin(u/4)/(u/4)]^2 I_0$
- 这是矩形孔夫琅和费衍射$(\sin x/x)^2$类型的强度分布，轴上强度的第一个零值决定于$u/4=\pi\theta^2 z/2\lambda=+/-\pi$, 即$z=+/-\lambda/2\theta^2$. (Max Born & Emil Wolf: << Principles of Optics>> (5th ed.) Pergamon Press, 1975. 中译本：《光学原理》，杨葭荪等译校。科学出版社，1978年。)

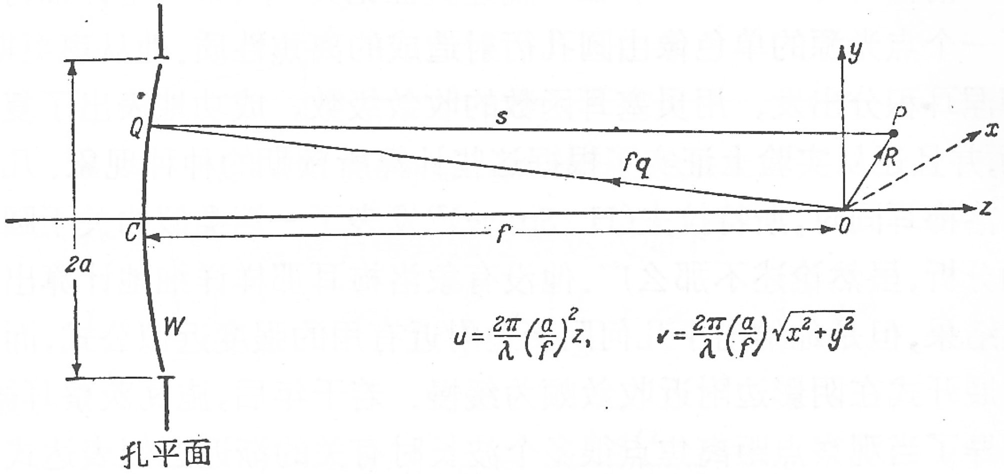


图 8.40 会聚球面波在圆孔上的衍射：符号

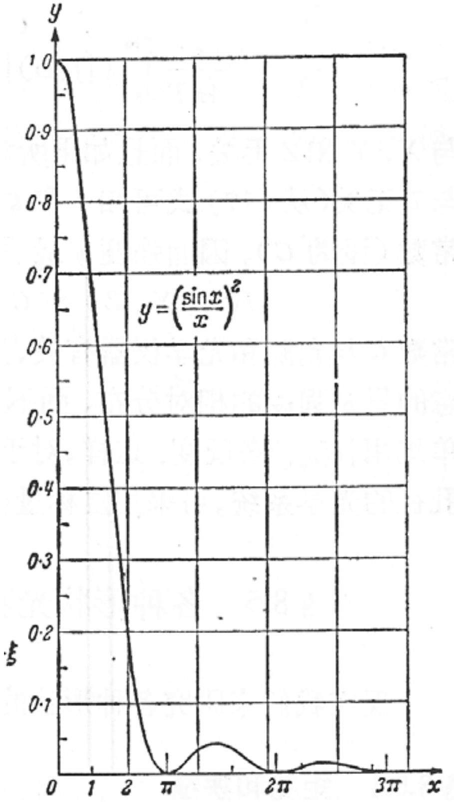


图 8.9 矩孔夫琅和费衍射函数 $y=\left(\frac{\sin x}{x}\right)^2$

用AC-STEM对晶体作层析

- 用束形成象差校正电镜可将电子束会聚到亚埃尺度，相应会聚角高达35mrad.套用光学焦长公式，300仟伏STEM的束斑在光轴方向收缩为1 nm。下一代仪器做到50mrad的话，光斑进一步缩短为5埃。这对于大晶胞晶体已适于作层析。

球差、色差对光斑长度的影响

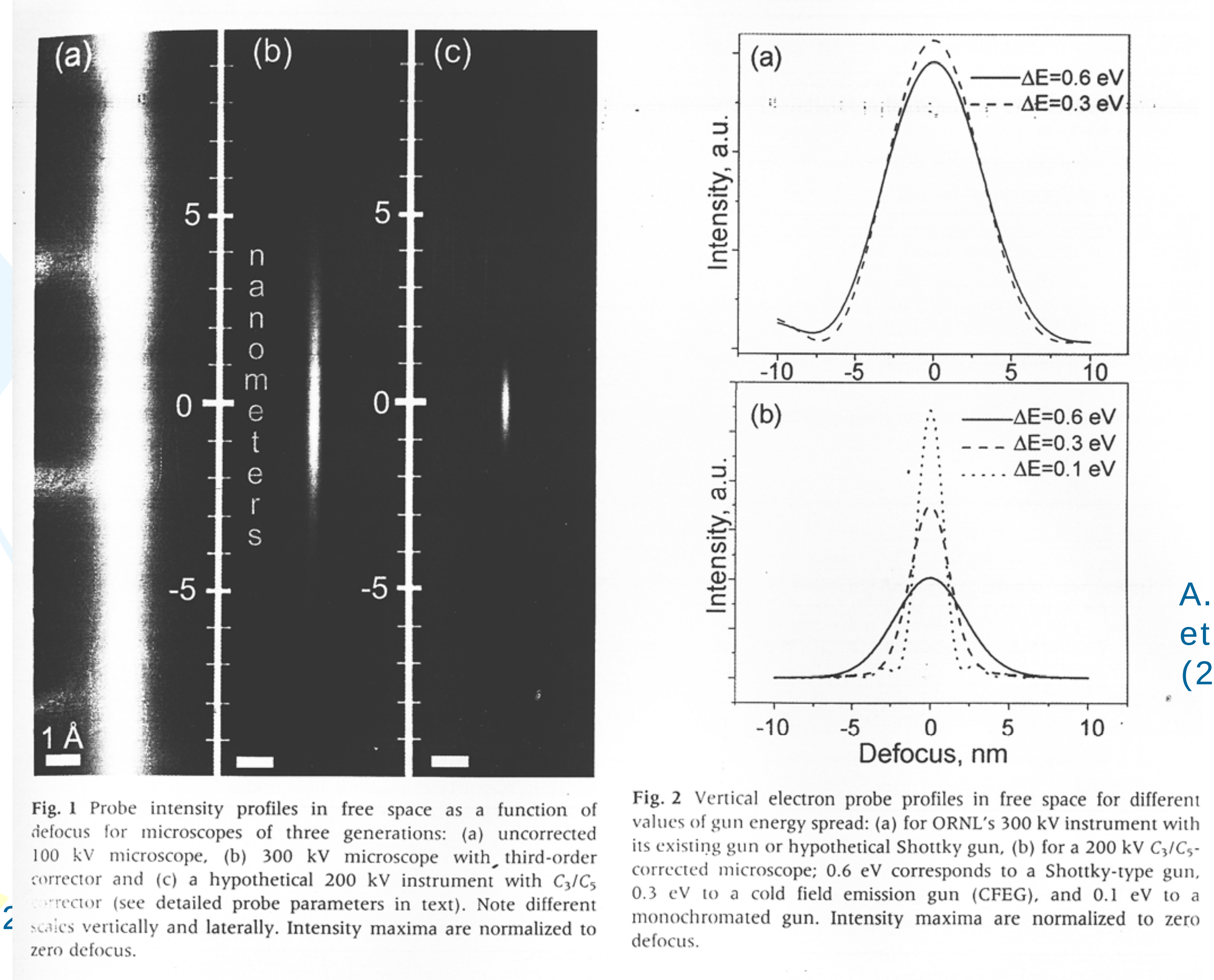


Fig. 1 Probe intensity profiles in free space as a function of defocus for microscopes of three generations: (a) uncorrected 100 kV microscope, (b) 300 kV microscope with third-order corrector and (c) a hypothetical 200 kV instrument with C_3/C_5 corrector (see detailed probe parameters in text). Note different scales vertically and laterally. Intensity maxima are normalized to zero defocus.

Fig. 2 Vertical electron probe profiles in free space for different values of gun energy spread: (a) for ORNL's 300 kV instrument with its existing gun or hypothetical Shottky gun, (b) for a 200 kV C_3/C_5-corrected microscope; 0.6 eV corresponds to a Shottky-type gun, 0.3 eV to a cold field emission gun (CFEG), and 0.1 eV to a monochromated gun. Intensity maxima are normalized to zero defocus.

A.Y.Borisevich et.al:J.EM, (2006) 55, 7.

深度敏感（变欠焦）扫描像的模拟

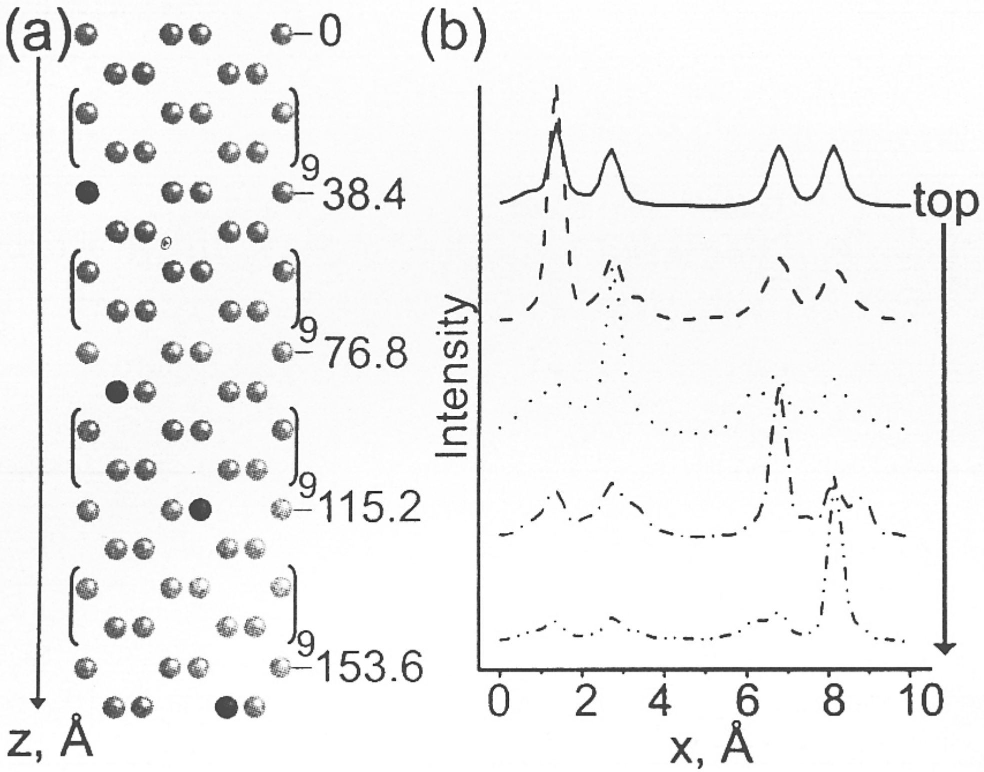


Fig. 3 (a) The model doped Si crystal with four Bi atoms at different depths (Bi, black; Si, gray); (b) simulated HAADF image intensity scans for an aberration-free probe with 35 mrad semiangle, detector angle from 70 to 300 mrad. Defocus varies from 0 (top) to 38.4, 76.8, 115.2 and 153.6 Å, consecutively.

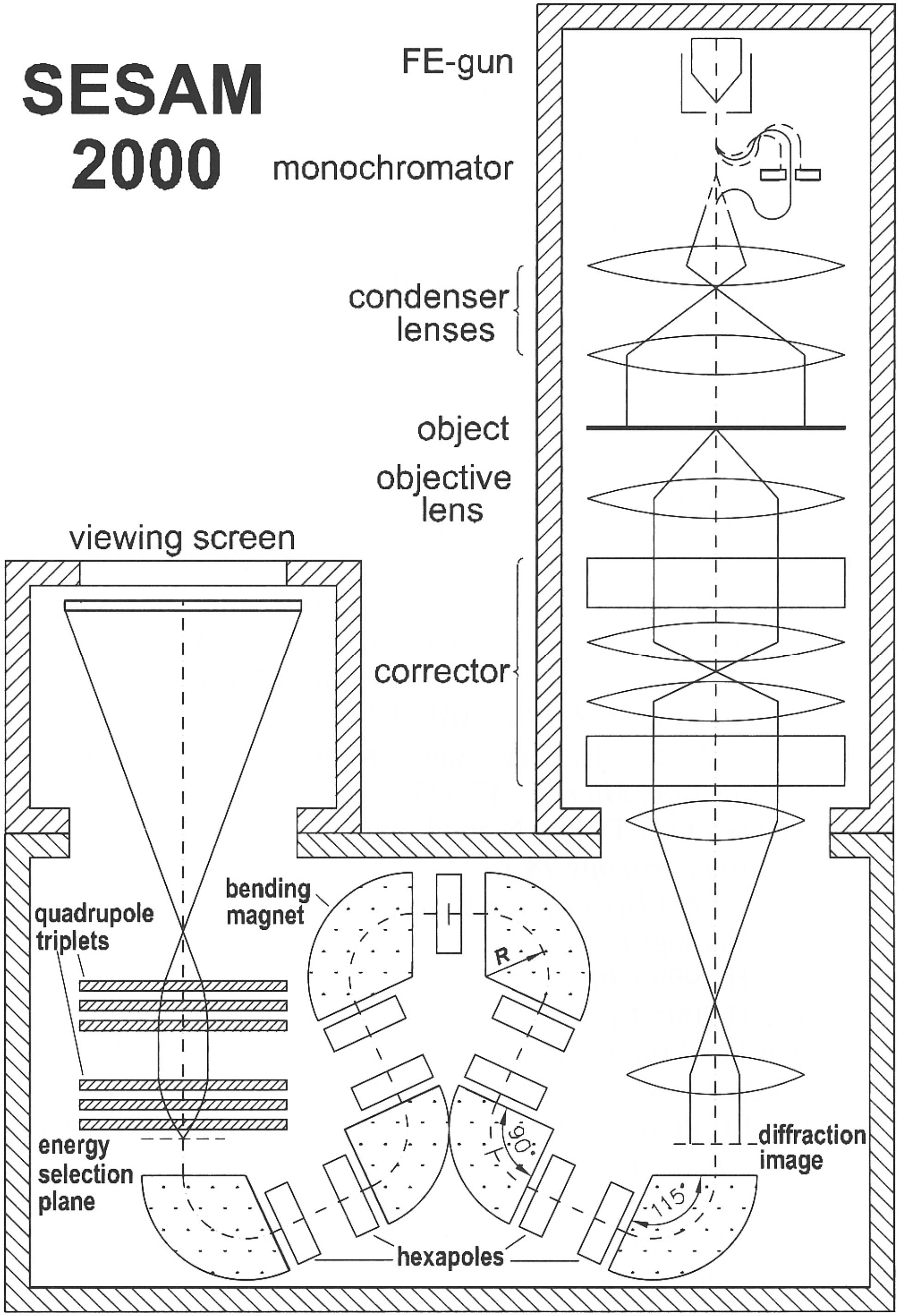
A.Y.Borisevich et.al:J.EM, (2006) 55, 7.

研制色差校正器成了当务之急

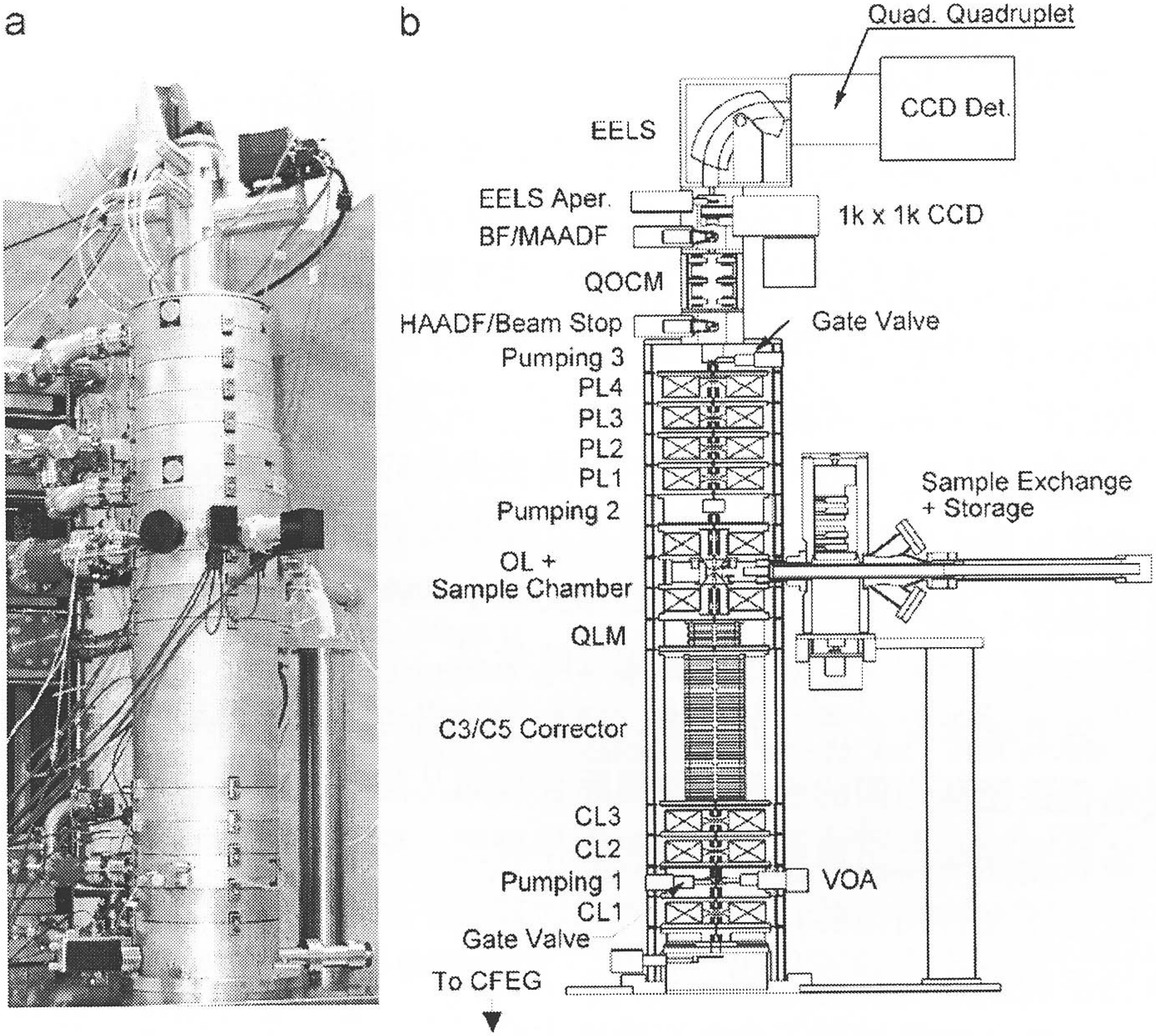
- 在相干成象的物镜传递函数的框架内，当**Cs**可以调整到零（甚至到负值），那么在**Cs**很小时，总可以找适当的Δ**f**值，把**Sin**χ曲线第一通带调整到极宽，即对应无限小的分辨率。因此由束的时间不相干性结合空间不相干性造成的衰减包络成了分辨率的限制因素。这其中，以色差的影响尤为突出。因此，研制色差校正器成了当务之急。美国的**TEAM**计划与德国科学家及**FEI**公司合作发展**0.5 Å**分辨电镜的项目，将光学消色差**-achromatic**与消球差**-aplanatic**两个字，合并成消色球差－**Achroplanat**作为新一代**Cc/Cs**校正器的命名。他们的主要结论是**[M.Haider, H.Muller, S.Uhlemann, J.Zach, U.Loebau, and R.Hoeschen: Ultramicroscopy 108 (2008) 167]**：（**1**）想象中的**Cc/Cs**校正器不限于单一的高分辨应用，也不限于**200KV**。当然每一种用途对校正器的要求会有所差别。如原位实验要求较大焦长；生物应用要求较大的的视场；能量选择成像及分析电镜或洛仑茨电镜的要求也各有不同等等。（**2**）表**1**列出的是在相应分辨率要求下相应象差的上限值，那是单项考虑的结果。显然**Cc**校正比单用**Cs**校正对信息极限的延伸好处大

Sub-ev-Sub-Å Microscope

H.H.Rose: Sci. Tech. Adv. Mat., 9 (1008) `14107 (30pp).



STEM-2008-NION



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谢谢