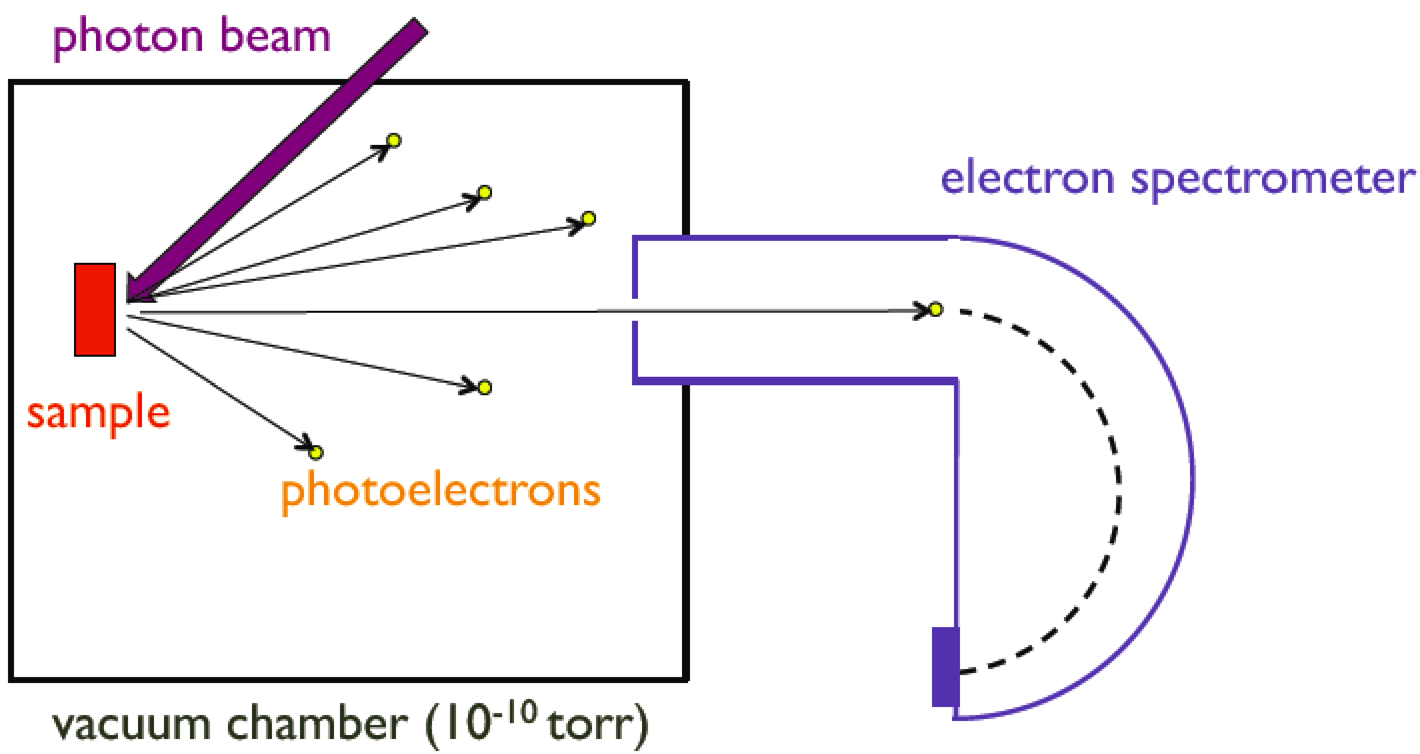
# 实验站真空系统

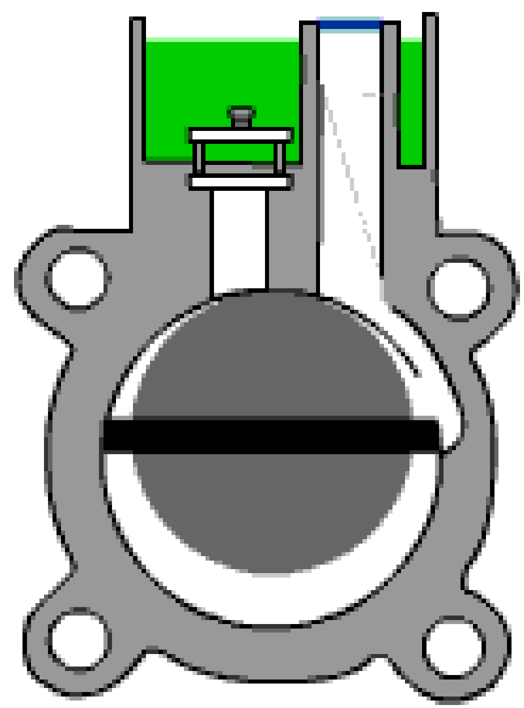
# Vacuum ! !



photon beam
electron spectrometer
sample
photoelectrons
vacuum chamber (10$^{-10}$ torr)

# Methods for Vacuum Generation: 1

- Positive displacement: use a mechanism to repeatedly expand a cavity, allow gases to flow in from the chamber, seal off the cavity, and exhaust it to the atmosphere (rotary vane, scroll pump, roots blower)

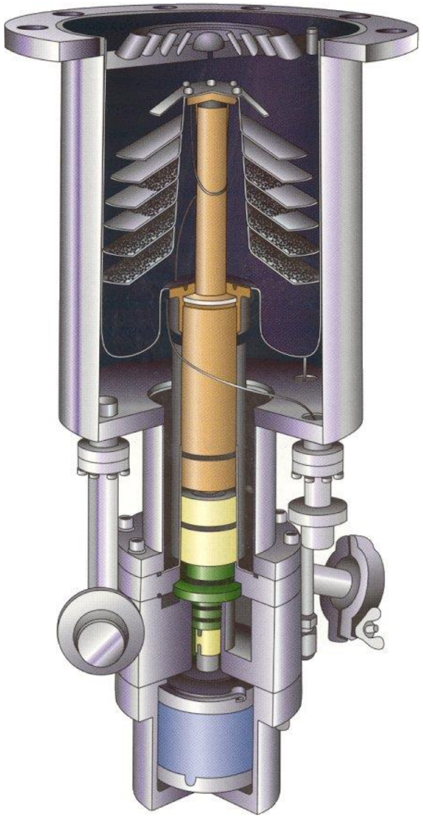


# Methods for Vacuum Generation: 2

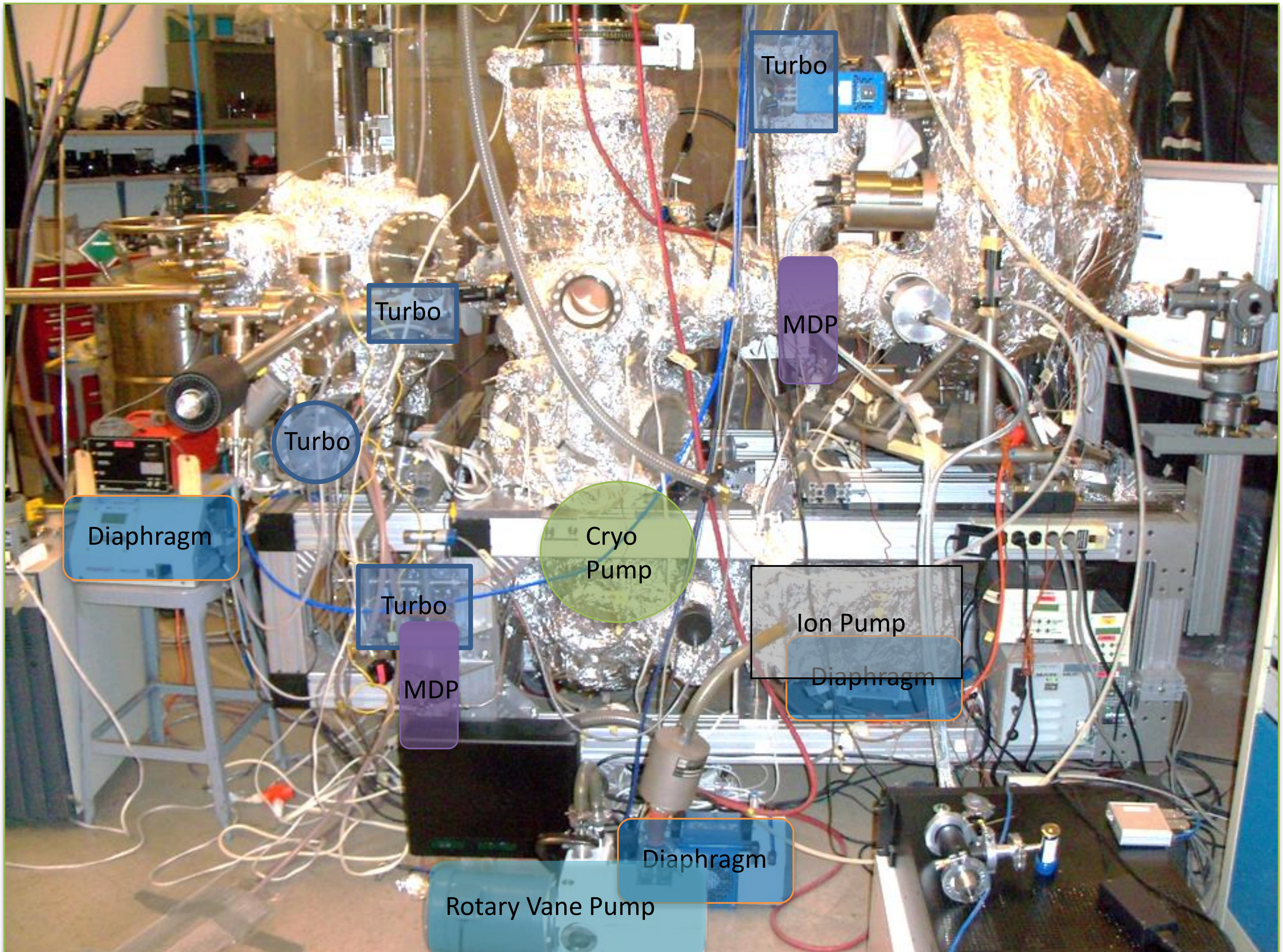
- Momentum transfer: use high speed jets of fluid or rotating blades to knock gaseous molecules out of the chamber (diffusion, turbomolecular)

# Methods for Vacuum Generation: 3

- Entrapment: capture gases in a solid or absorbed state (cryopumps, getters, ion pumps)

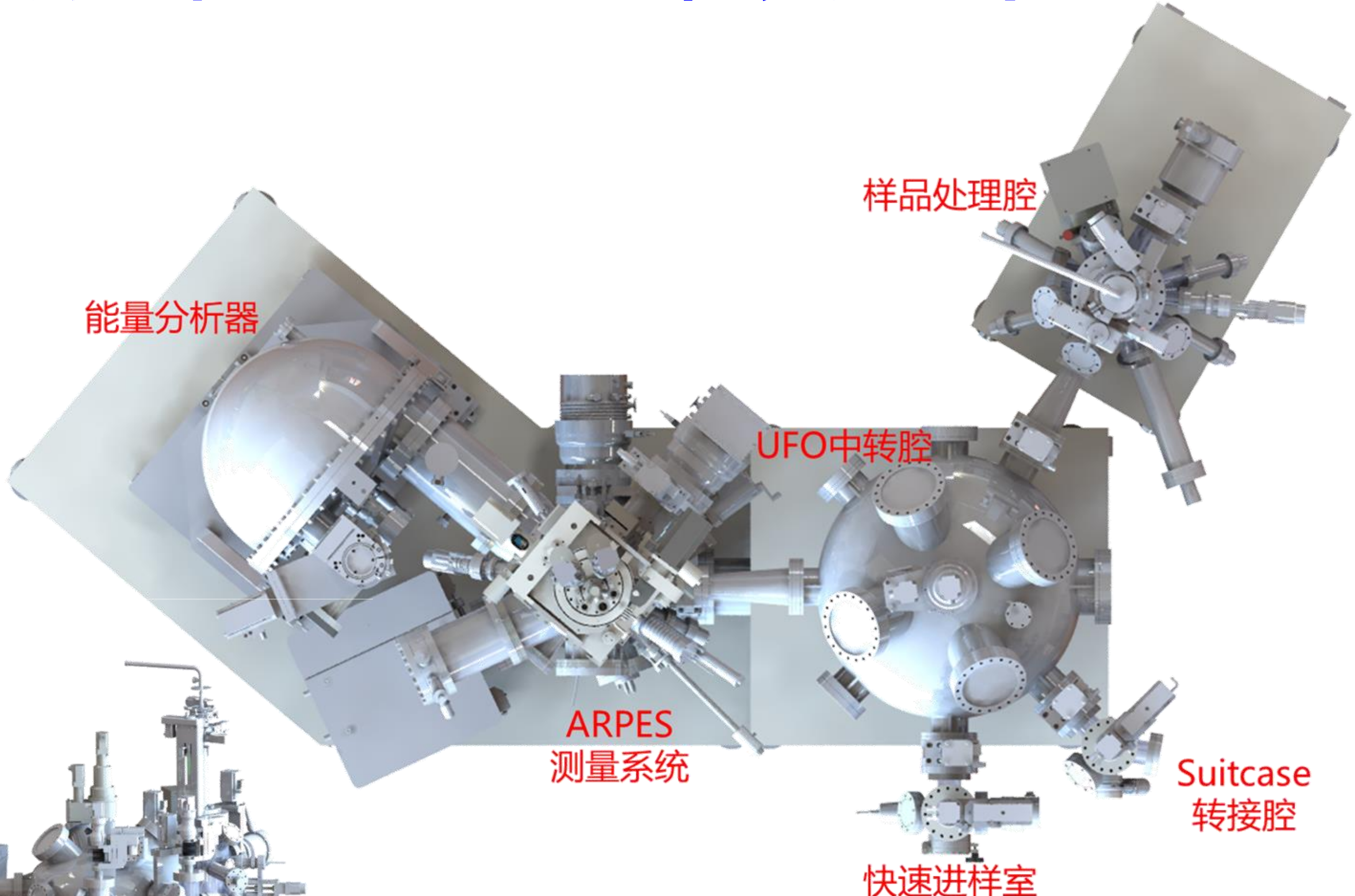


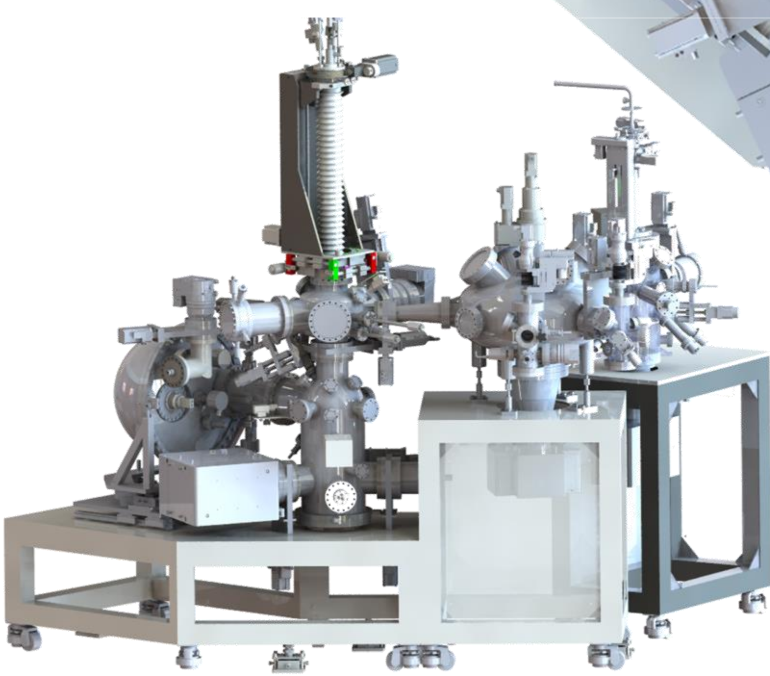
# 角分辨光电子能谱实验站




Probability of everything working at once ~ $(98\%)^{30}$ = 55%

# 角分辨光电子能谱实验站



# 角分辨光电子能谱实验站

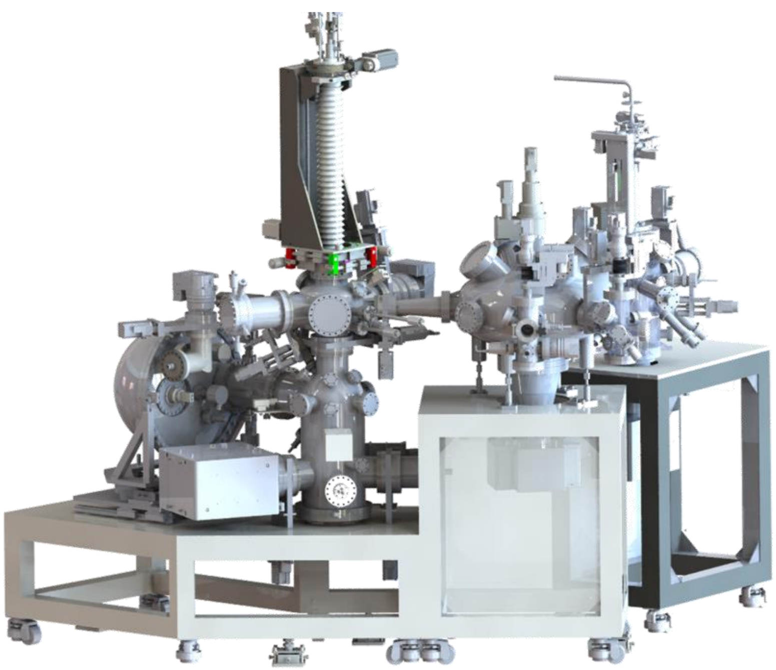
- **上下腔构造**

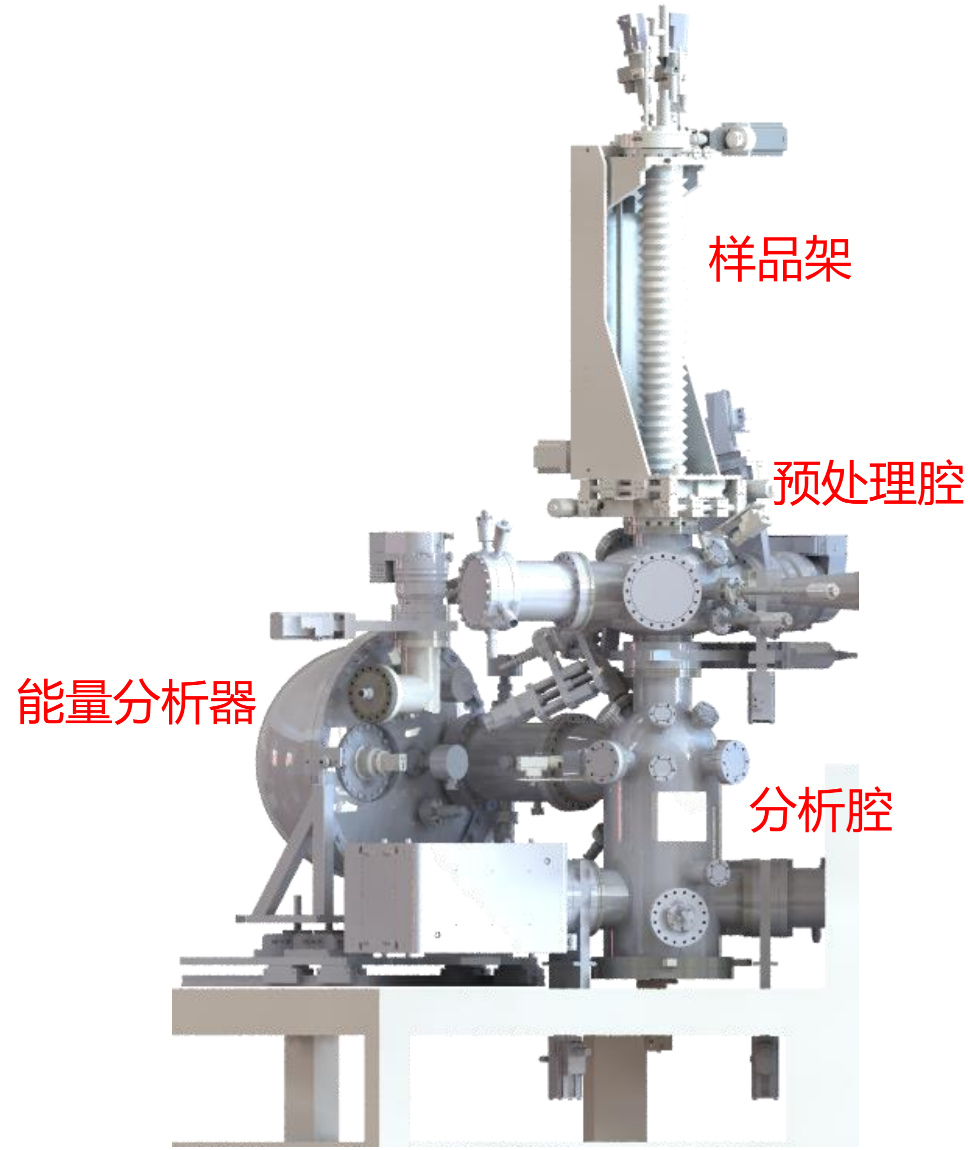
  **保护主腔超高真空**

  **易于维护**

  **上腔集成多种功能**

  **配备LEED、碱金属蒸发源**

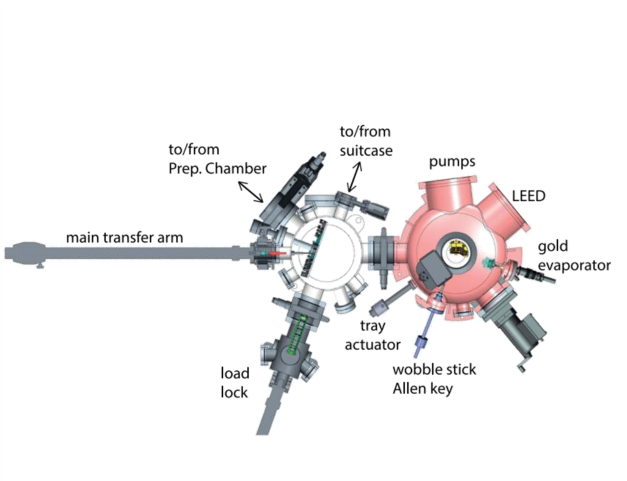




# 角分辨光电子能谱实验站

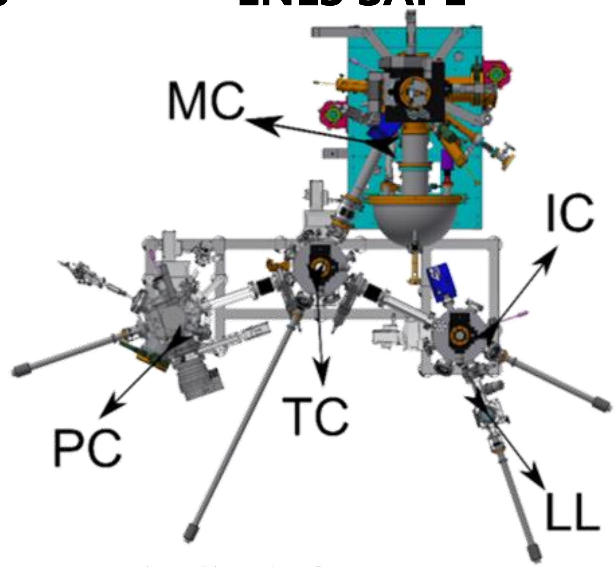
## 中转传样的选择

### Diamond I05 HR-ARPES



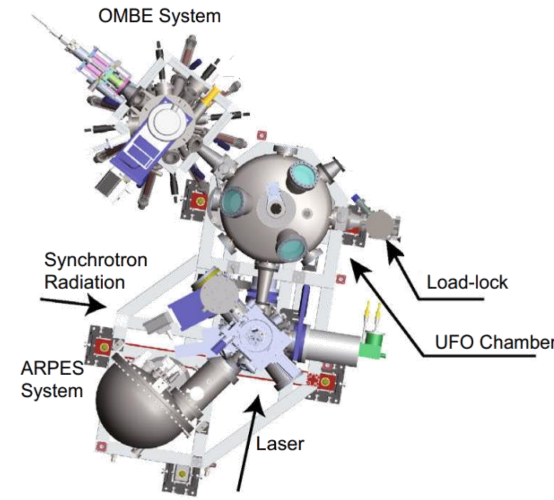

- 传样距离短
- 功能扩展受限

### LNLS SAPE




- 传样杆过长/操作不便
- 布局不紧凑
- 功能扩展受限

### SSRF ME$^2$




- UFO传样距离合适
- 操作便利
- 布局紧凑
- 功能扩展强

# 在真空方面需要注意的问题

**不能使用的材料:**

-S, Pb, Zn, Cd, Hg

-润滑油

-有机物 (指纹)

-不能承受200℃烘烤的材料

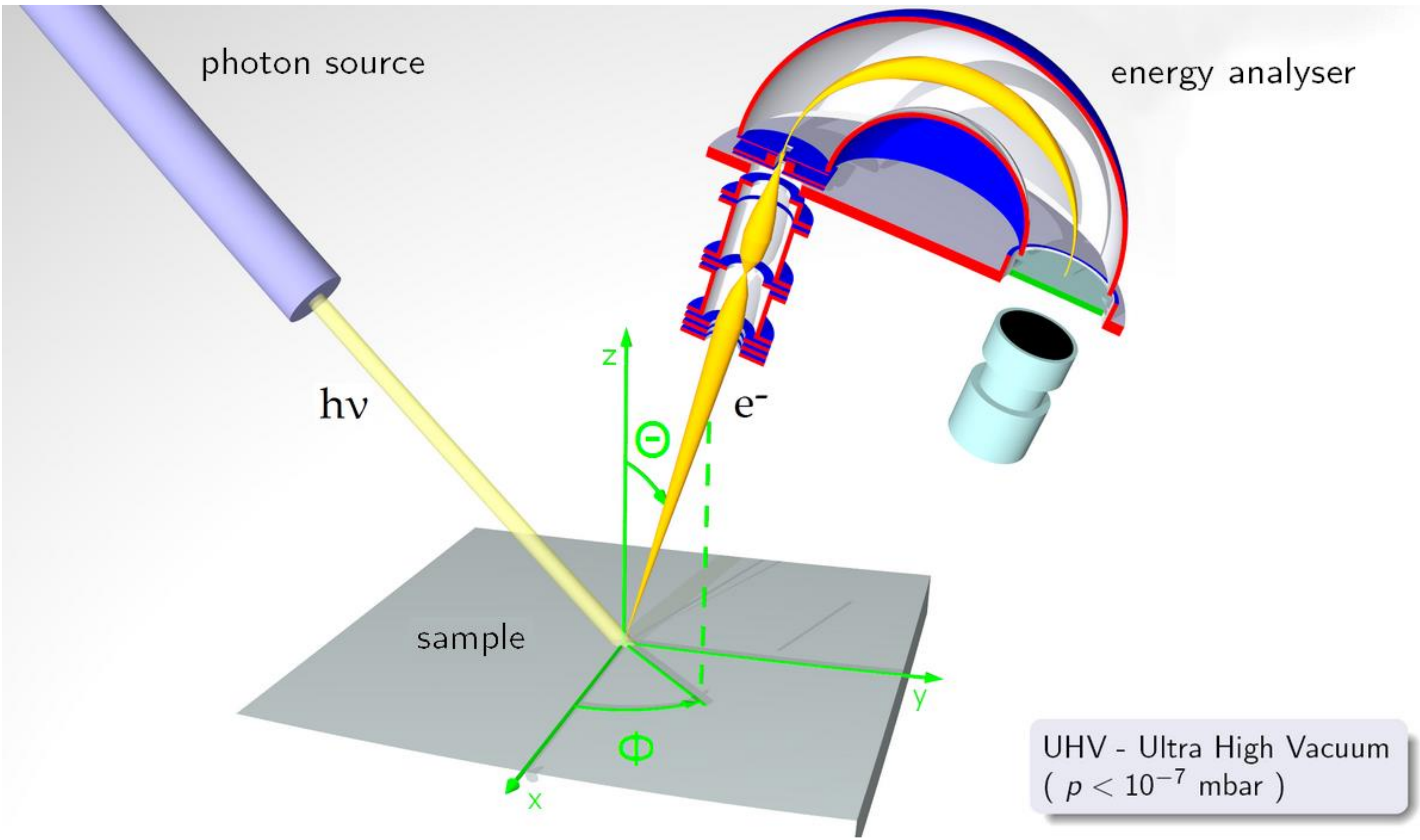
**虚漏:**

-腔体焊接问题，未通气的孔洞

**磁性材料(ARPES):**

-大多数不锈钢、铁、镍等

# 实 验 中 的 问 题


photon source
energy analyser
hν
e⁻
z
Θ
sample
y
x
Φ
UHV - Ultra High Vacuum
( $p < 10^{-7}$ mbar )

# 实验中的问题

样品荷电问题 – 绝缘体、弱绝缘体、
样品制备问题

1. 改变光通量，观察特征峰或费米能级的移动

2. 提高样品温度

3. 用电子枪补偿电子

# 实验中的问题

## Space charge effect – 高光通量

1. 使谱峰变宽、移动

2. 在高光强、高分辨率时出现

3. 调整光强度

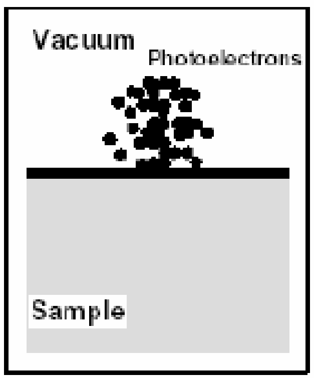
3. 让光斑弥散开

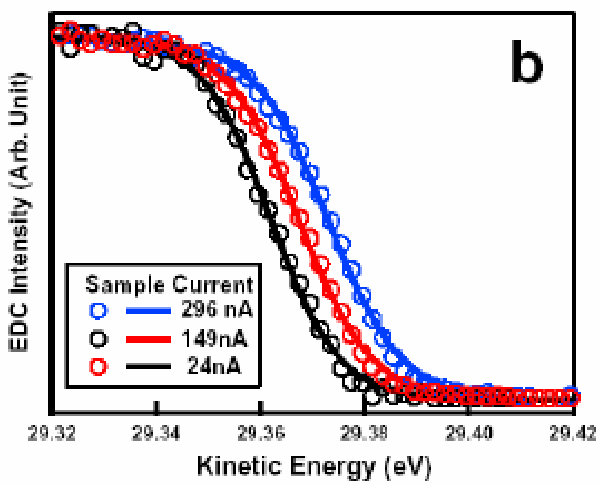
# Space charge effect

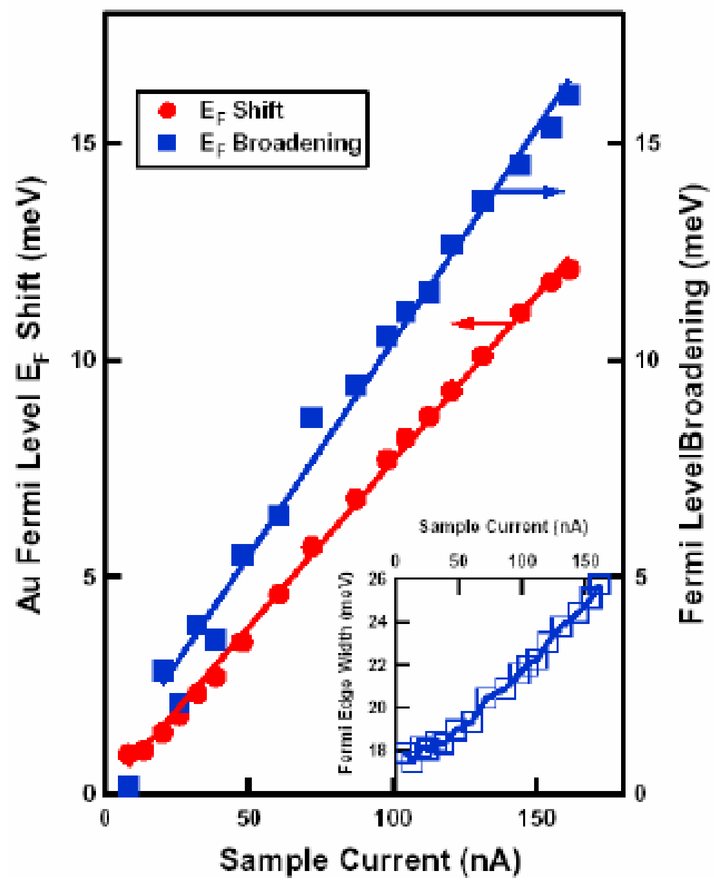
Space charge effect and mirror charge effect in photoemission spectroscopy

X.J. Zhou[a,b,*], B. Wannberg[c], W.L. Yang[a,b], V. Brouet[a,b], Z. Sun[d], J.F. Douglas[d], D. Dessau[d], Z. Hussain[b], Z.-X. Shen[a]

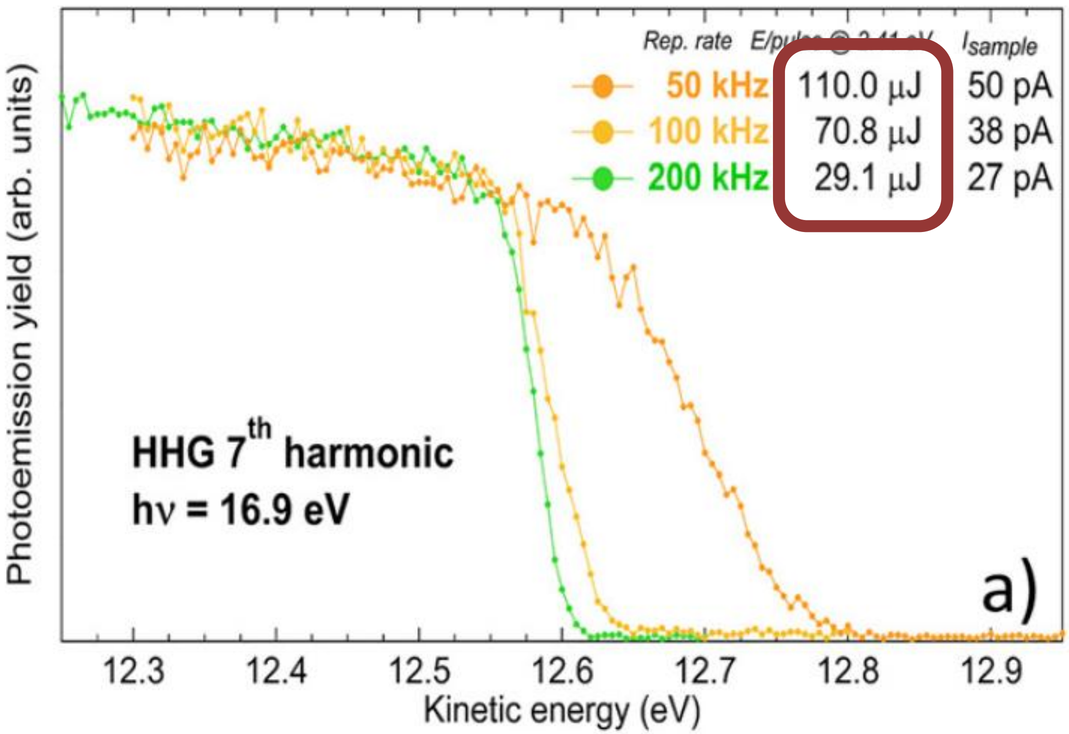
From ALS undulator beamline 10.0.1



# Space charge的影响




Struct. Dyn. 7, 014303 (2020)

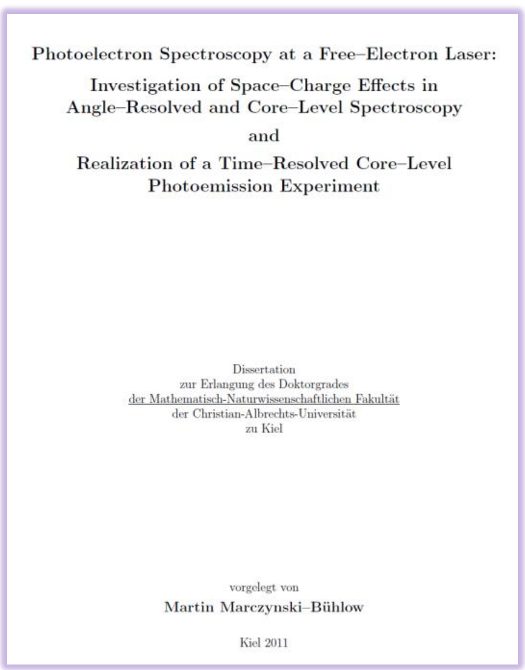
**能量尺度上：**

- **展宽**
- **移动**

# Space charge的影响

**Space charge的影响在三代光源上已经比较明显，在FEL上对数据的影响更显著：**

- **数据质量——谱线展宽**
- **数据可靠性——能量尺度上移动**
- **非线性效应——色散不准确**


Photoelectron Spectroscopy at a Free–Electron Laser:

Investigation of Space–Charge Effects in Angle–Resolved and Core–Level Spectroscopy

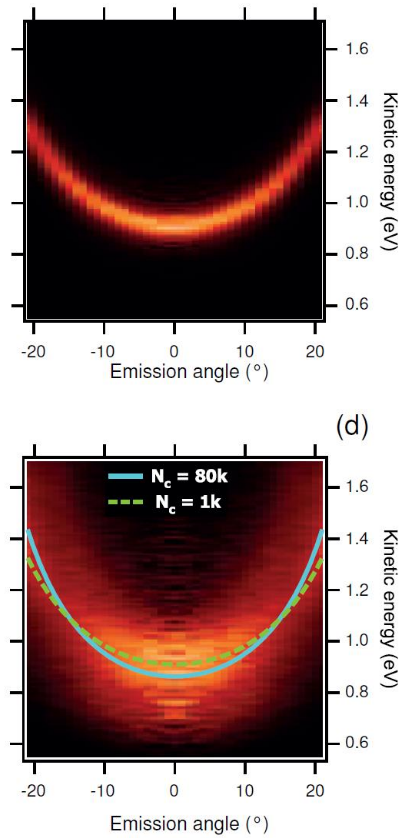
and

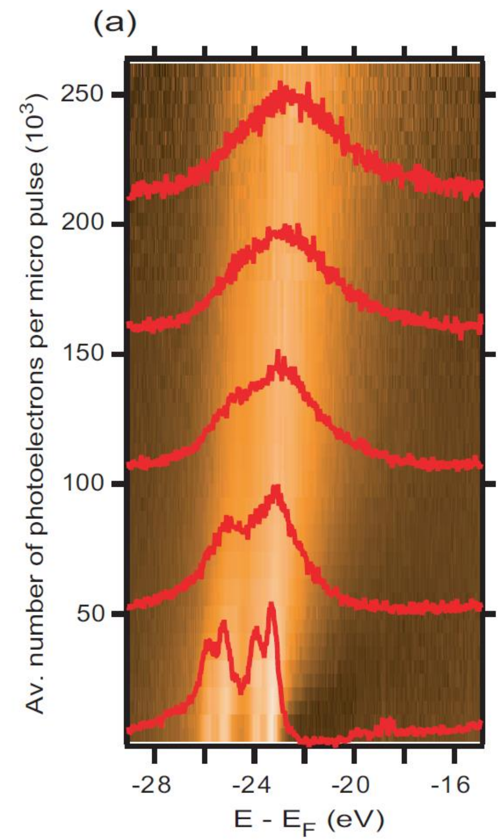
Realization of a Time–Resolved Core–Level Photoemission Experiment

Dissertation
zur Erlangung des Doktorgrades
der Mathematisch-Naturwissenschaftlichen Fakultät
der Christian-Albrechts-Universität
zu Kiel

vorgelegt von
Martin Marczynski–Bühlow

Kiel 2011



# 实验中的问题

## 样品变性

1. 气体物理吸附、化学吸附，升温可能有帮助
2. 氧原子离开样品表面，低温有帮助
3. 光损伤，用低能光子、低光通量
4. 快速测量、在多个样品测不同信息

# 实验中的问题

## 表面质量

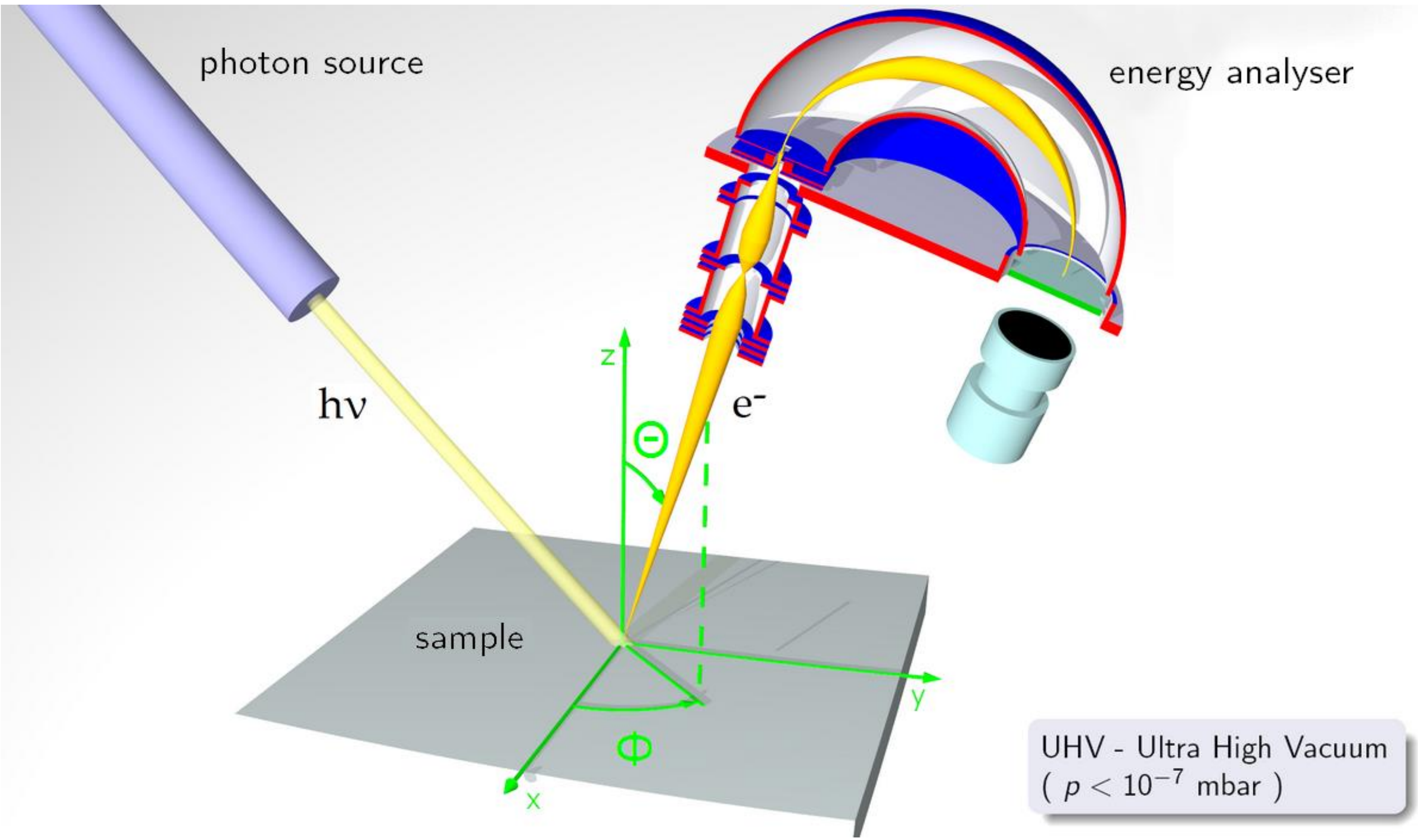
1. 对角分辨实验特别重要

2. 缺陷、杂质、台阶

3. 不同区域功函数问题

# 能量分析器

# 能量分析器



photon source
energy analyser
hν
e⁻
z
Θ
sample
y
Φ
x
UHV - Ultra High Vacuum
( p < 10⁻⁷ mbar )

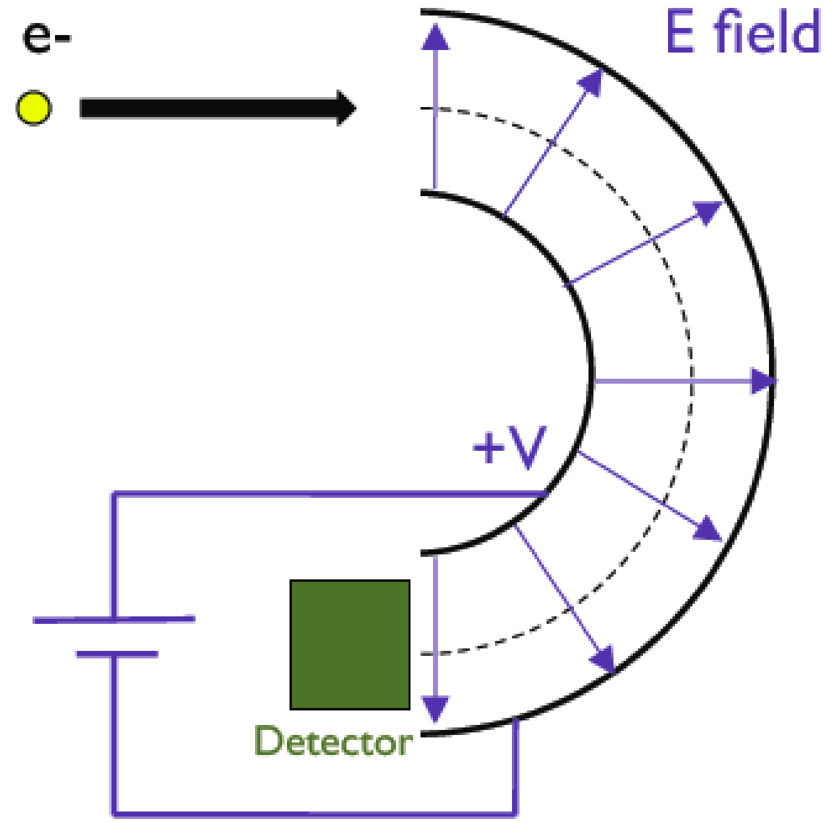
# 能量分析器

• typical energy resolution ~ 0.1 to 0.01 eV. Best systems are ~ 0.001 eV.

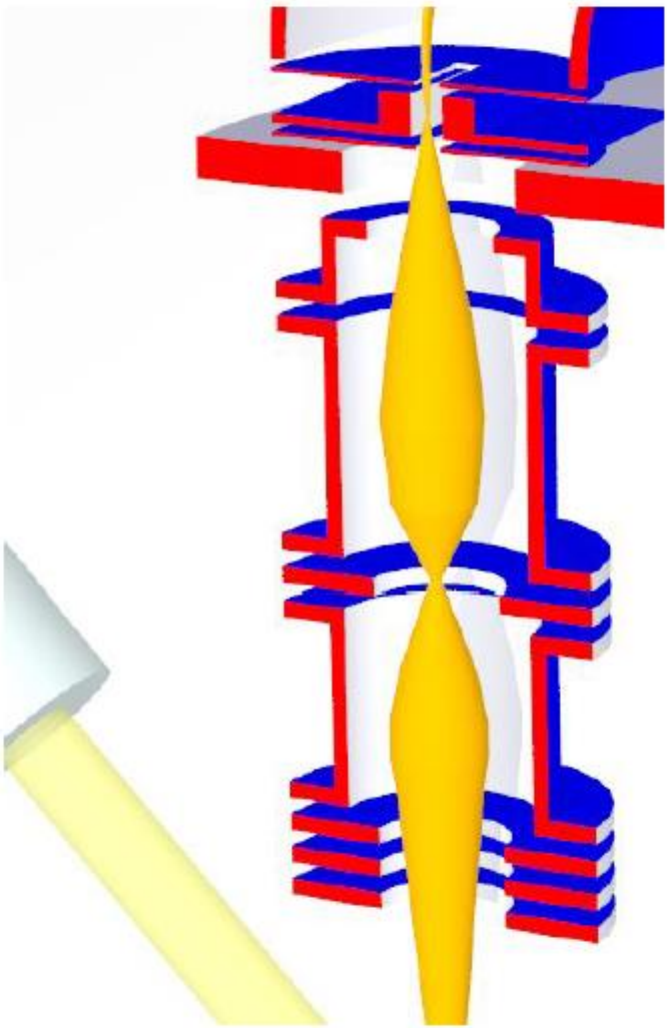
• most electron analyzers operate using electrostatic optics (magnetic fields harder to control)

• detectors are typically channel plates (electron multipliers) with a CCD or current pulse output

• detecting & manipulating electrons is relatively easy



# Retarding and focusing

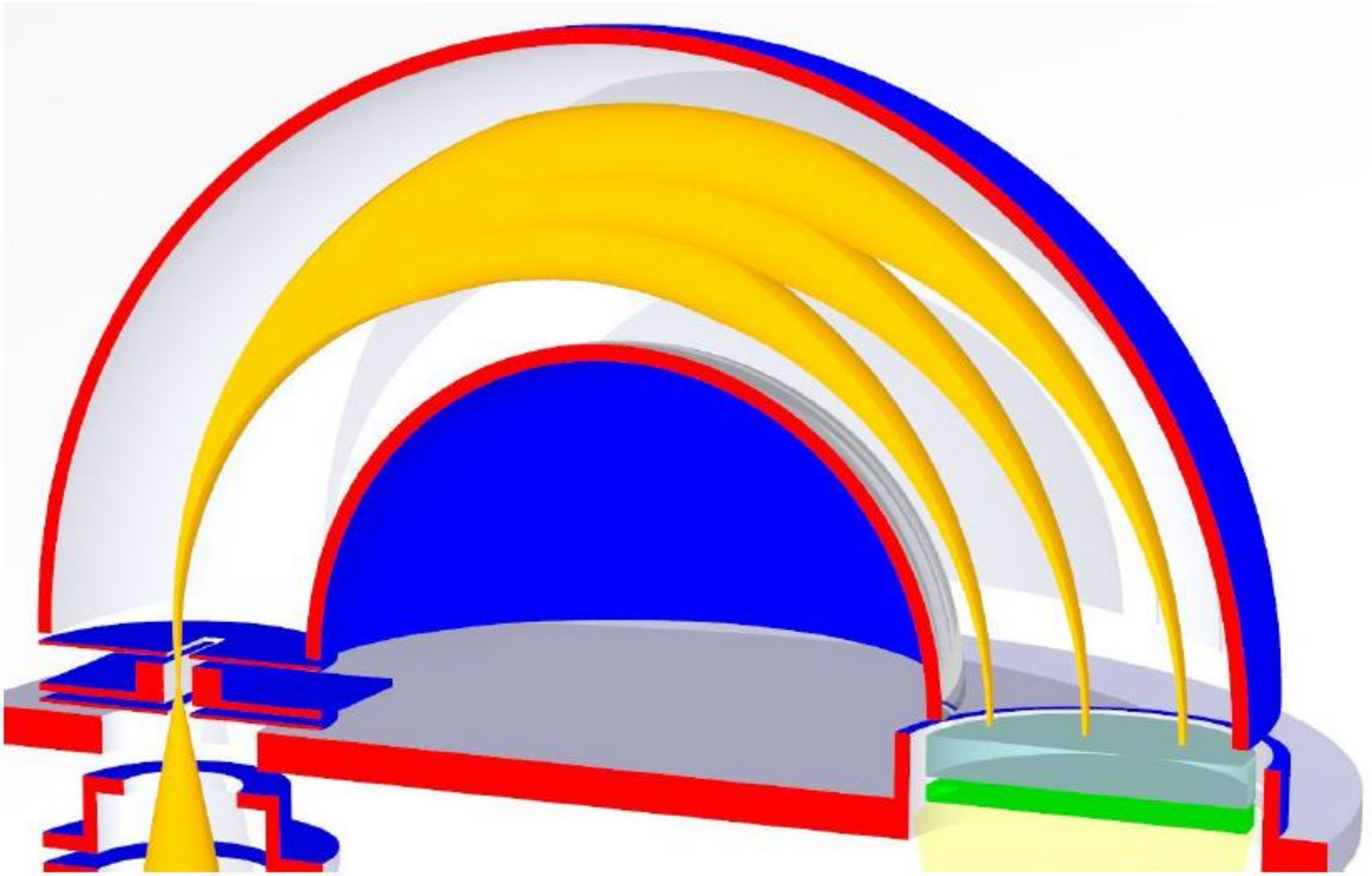


**Preretarding stage**

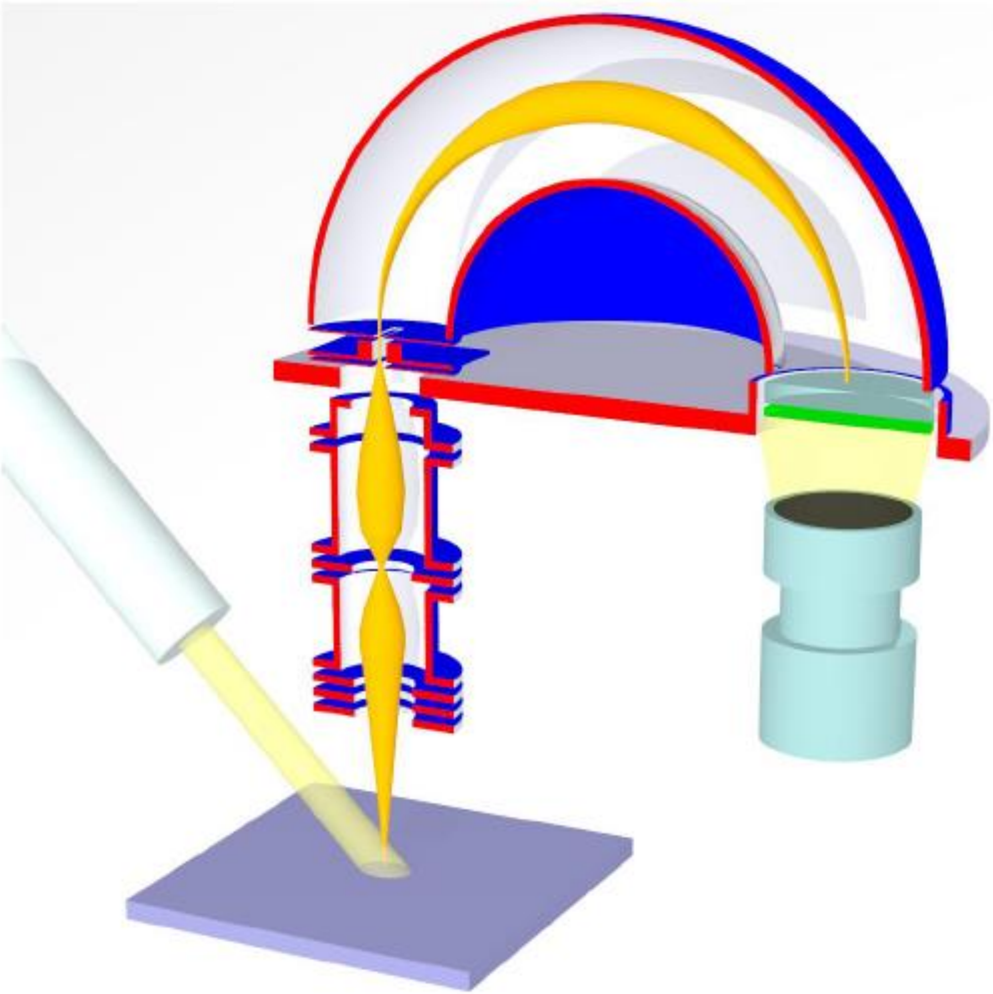
Usually a preretarding stage is used prior to the energy analysis. Electrons enter the analyser with a specified pass energy. One can decelerate (or accelerate) electrons (almost) without changing their absolute energy spread. Measured kinetic energy:

$$E_{kin,A} = E_{pass} - U_{ret}$$

# 能量分辨



# 能量分辨率



## Potentials on hemispheres

For transmission of electrons with initial emergy $E_0$ along a path with $R_0 = (R_{in} + R_{out})/2$ the potential has to be

$$V_{out} = E_0[3 - 2(R_0/R_{out})]$$

$$V_{in} = E_0[3 - 2(R_0/R_{in})]$$

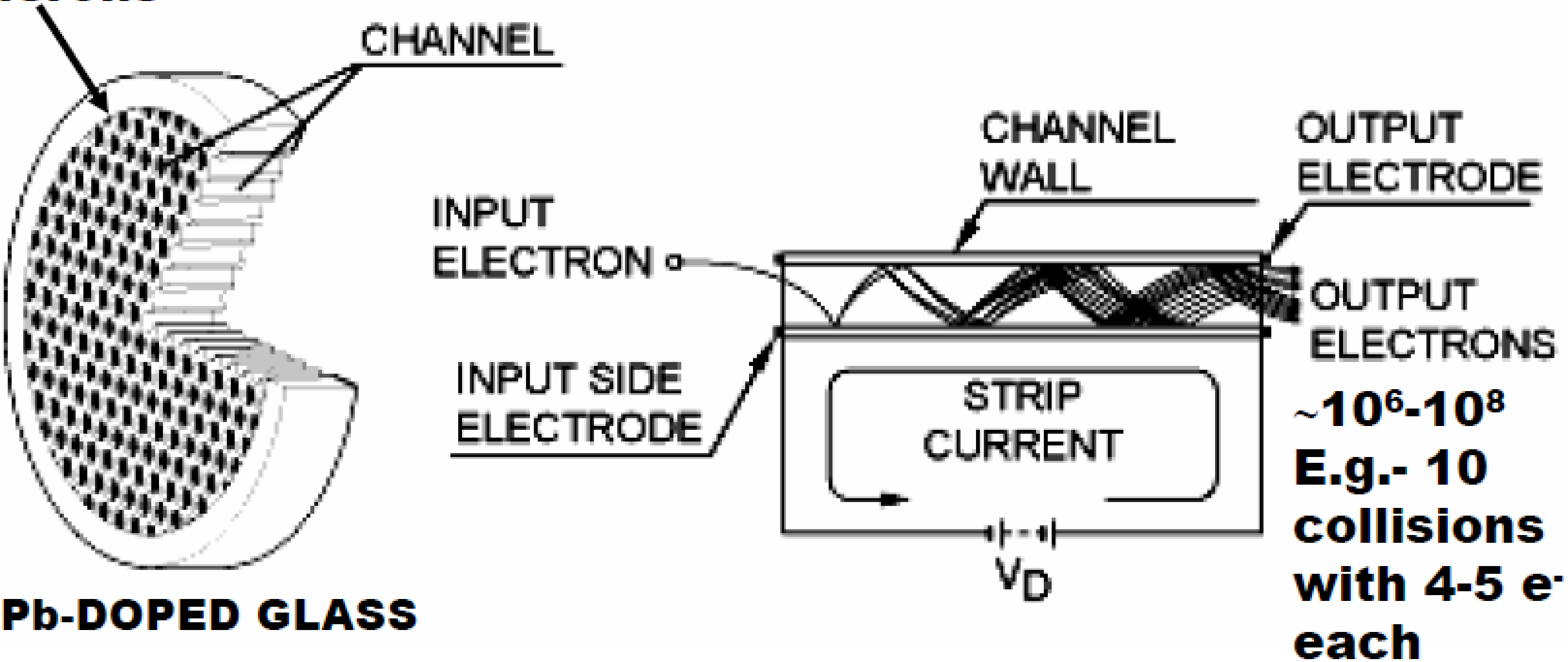
## Resolution

$$\frac{\Delta E}{E_{pass}} = \frac{w}{2R_0} + \alpha^2$$

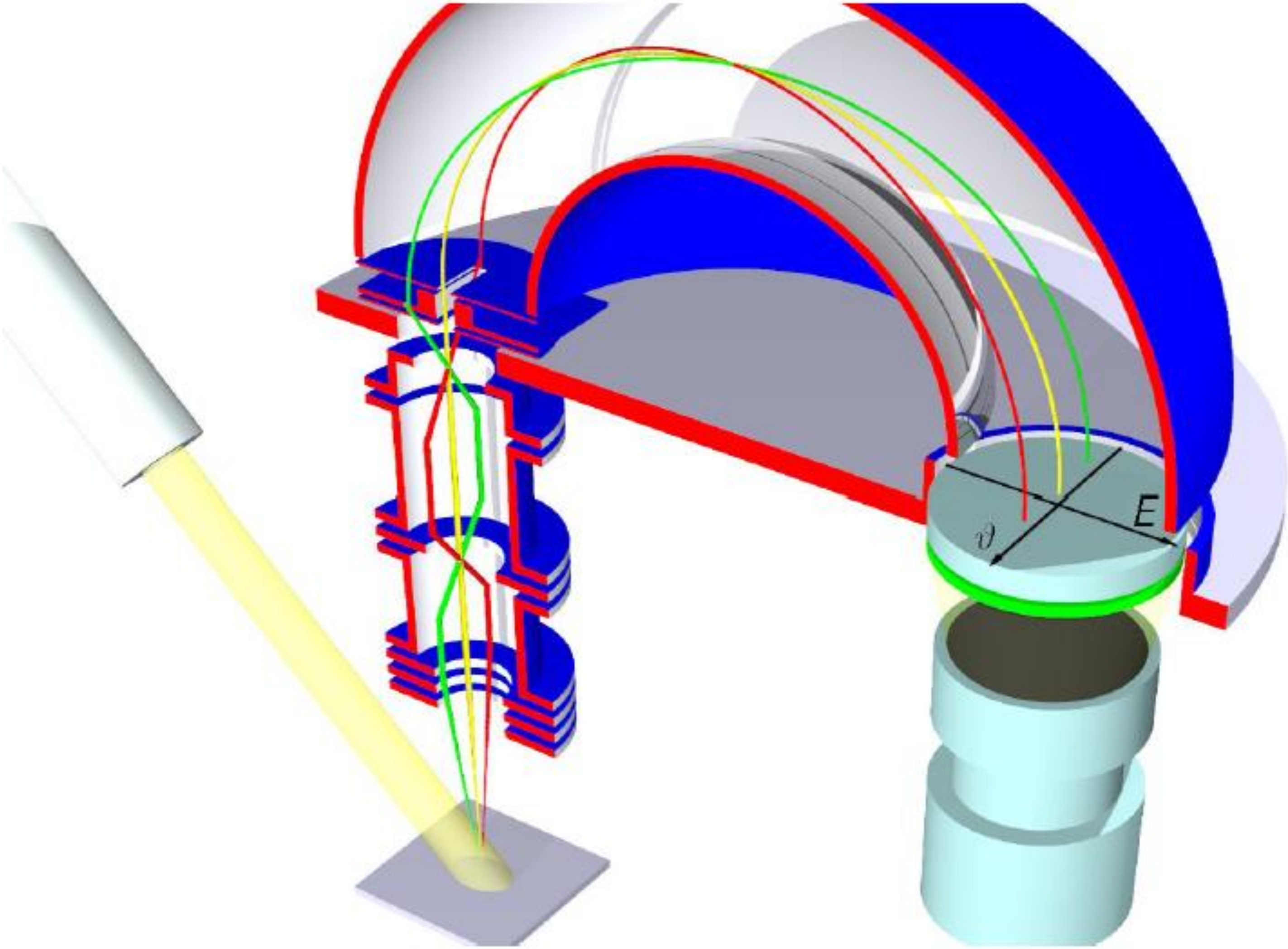
| | |
|---|---|
| w | width entrance slit |
| $\alpha$ | acceptance angle |

# Microchannel Plate

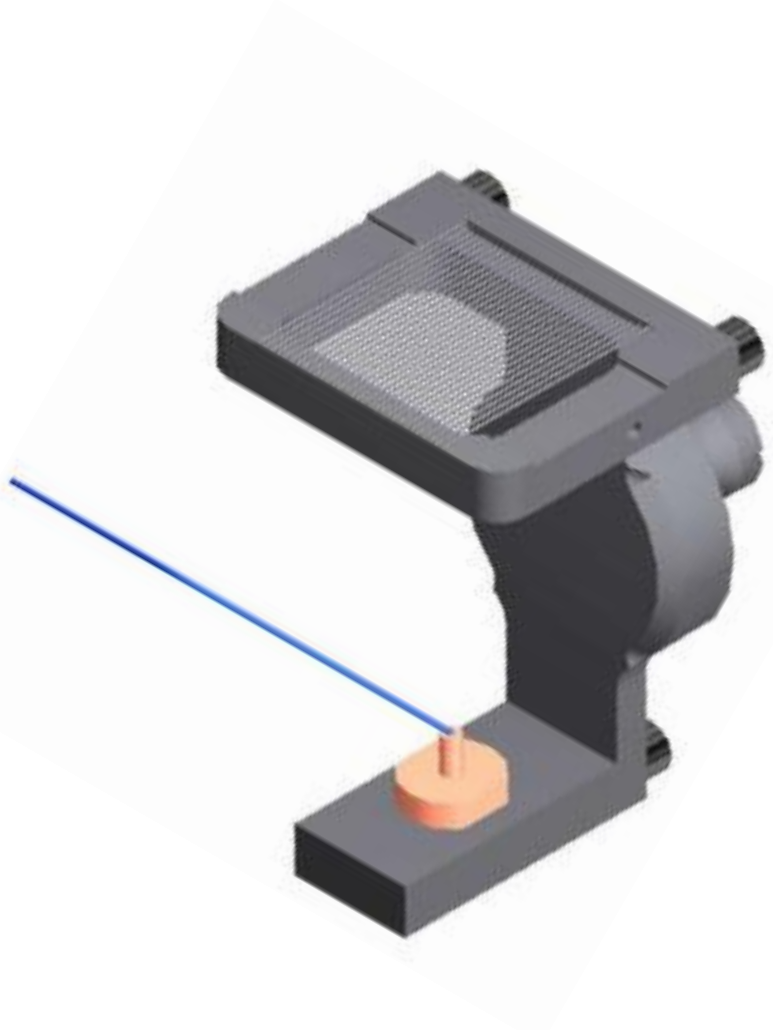
**Diam.**
**Down to 5**
**microns**

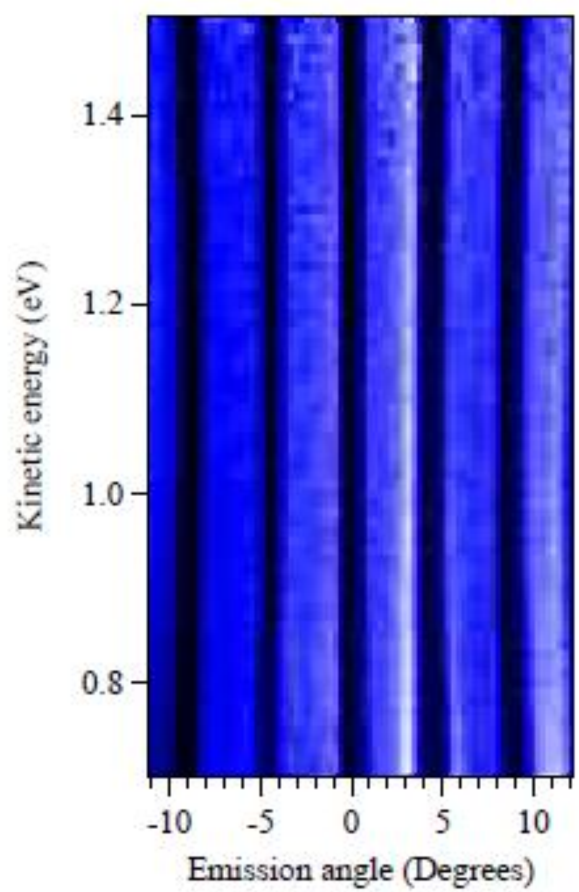


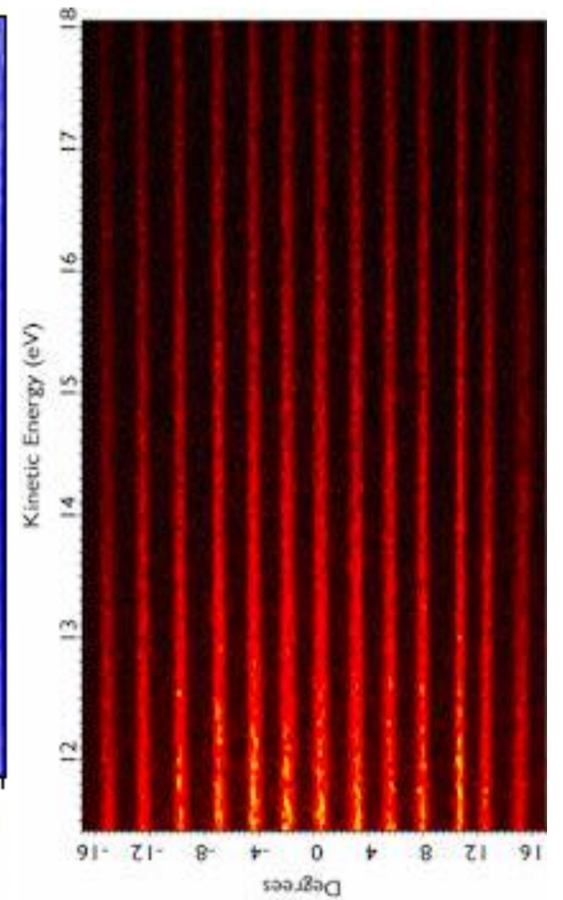
# 角度分辨



# 角度分辨率测量



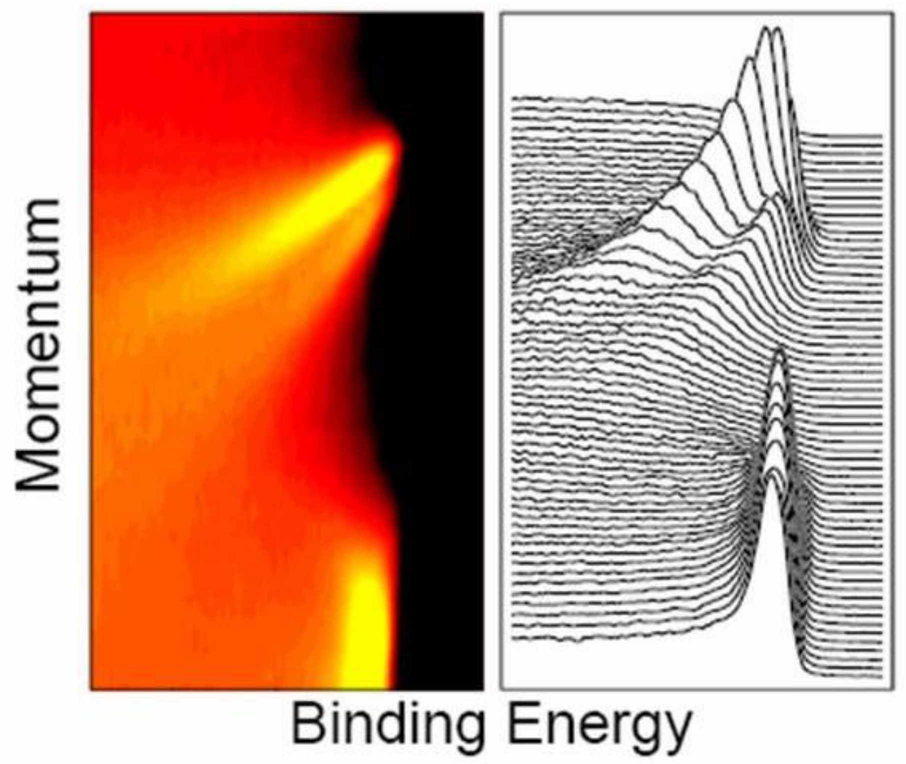

Kinetic energy (eV)
1.4
1.2
1.0
0.8
-10
-5
0
5
10
Emission angle (Degrees)


Kinetic Energy (eV)
12
13
14
15
16
17
18
Degrees

# 现代的能量分析器的发明者

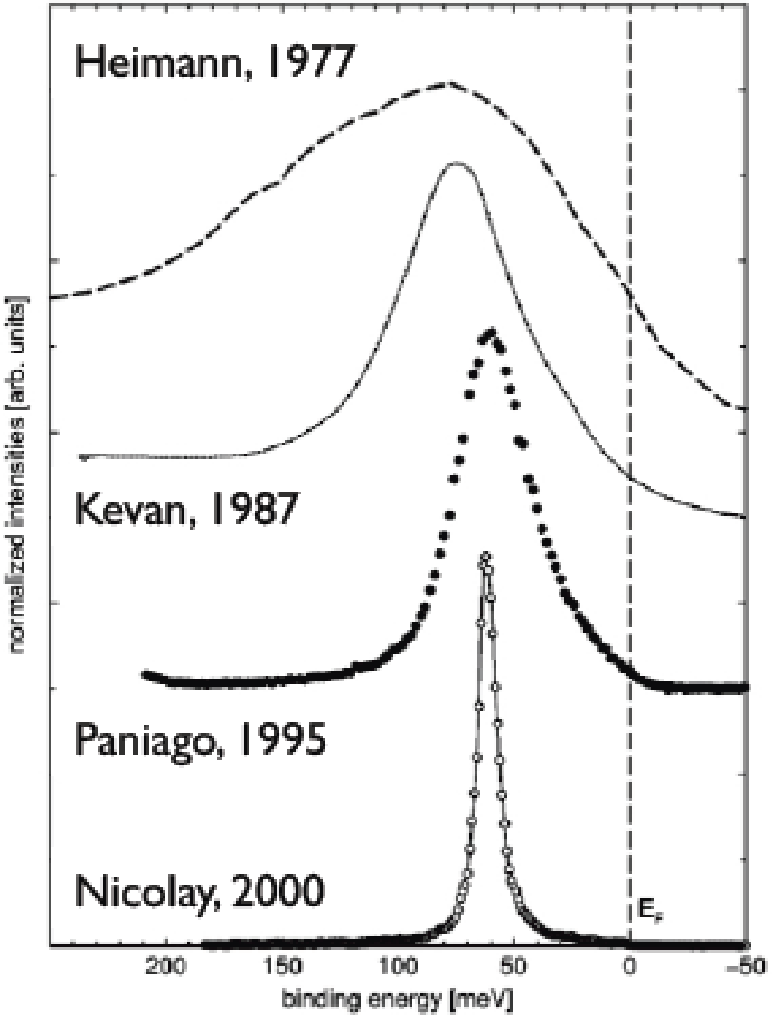
Bjorn Wannberg

2008 APS
Keithley Award

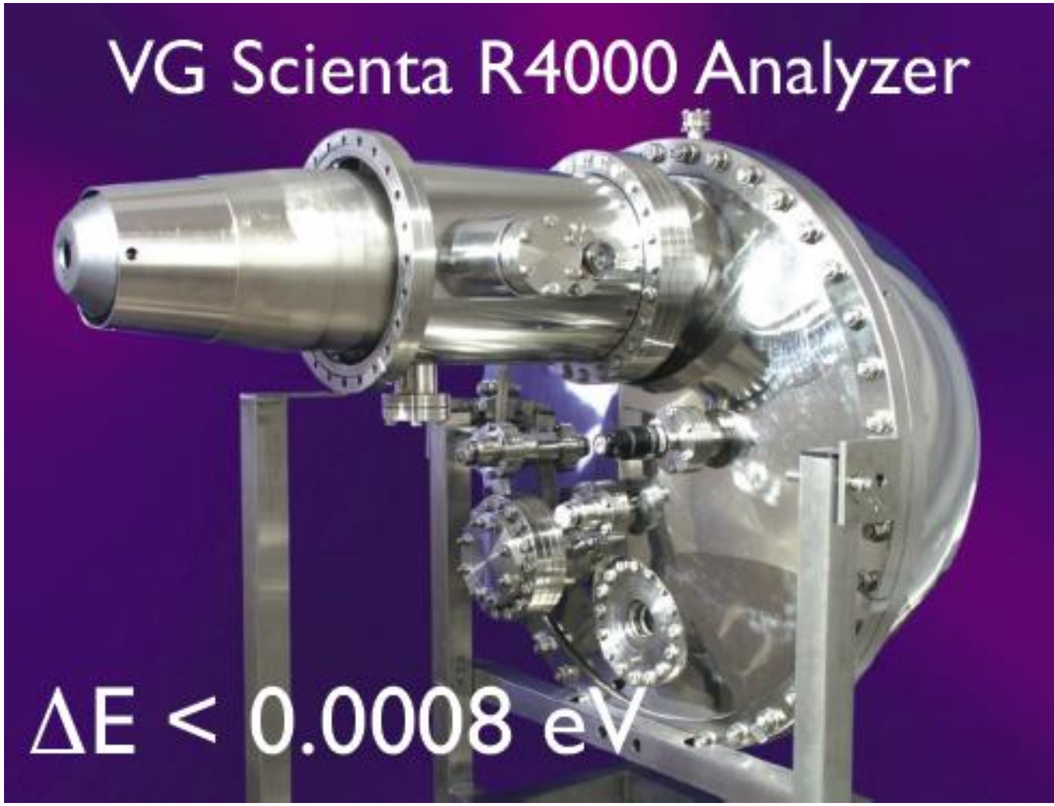



能量分辨率1meV，提高20倍
角分辨率0.2度，提高10倍
采集效率极大地提高

# 能量分析器

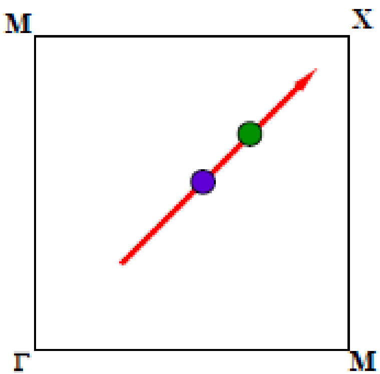



F. Reinert *et al.*, PRB (2001)

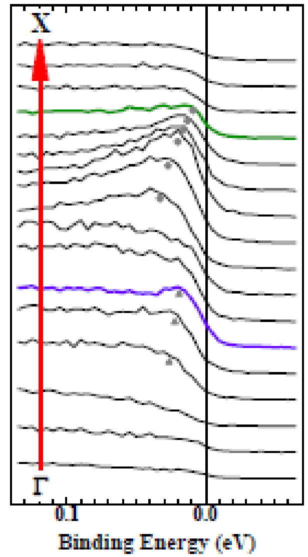


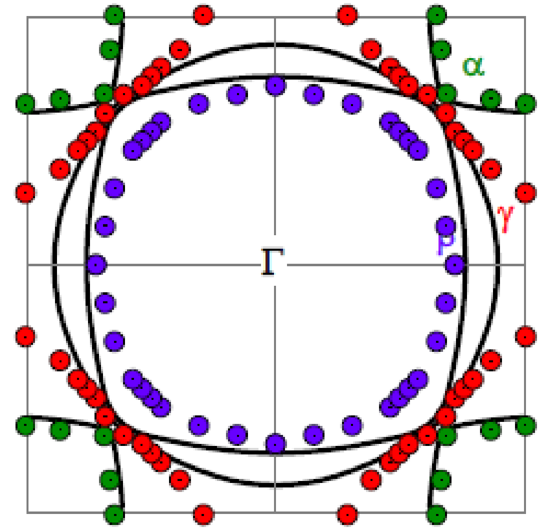
# 过去与现在

## ***ARPES : circa 1996***



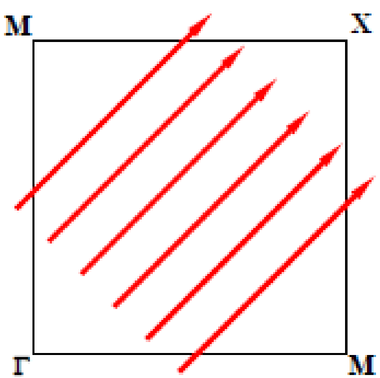

D.H. Lu *et al.*, PRL **76**, 4845 (1996)



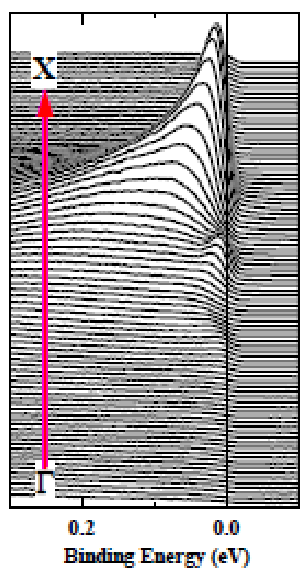



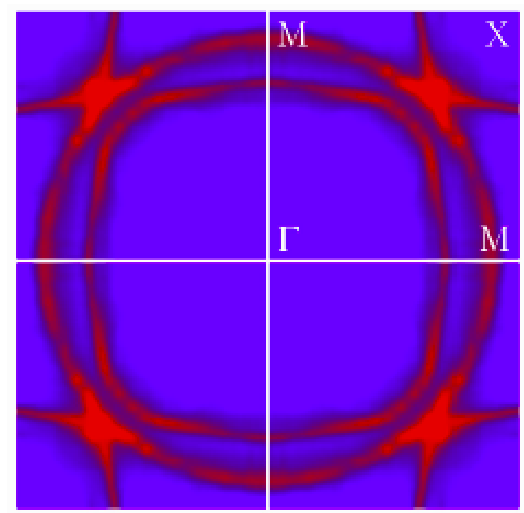

D.J. Singh, PRB **52**, 1358 (1995)

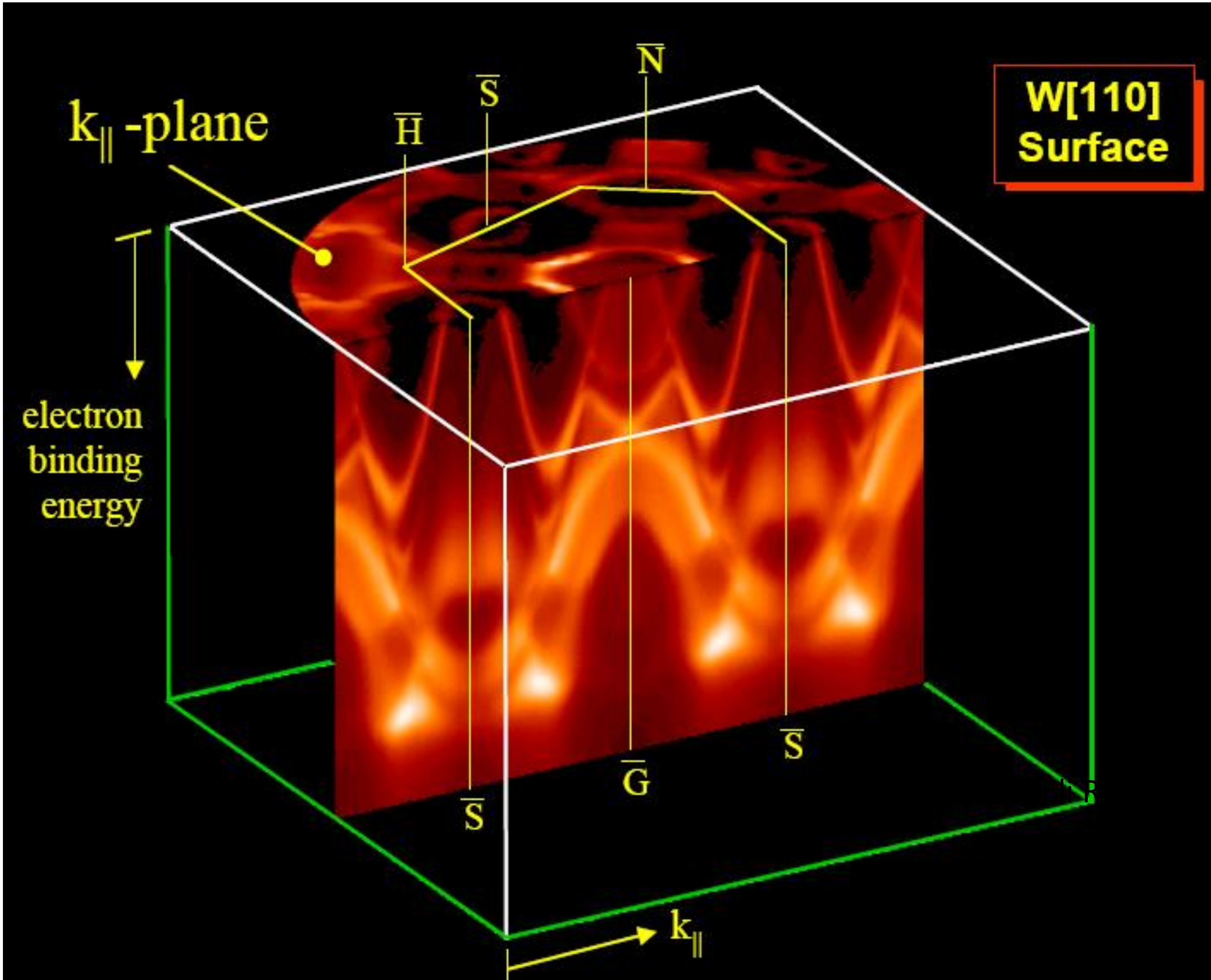
## ***ARPES : present day***




A. Damascelli *et al.*, PRL **85**, 5194 (2000)

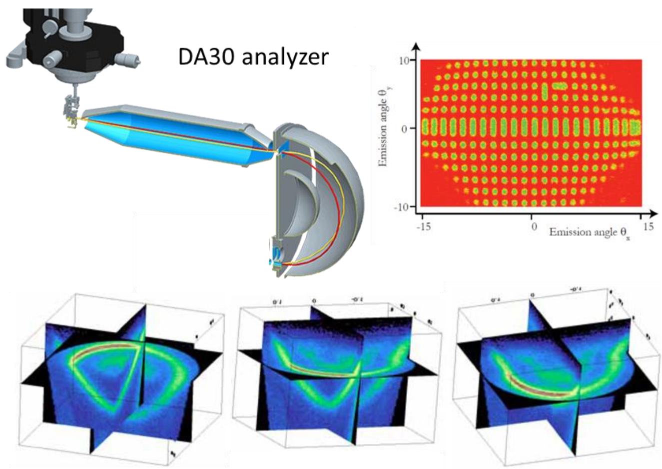




$k_{\parallel}$ -plane
W[110]
Surface
$\bar{H}$
$\bar{S}$
$\bar{N}$
electron
binding
energy
$\bar{S}$
$\bar{G}$
$\bar{S}$
$\bar{S}$
$k_{\parallel}$

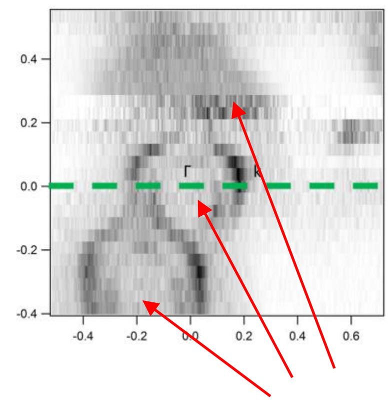
# 新一代高效率能量分析器

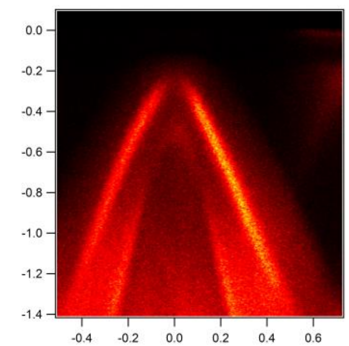




## R4000分析器

TiSe$_2$

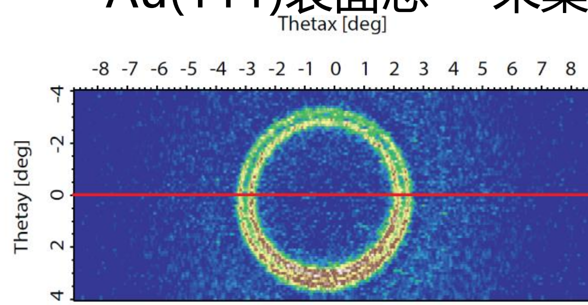


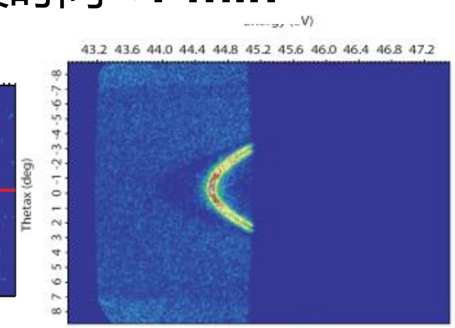


数据来自样品上不同区域，无法保证可靠性

## DA30L分析器

Au(111)表面态　采集时间<**1 min**




- Energy Resolution: better than 2meV
- Angular Resolution: 0.1°
- Angular Acceptance: 2D ±15°
- Deflection mode: ±15°

**新型分析器**

Scienta Omicron: DA30L

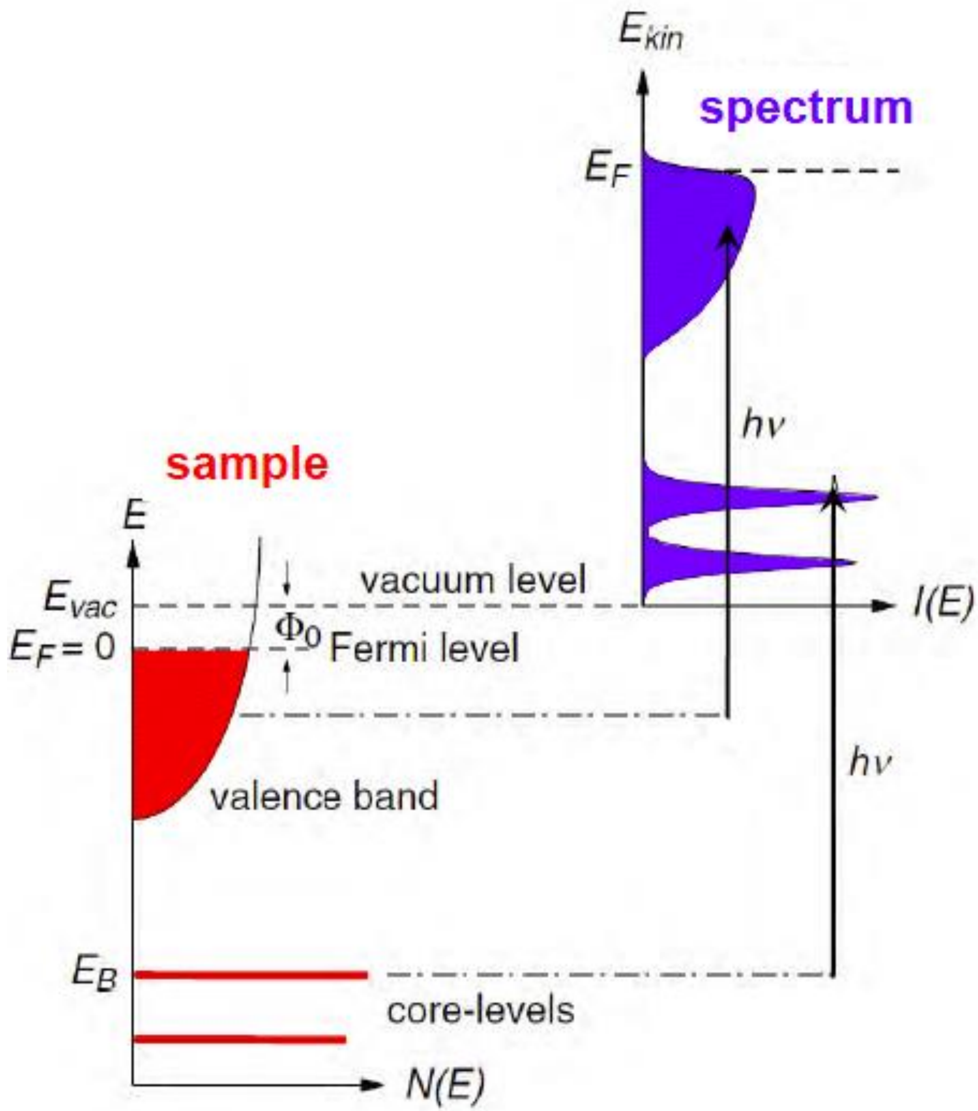
Specs: Phoibos 150 SAL

MBS: A-1 lens-4

Dr. Vobornik, ELETTRA

# 光电子过程

# 光电激发



$E_{kin}$
spectrum
$E_F$
$h\nu$
sample
$E$
vacuum level
$I(E)$
$E_{vac}$
$\Phi_0$
$E_F = 0$
Fermi level
$h\nu$
valence band
$E_B$
core-levels
$N(E)$

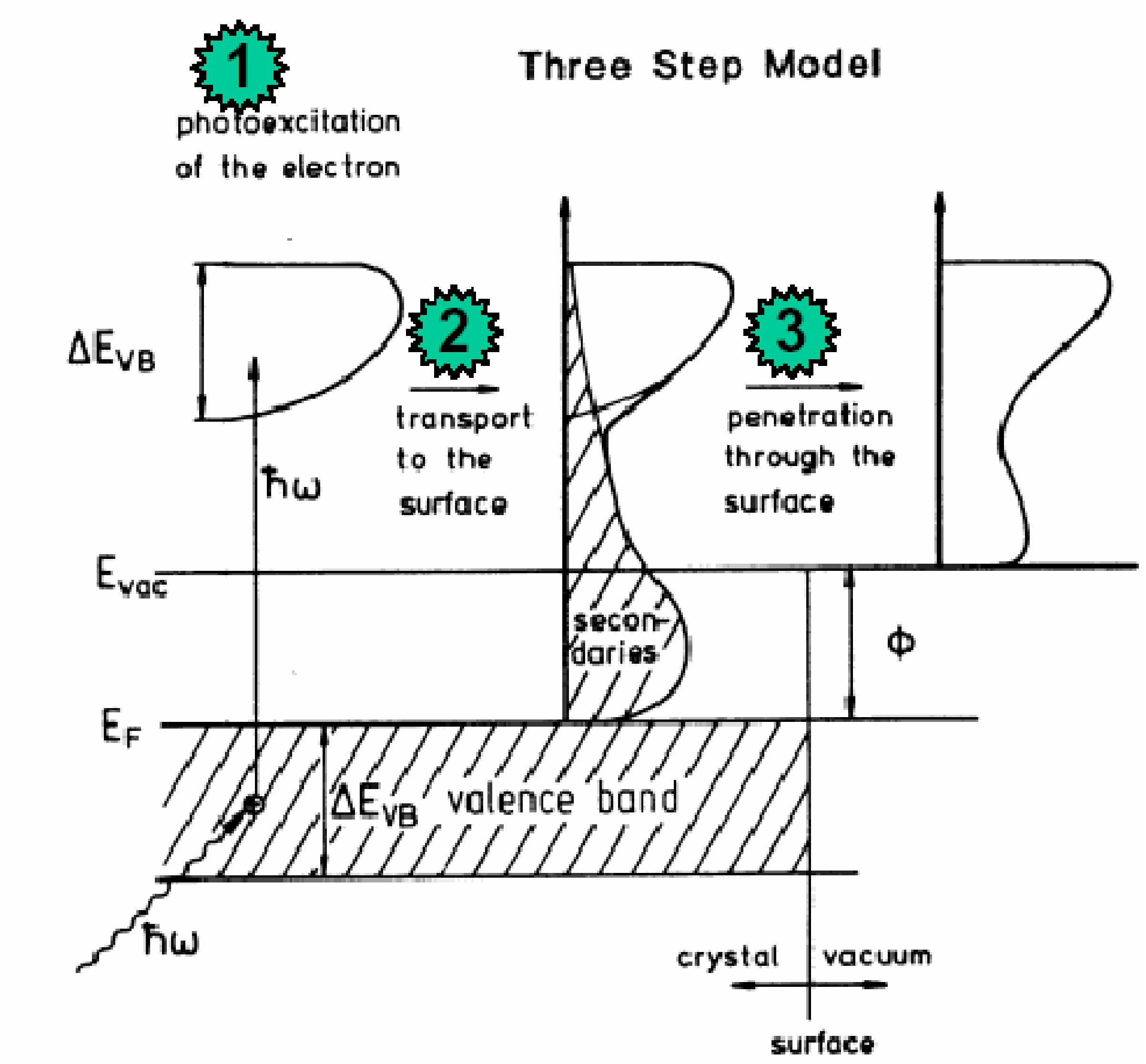
# 光电激发的三步模型

第一步：单个电子的光激发。

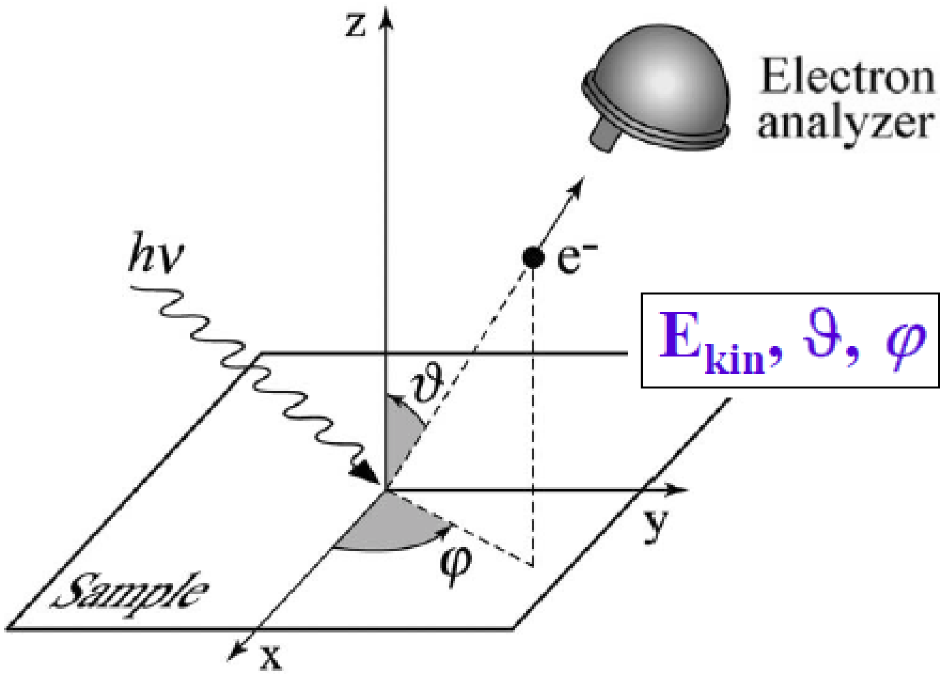
第二步：被激发的电子在固体中传输到表面，在此过程中，电子可能会受到非弹性散射。

第三步：具有足够动能的电子越过表面势垒，发射到真空中去。

# 光电激发的三步模型


Three Step Model
1
photoexcitation
of the electron
2
transport
to the
surface
3
penetration
through the
surface
$\Delta E_{VB}$
$\hbar\omega$
$E_{vac}$
secon-
daries
$\Phi$
$E_F$
$\Delta E_{VB}$ valence band
$\hbar\omega$
crystal
vacuum
surface

# 基本公式




$$\mathbf{K} = \mathbf{p}/\hbar = \sqrt{2mE_{kin}}/\hbar$$

$$K_x = \frac{1}{\hbar}\sqrt{2mE_{kin}}\sin\vartheta\cos\varphi$$

$$K_y = \frac{1}{\hbar}\sqrt{2mE_{kin}}\sin\vartheta\sin\varphi$$

$$K_z = \frac{1}{\hbar}\sqrt{2mE_{kin}}\cos\vartheta$$

---

**Vacuum**

$E_{kin}$

$\mathbf{K}$

**Conservation laws**

$$E_f - E_i = h\nu$$

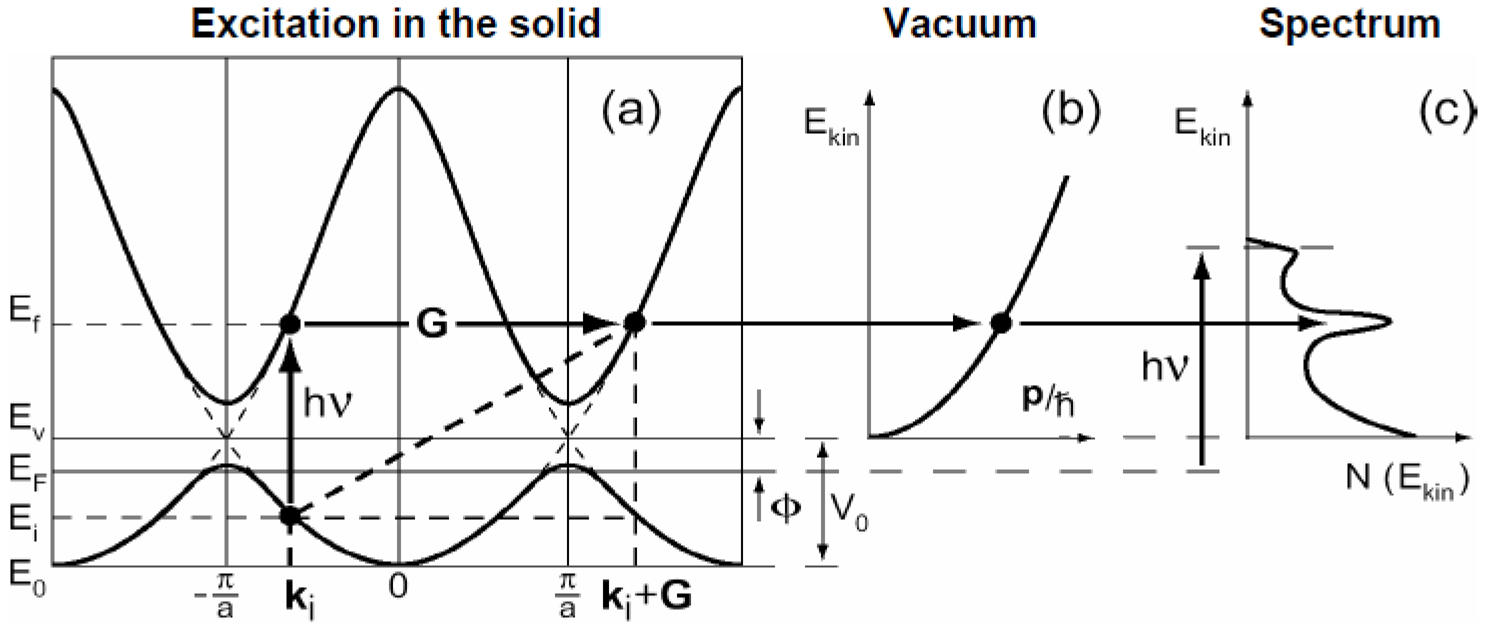
$\mathbf{k}_f - \mathbf{k}_i =$ ~~$\mathbf{k}_{h\nu}$~~

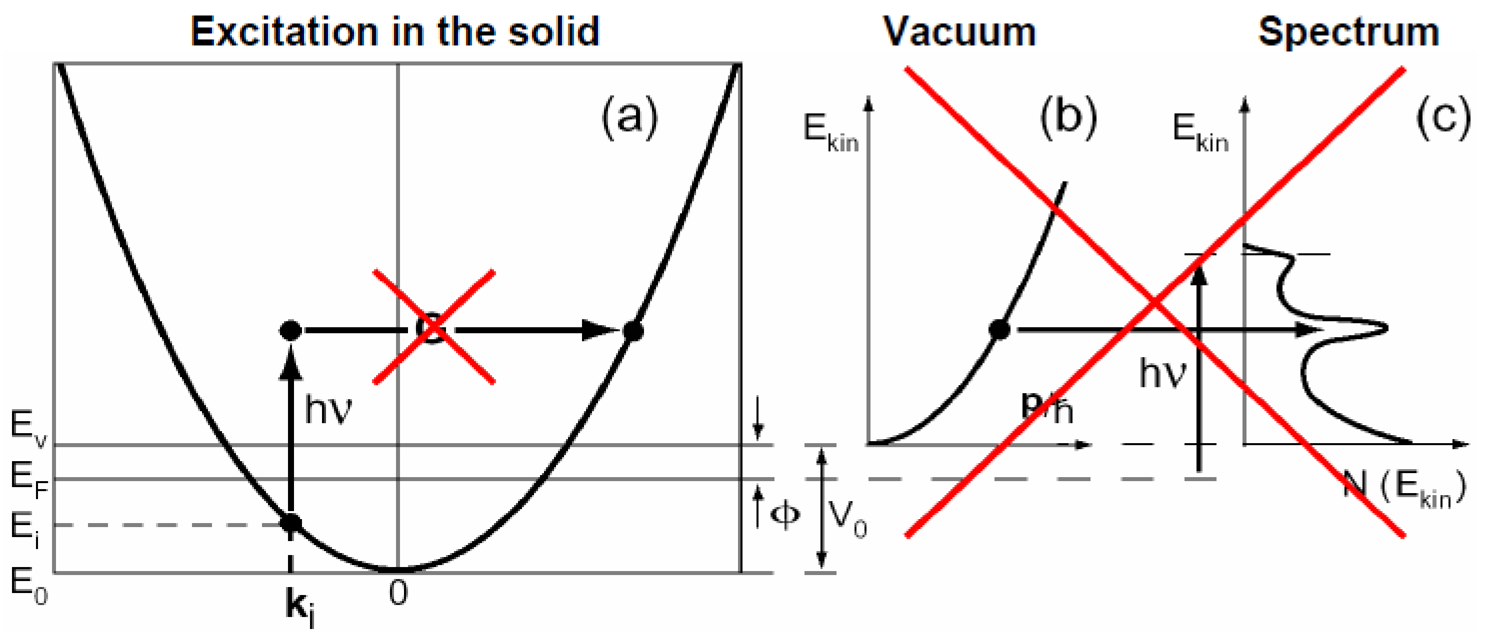
**Solid**

$E_B$

$\mathbf{k}$

# Direct transition



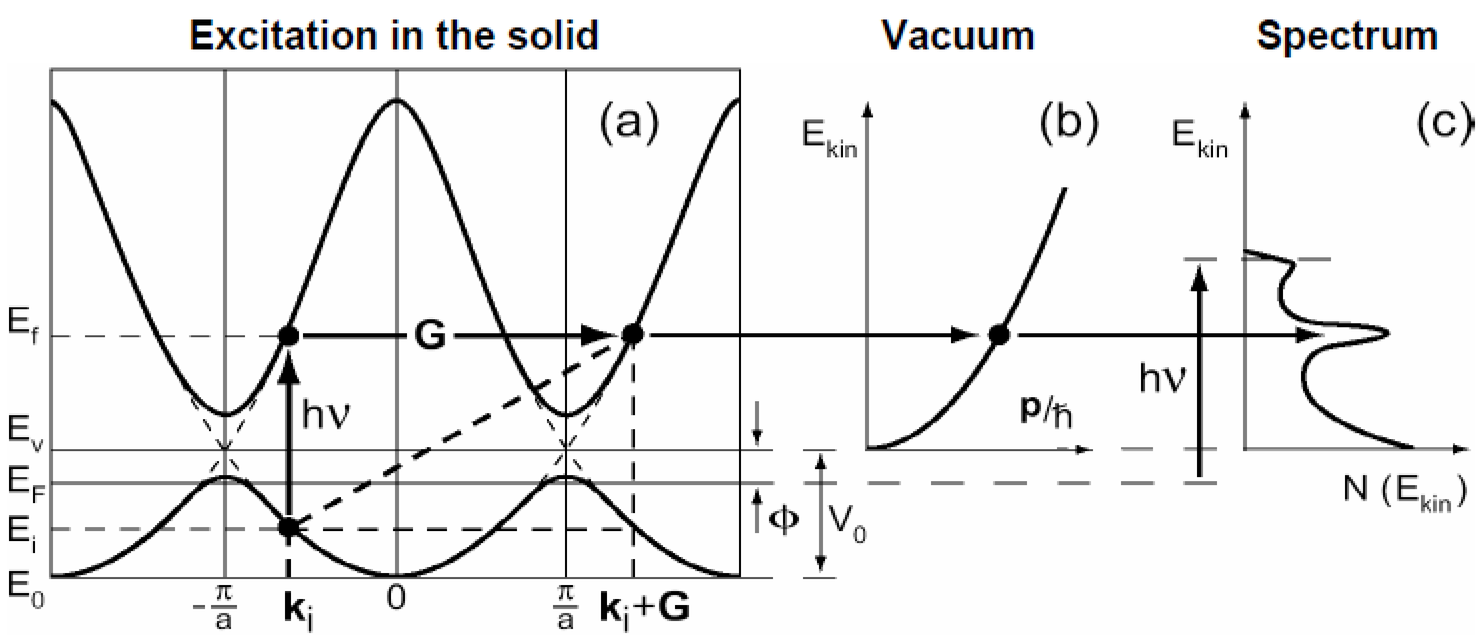



# Inner potential and determination of $k_z$

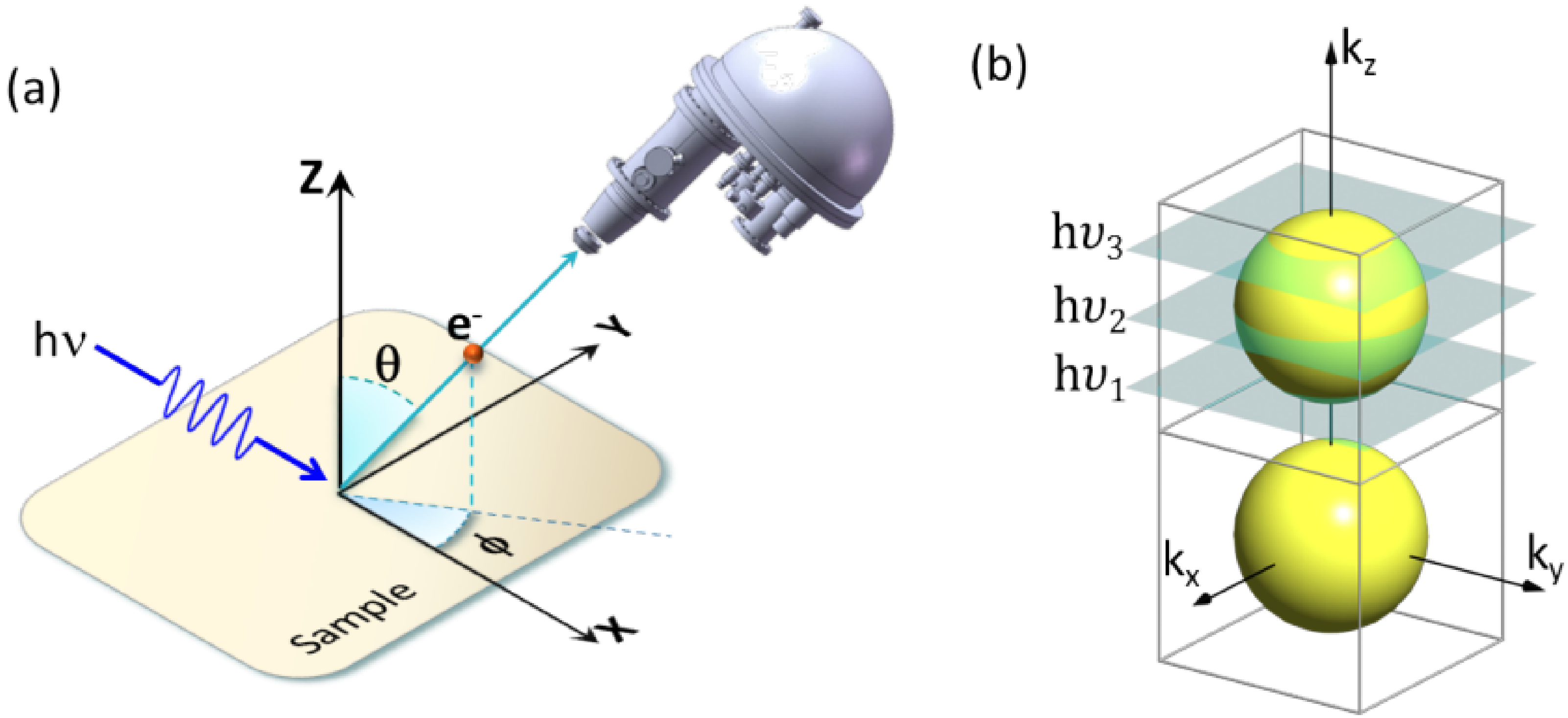
**Free-electron final state** $E_f(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m} - |E_0| = \frac{\hbar^2 (\mathbf{k}_\parallel{}^2 + \mathbf{k}_\perp{}^2)}{2m} - |E_0|$

**because** $\hbar^2 \mathbf{k}_\parallel^2 / 2m = E_{kin} \sin^2 \vartheta$ $E_f = E_{kin} + \phi$ $V_0 = |E_0| + \phi$

$$\mathbf{k}_\perp = \frac{1}{\hbar}\sqrt{2m(E_{kin}\cos^2\vartheta + V_0)}$$



# Inner potential and determination of $k_z$




(c)

$$E_k = h\upsilon - w - E_B$$

In vacuum:

$$k^V{}_x = \frac{\sqrt{2m_eE_k}}{\hbar}\sin(\theta)\cos(\Phi)$$

$$k^V{}_y = \frac{\sqrt{2m_eE_k}}{\hbar}\sin(\theta)\sin(\Phi)$$

$$k^V{}_z = \frac{\sqrt{2m_eE_k}}{\hbar}\cos(\theta)$$

In crystal:

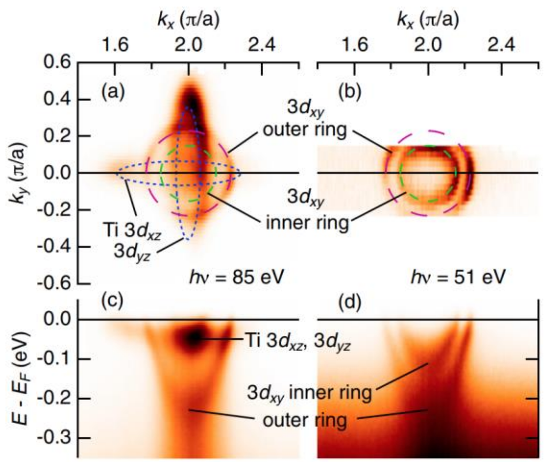
$$k_x = \frac{\sqrt{2m_eE_k}}{\hbar}\sin(\theta)\cos(\Phi) \quad = k^V{}_x$$

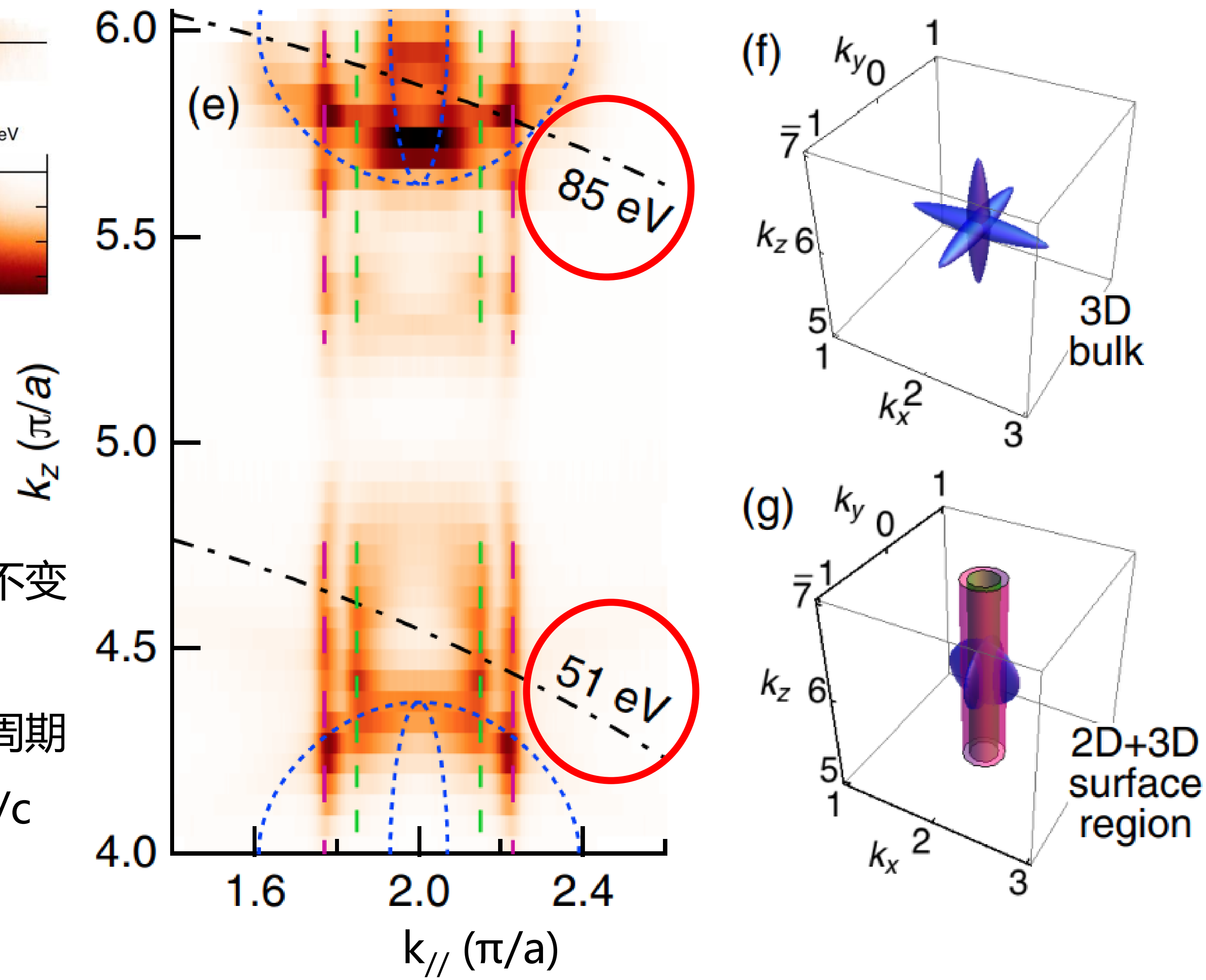
$$k_y = \frac{\sqrt{2m_eE_k}}{\hbar}\sin(\theta)\,sin(\Phi) \quad = k^V{}_y$$

$$k_z = \sqrt{\frac{2m_e{}^*}{\hbar^2}(E_k + V_0) - \frac{2m_eE_k}{\hbar^2}\sin^2\theta} \neq k^V z$$

DOI: 10.1126/science.1245085

# Inner potential and determination of $k_z$

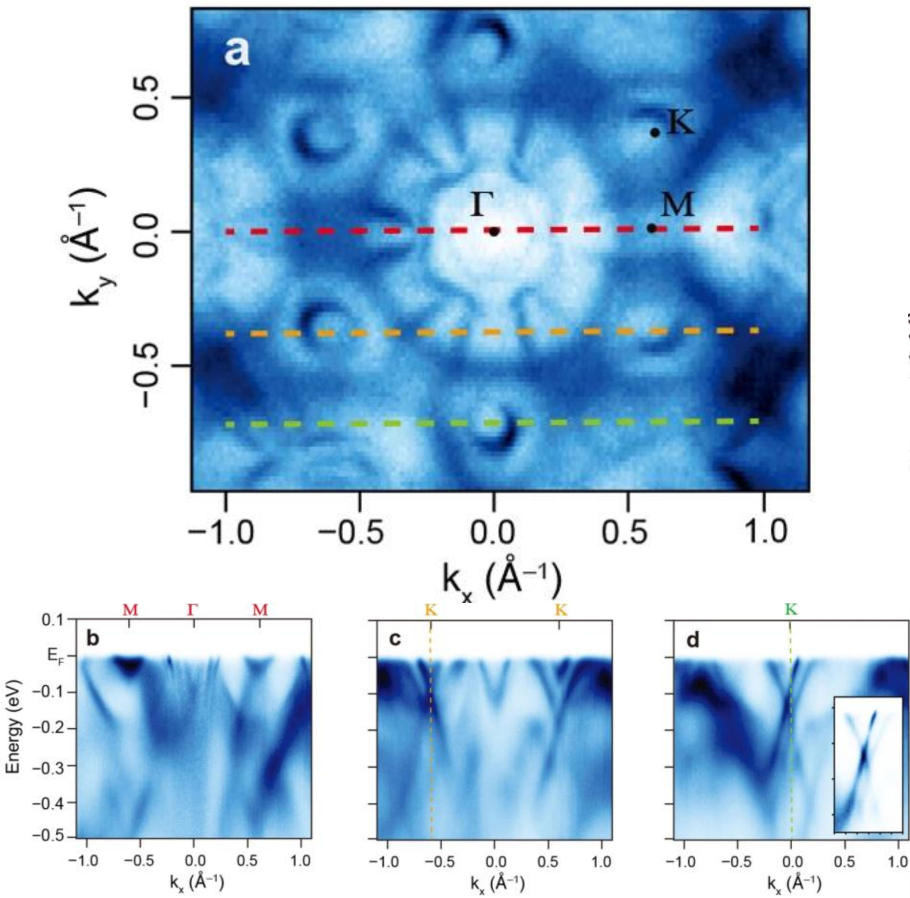


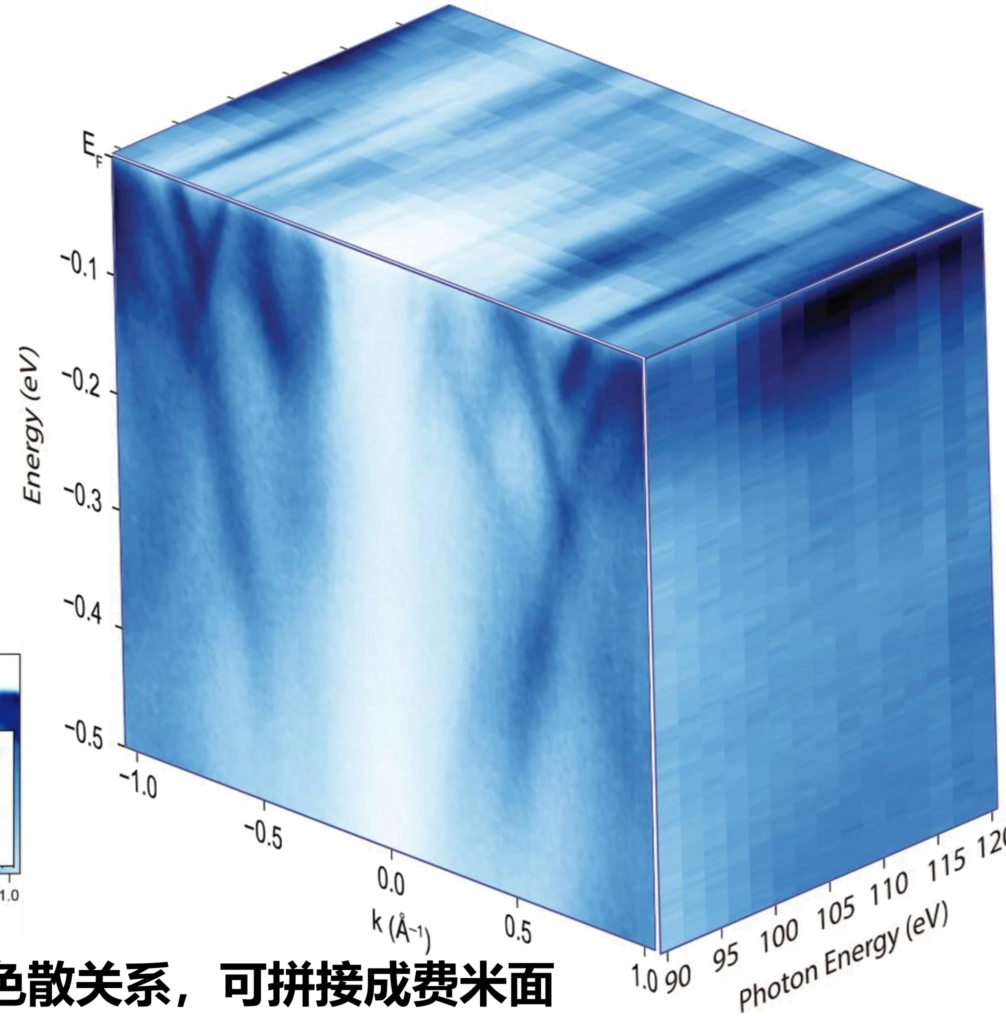




- 二维电子态kz色散不变 (无kz色散)
- 三维电子态kz色散周期性变化，周期为2π/c

PRL 113, 086801 (2014)

# Photon-energy dependence of ARPES

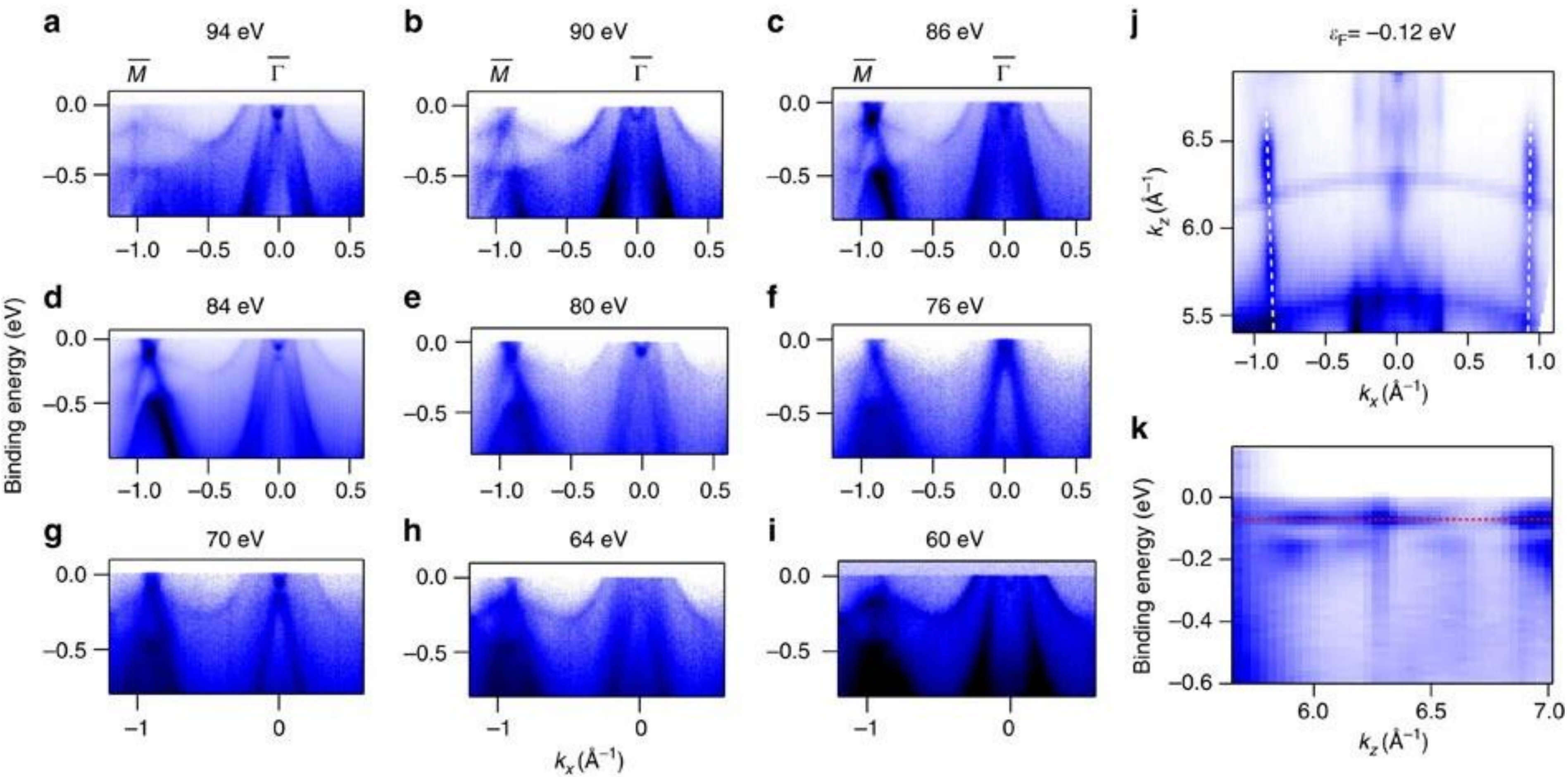



Nature 555, 638 (2018)

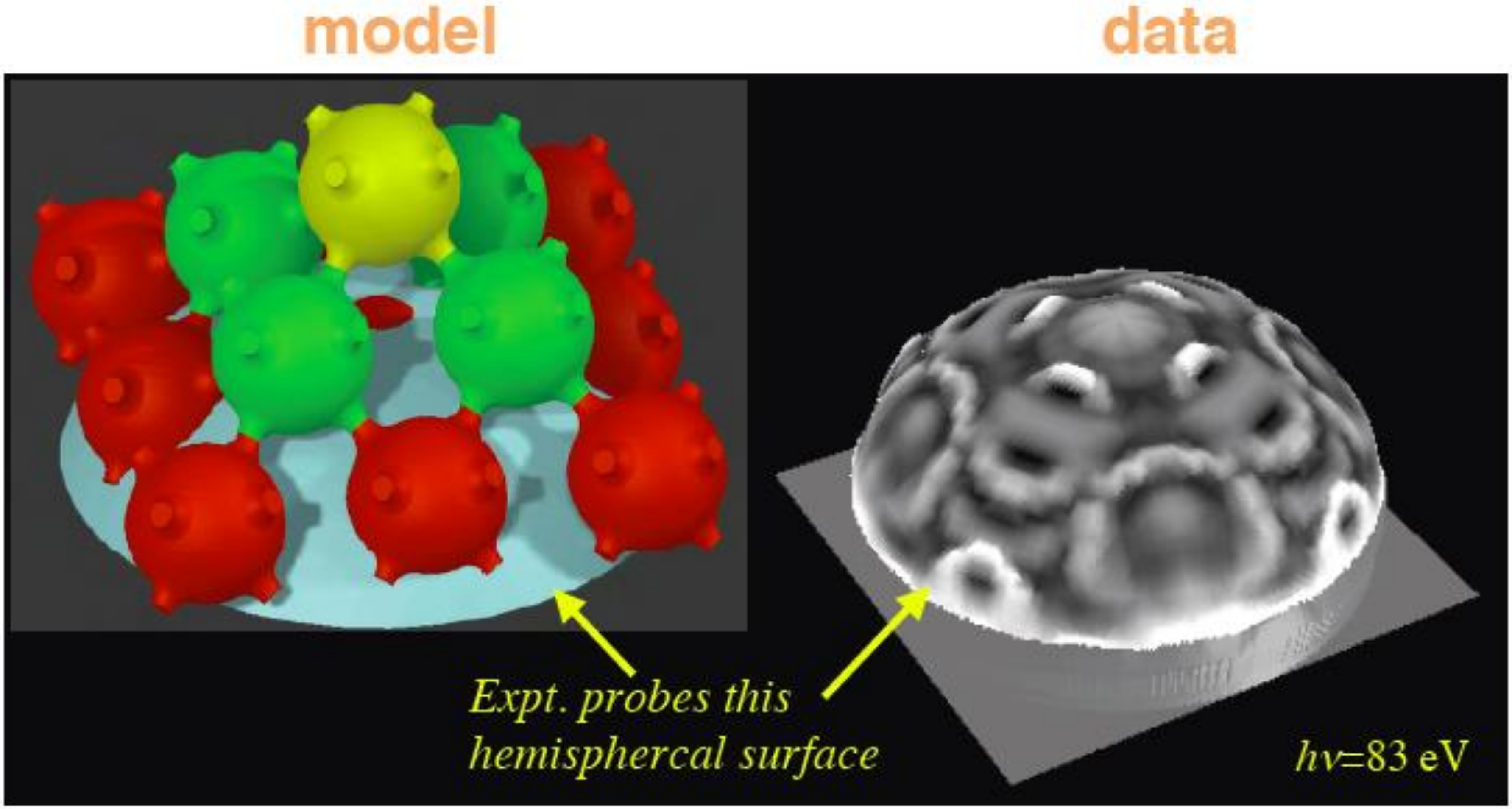
- 固定能量下，数据形式为能量-动量色散关系，可拼接成费米面
  - 如上面小图中，每一幅图展示固定ky时沿着kx方向的色散
- 确定Γ点后，改变光子能量，在高对称方向采集数据，如右图所示
  - 通过$k_F$随能量的变化，可以看到沿着kz方向的规律，帮助判断电子态的维度

# Photon-energy dependence of ARPES

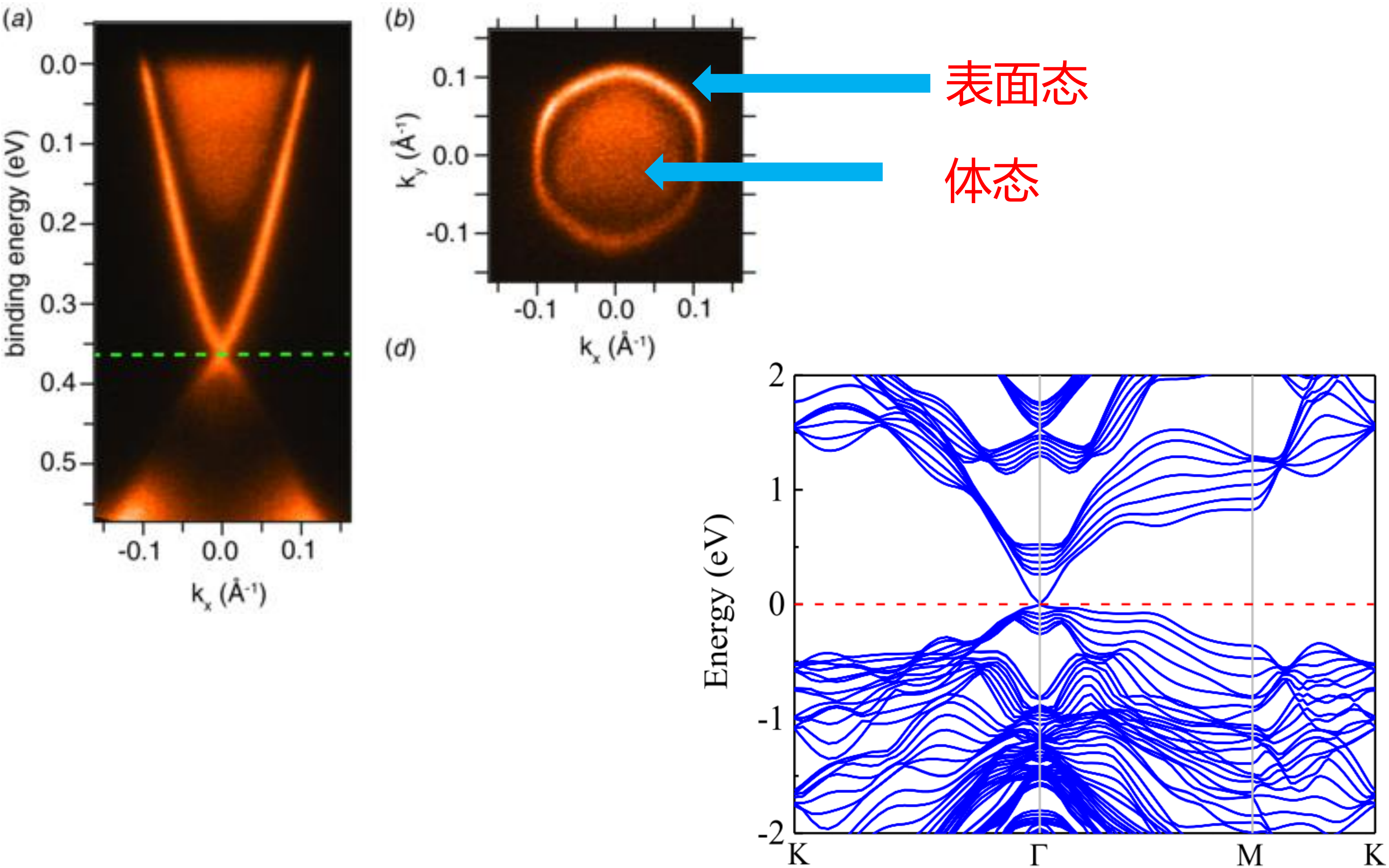



Nature Communications 8, 13942 (2017)

# 等动量面



# 三维体态与二维表面态的展宽



PHYSICAL REVIEW B VOLUME 21, NUMBER 8 15 APRIL 1980

# Angle-resolved photoemission, valence-band dispersions $E(\vec{k})$, and electron and hole lifetimes for GaAs

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(Received 3 December 1979)

$$E_f(\vec{k}) = \hbar^2 |\vec{k}|^2/2m + E_0 = \hbar^2(k_\parallel^2 + k_\perp^2)/2m + E_0$$

Final Bloch states.

$E_o$ = "bottom of Muffin tin" – starting point for parabolic band dispersions = -9.34 eV for GaAs.

$$E_f(\vec{k}) = E_i(\vec{k}) + h\nu$$

$$E_f = E_k + e\Phi$$

Direct or k-conserving transitions.

$e\phi$ = work function of sample,

$E_k$=kinetic energy

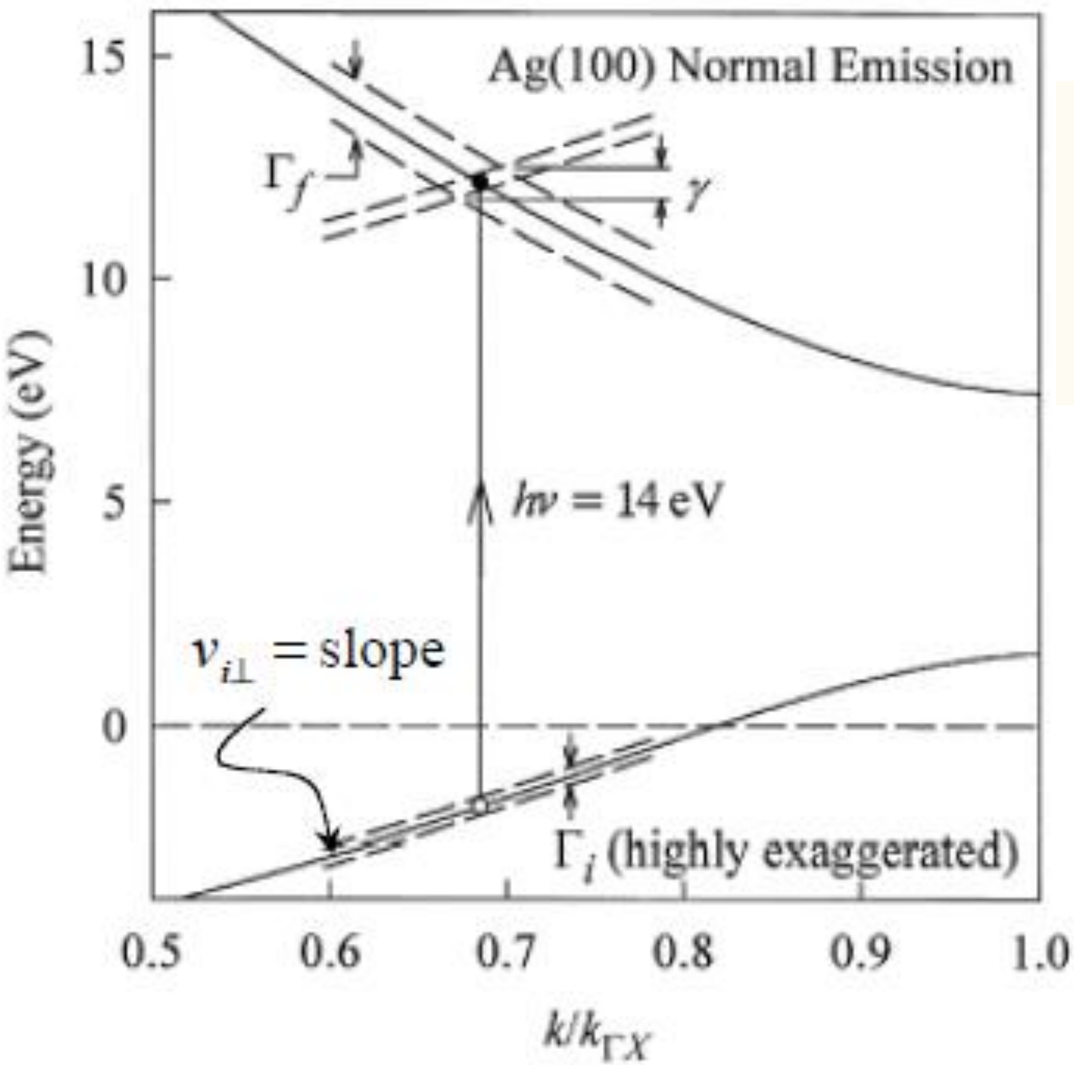
$$\hbar k_\parallel = (2mE_k)^{1/2}\sin\theta = [2m(E_i + h\nu - e\Phi)]^{1/2}\sin\theta$$

$$\hbar k_\perp = [2m(E_k\cos^2\theta - V_0)]^{1/2} = \{2m[(E_i + h\nu - e\Phi)\cos^2\theta - V_0]\}^{1/2}$$

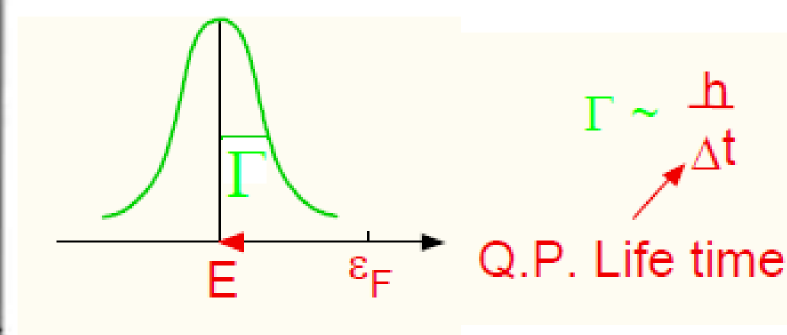
$V_o=E_o- e\phi$ ="Inner potential".
Usually just a fitting parameter.

Normal emission: theta=0 $\hbar k_\parallel = 0$ $\hbar k_\perp = [2m(E_i + e\Phi - E_0)]^{1/2}$

# 谱线宽度




Interpretation of Line Widths




$$\gamma = \frac{\dfrac{\Gamma_i}{|v_{i\perp}|} + \dfrac{\Gamma_f}{|v_{f\perp}|}}{\left|\dfrac{1}{v_{i\perp}} - \dfrac{1}{v_{f\perp}}\right|}$$

正出射

# 谱线宽度

**FWHM of an ARPES peak** $\Gamma = \dfrac{\dfrac{\Gamma_i}{|v_{i\perp}|} + \dfrac{\Gamma_f}{|v_{f\perp}|}}{\left|\dfrac{1}{v_{i\perp}}\left[1 - \dfrac{mv_{i\parallel}\sin^2\vartheta}{\hbar k_\parallel}\right] - \dfrac{1}{v_{f\perp}}\left[1 - \dfrac{mv_{f\parallel}\sin^2\vartheta}{\hbar k_\parallel}\right]\right|}$

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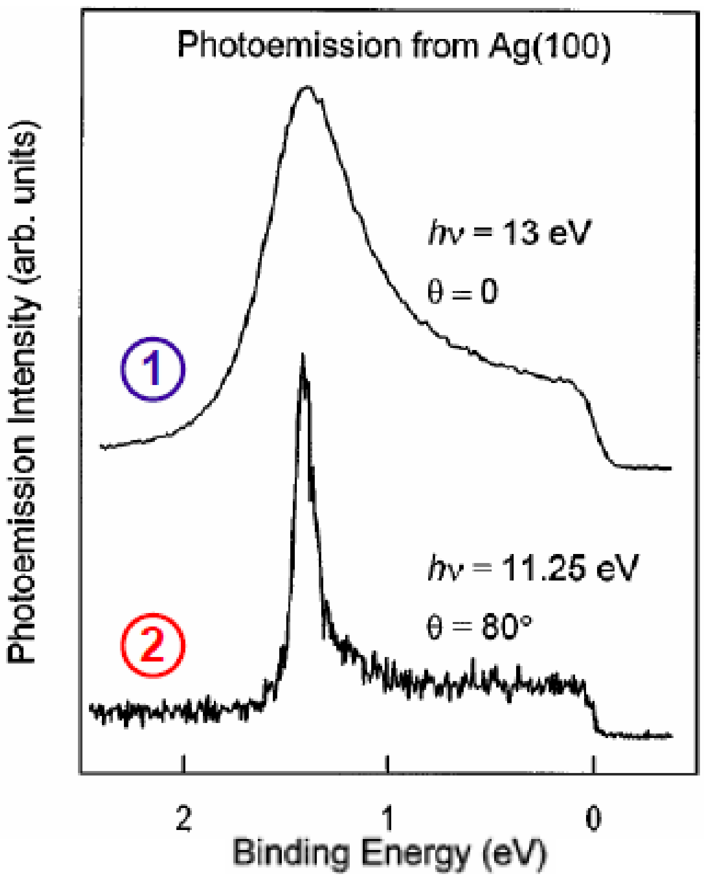
Hansen *et al*., PRL **80**, 1766 (1998)




① if $E_i \simeq E_F$

→ $\Gamma_i \longrightarrow 0$ → $\Gamma \propto \Gamma_f$

② if $|v_{i\perp}| \simeq 0$ 二维、准二维系统

→ $\Gamma = \dfrac{\Gamma_i}{\left|1 - \dfrac{mv_{i\parallel}\sin^2\vartheta}{\hbar k_\parallel}\right|} \equiv C\,\Gamma_i$

if $v_{i\parallel} < 0$, large; $\theta$ large; $k_\parallel$ small

→ $C < 1$, and $\Gamma < \Gamma_i$