

Angle resolved photoemission spectroscopy

각분해능 광전자 분광



김용관
한국과학기술원 물리학과

목차

- ✓ 각분해능 광전자 분광의 기초
 - ✓ 광전효과- 각분해능?
 - ✓ 관측법 및 관측결과를 전자구조로 매팅 하는 법
 - ✓ 기본 데이터 읽는 법
- ✓ 심화- ARPES로 얻을 수 있는 정보 / Intensity에 숨겨진 정보
 - ✓ Light polarization dependence
 - ✓ Electron self energy info. in ARPES spectrum
- ✓ 심화- 최신 ARPES 기법 리뷰
 - ✓ 빛
 - ✓ 샘플
 - ✓ 전자 분광 및 검출

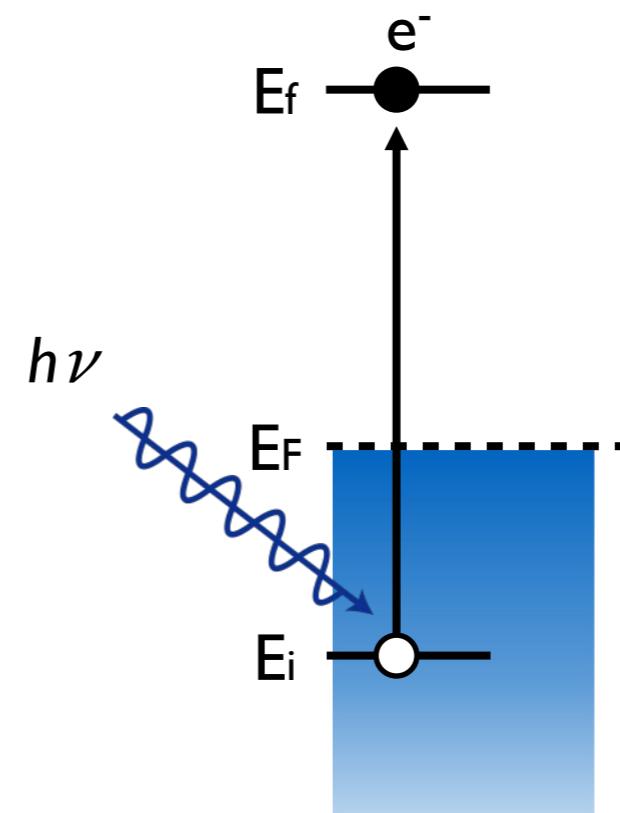
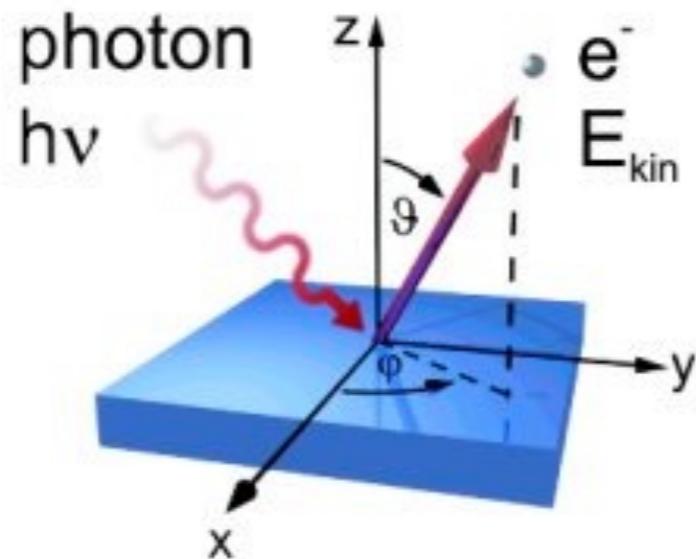
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광전자 분광

Photoemission spectroscopy

광전효과

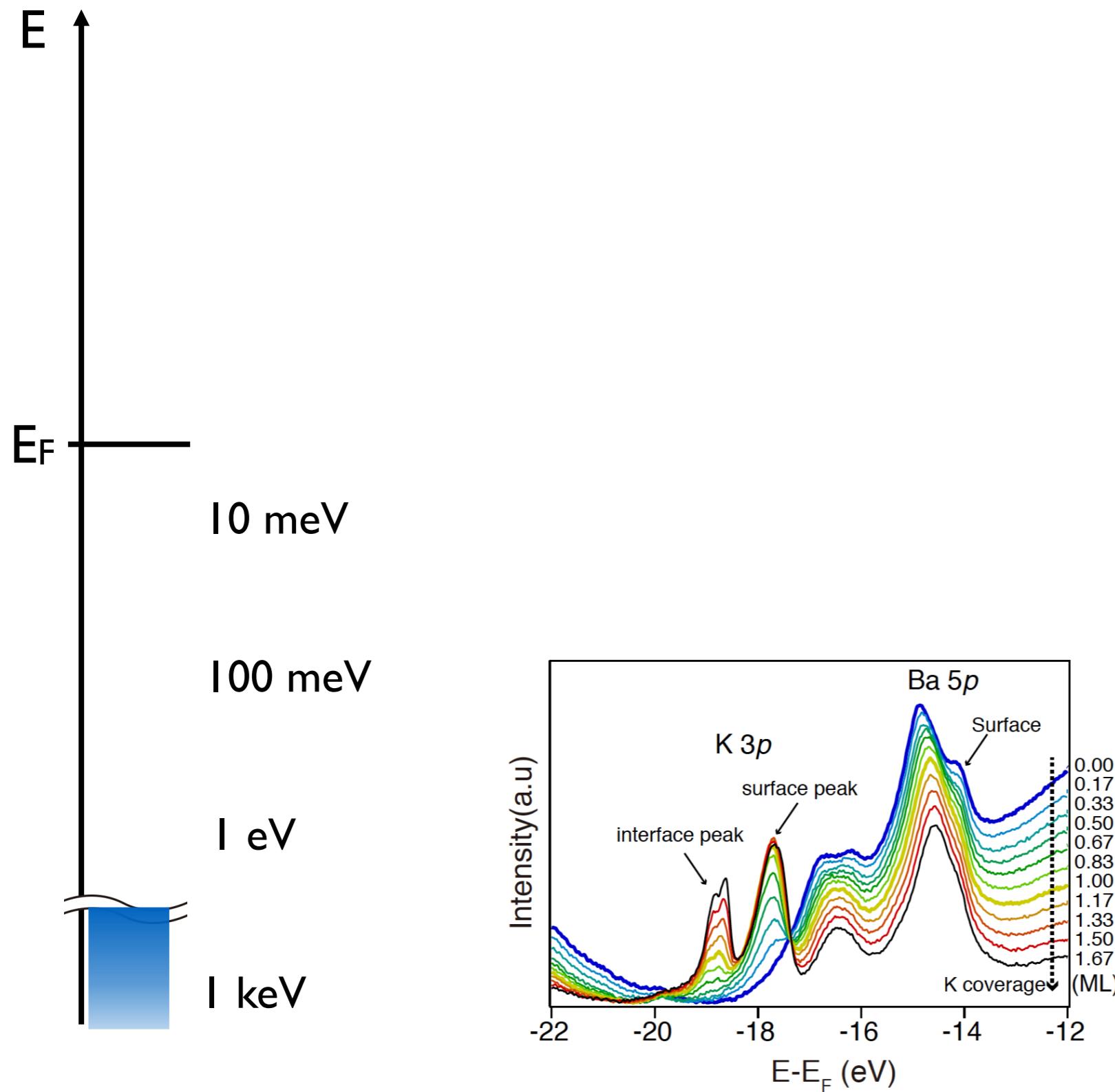


XPS - X-ray photoemission spectroscopy

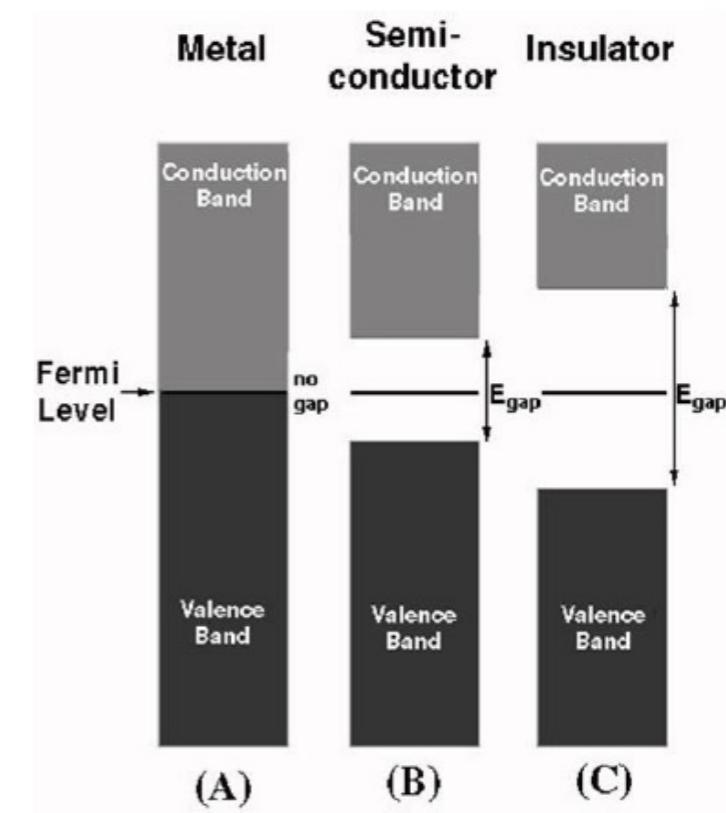
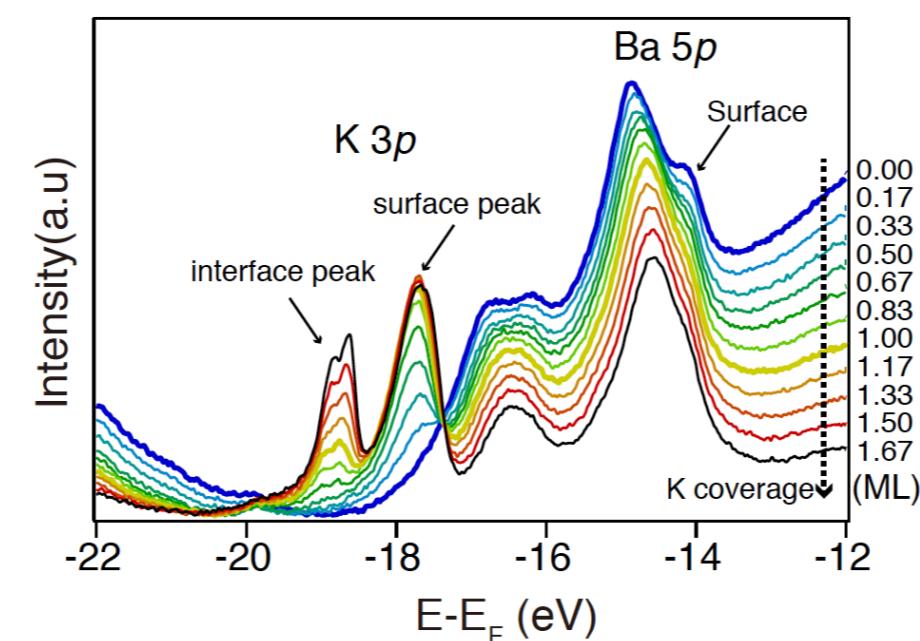
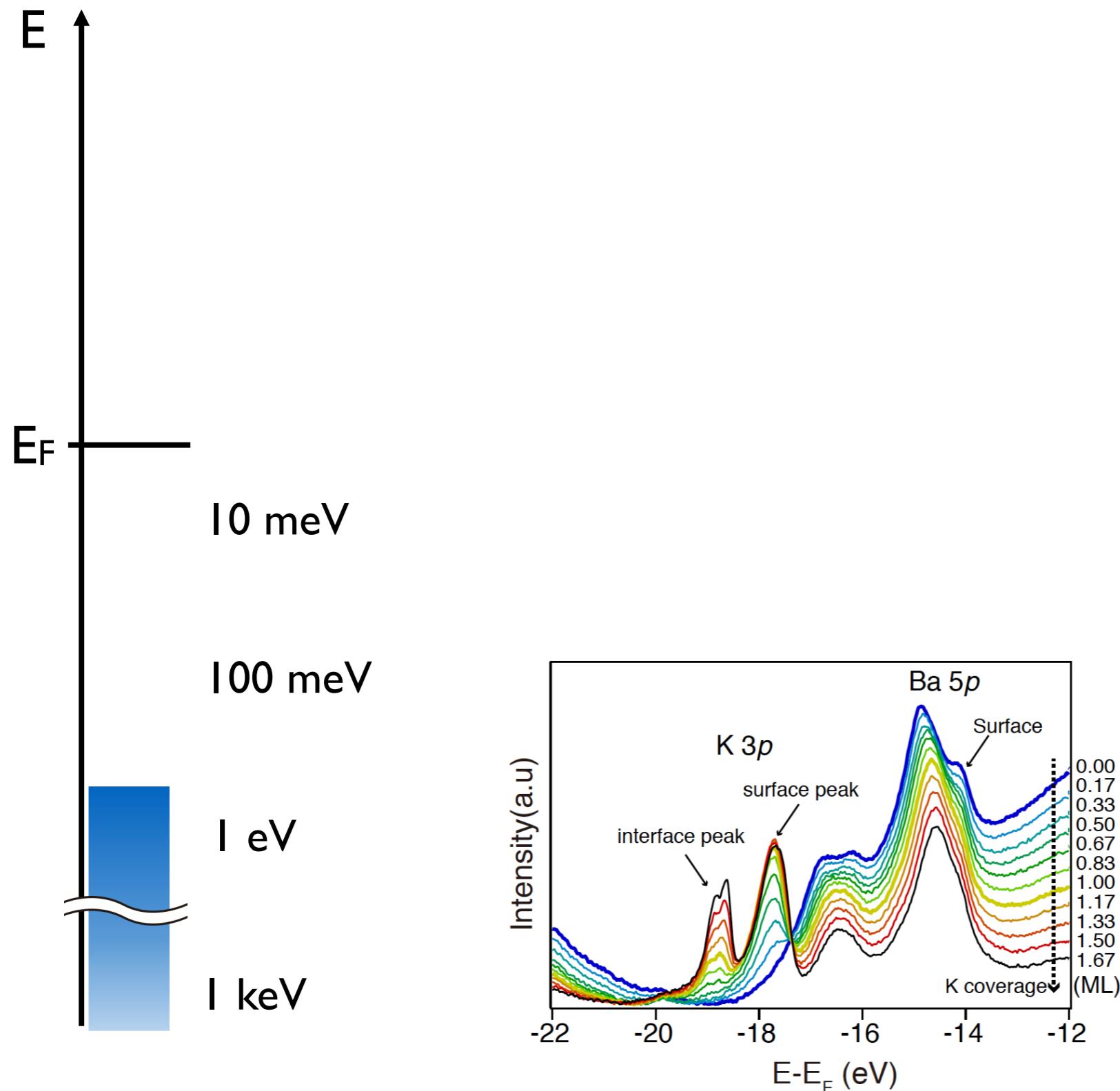
UPS - UV photoemission spectroscopy

ARPES - angle-resolved photoemission spectroscopy

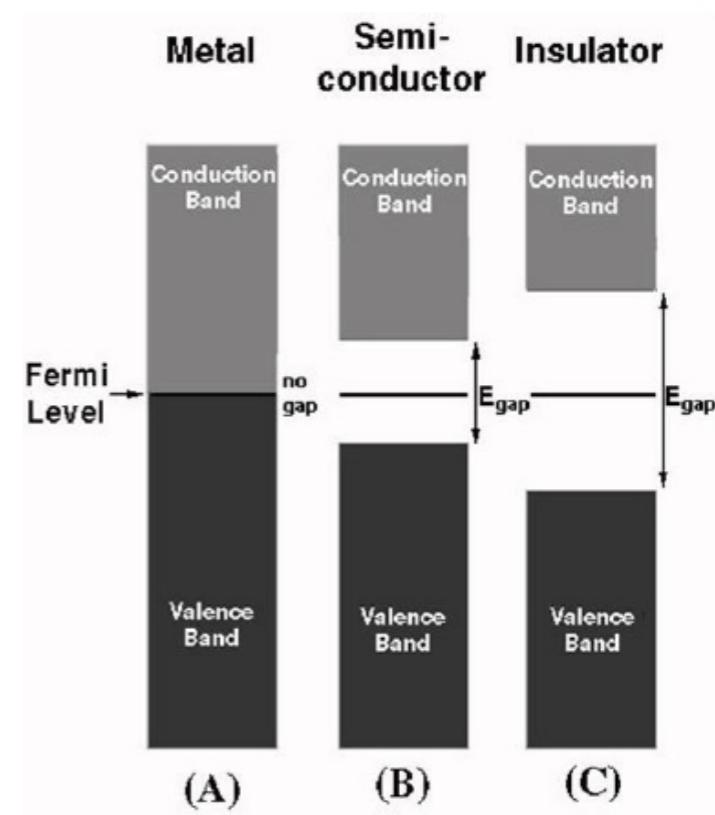
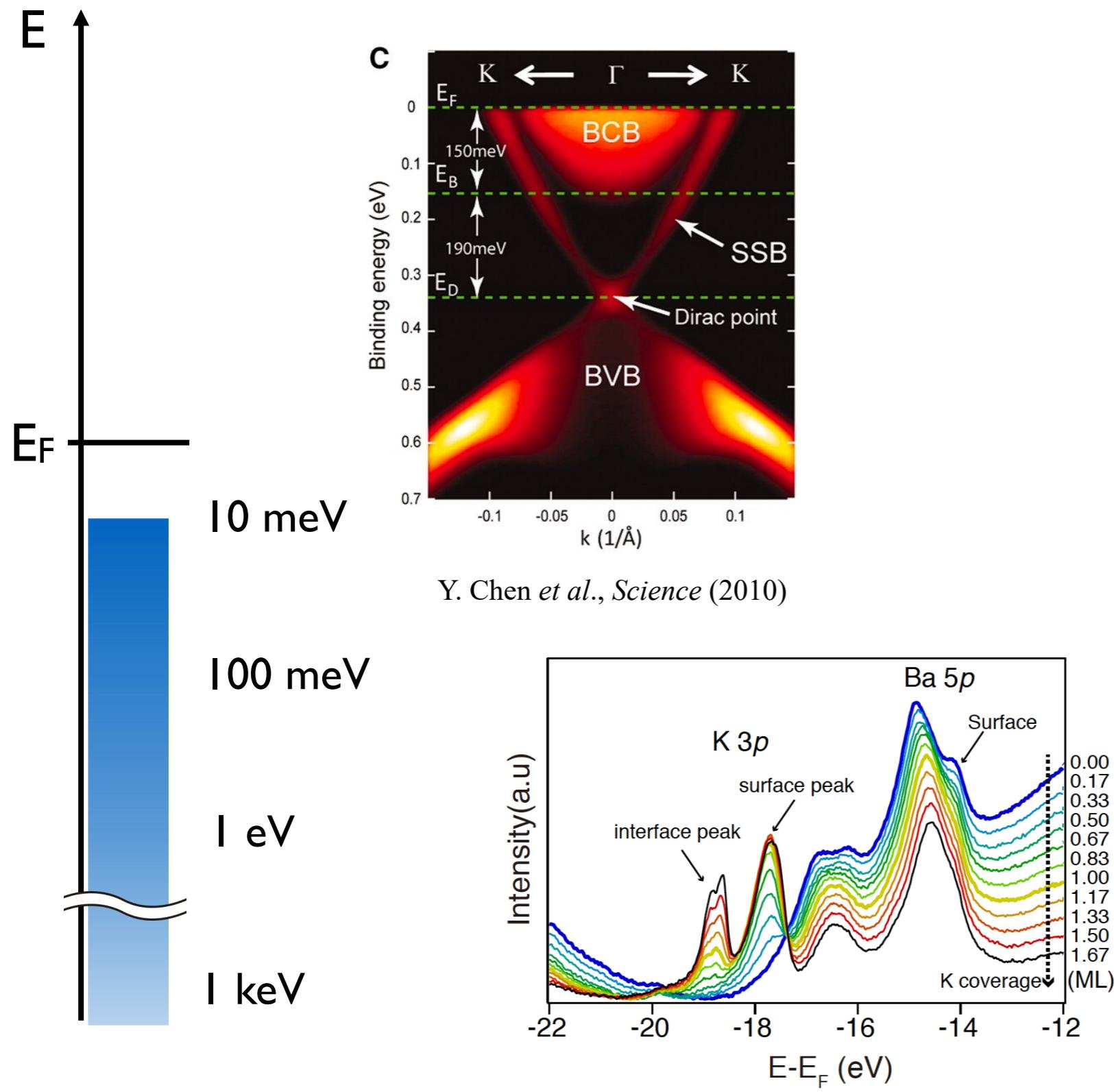
광전자 분광으로 얻을 수 있는 정보 - XPS



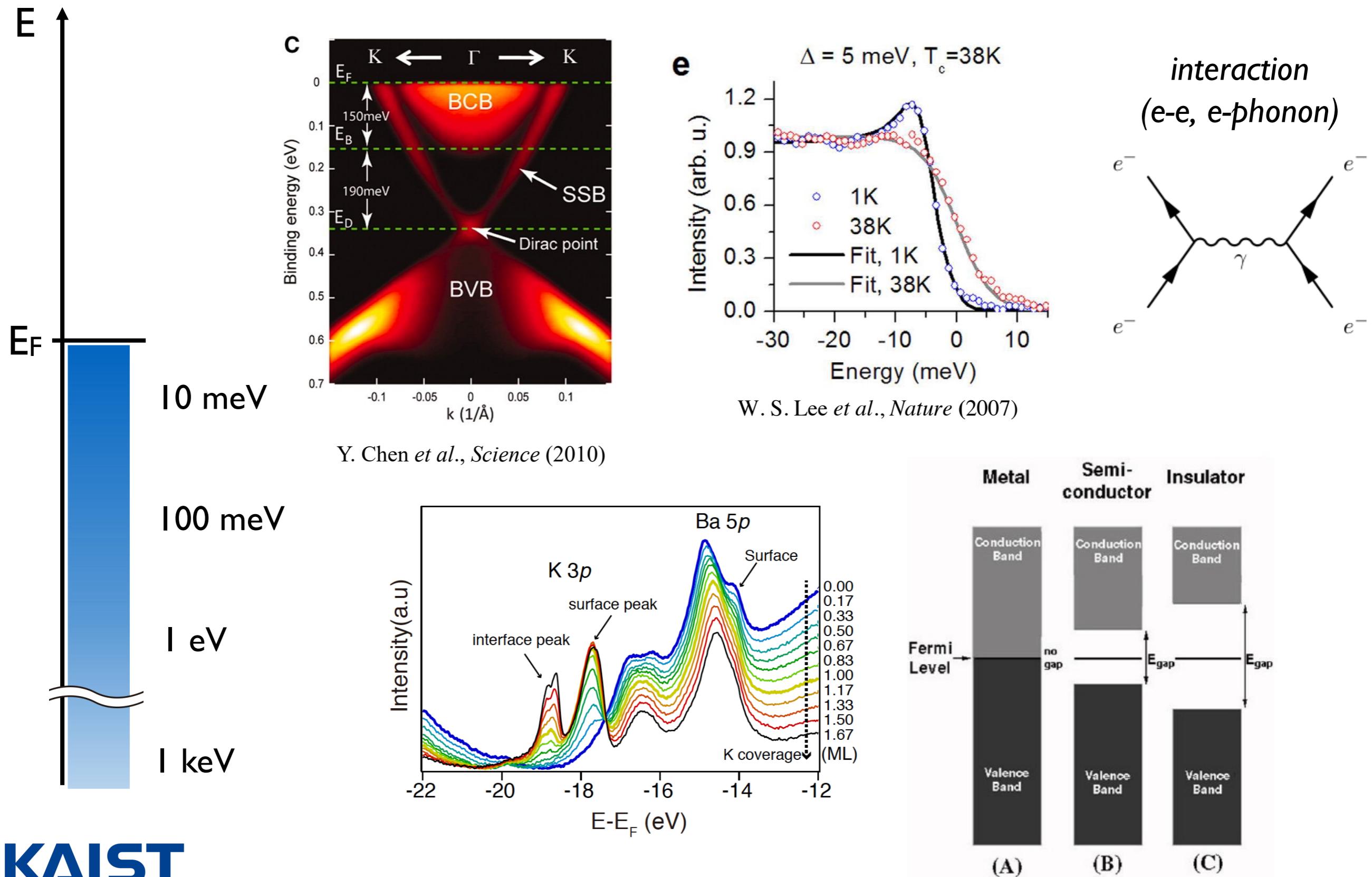
광전자 분광으로 얻을 수 있는 정보 - UPS



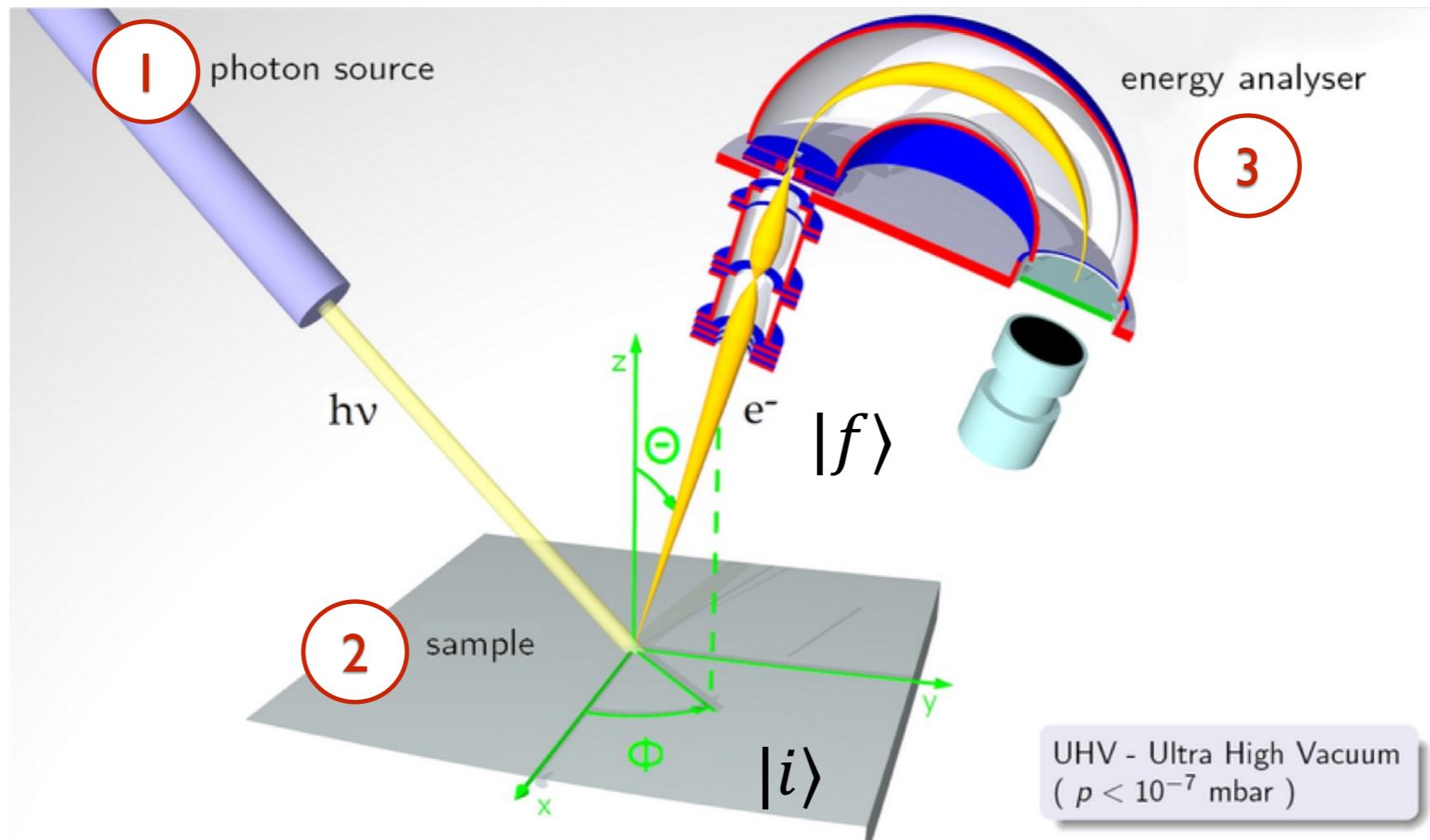
광전자 분광으로 얻을 수 있는 정보 -ARPES



광전자 분광으로 얻을 수 있는 정보 -ARPES



각분해능 광전자 분광 구성 요소 및 과정



우리가 알고 싶은 상태 $\rightarrow |i\rangle \rightarrow |f\rangle \leftarrow$ 우리가 관측하는 상태

$B(k_x, k_y, k_z \text{ & } B.E)$

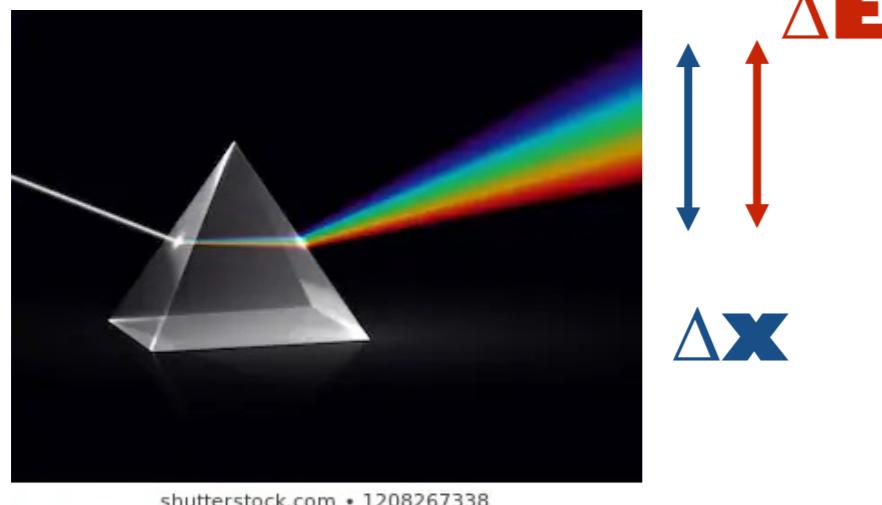
Dipole transition

$$H' = -\frac{e}{mc} \mathbf{A} \cdot \mathbf{p}$$

$F(k_x, k_y, k_z \text{ & } K.E)$

에너지 분광

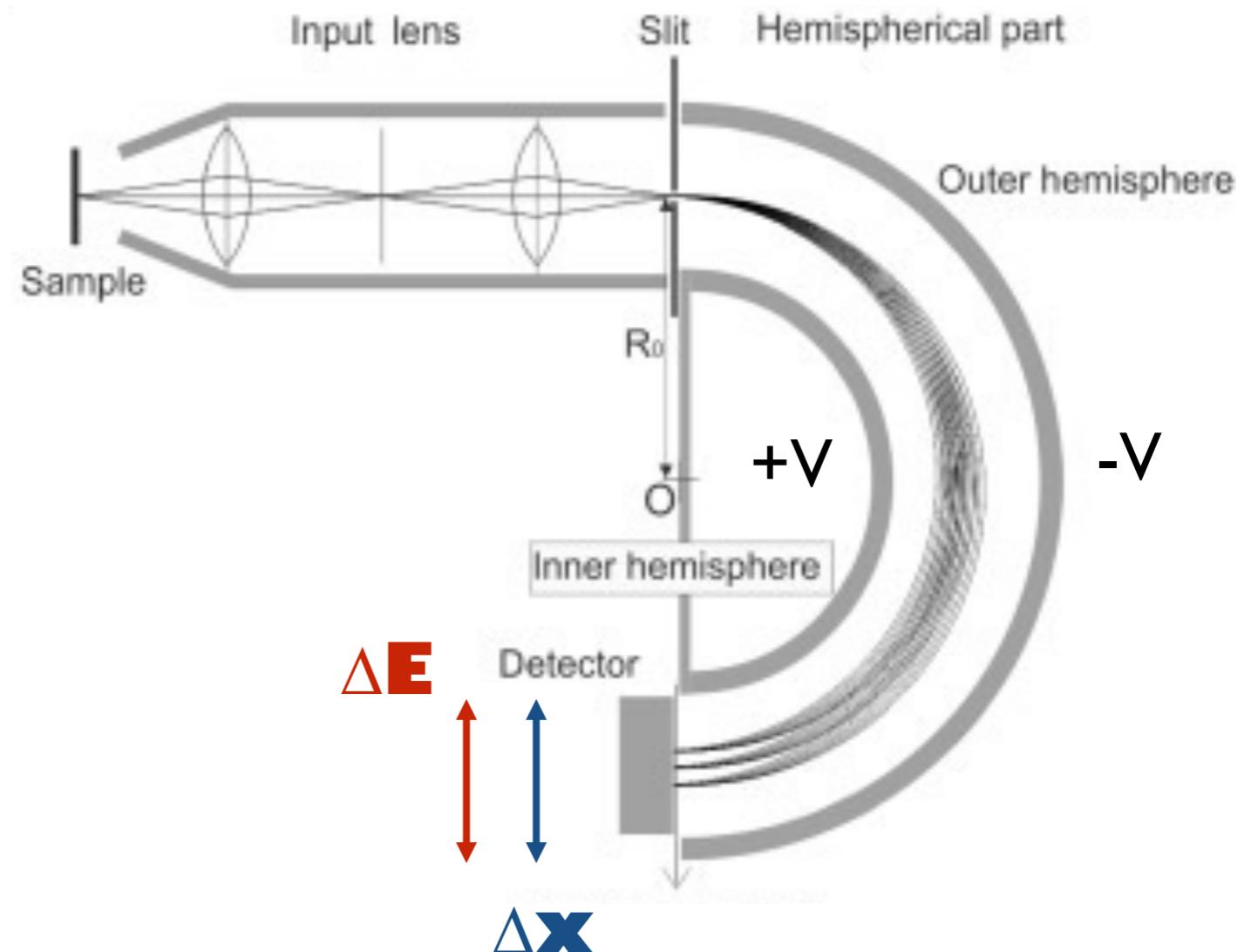
온동 에너지를 어떻게 선별해 낼 것인가?



hemisphere electron analyzer



electron lens + electron prism



운동량 측정 - 각분해능

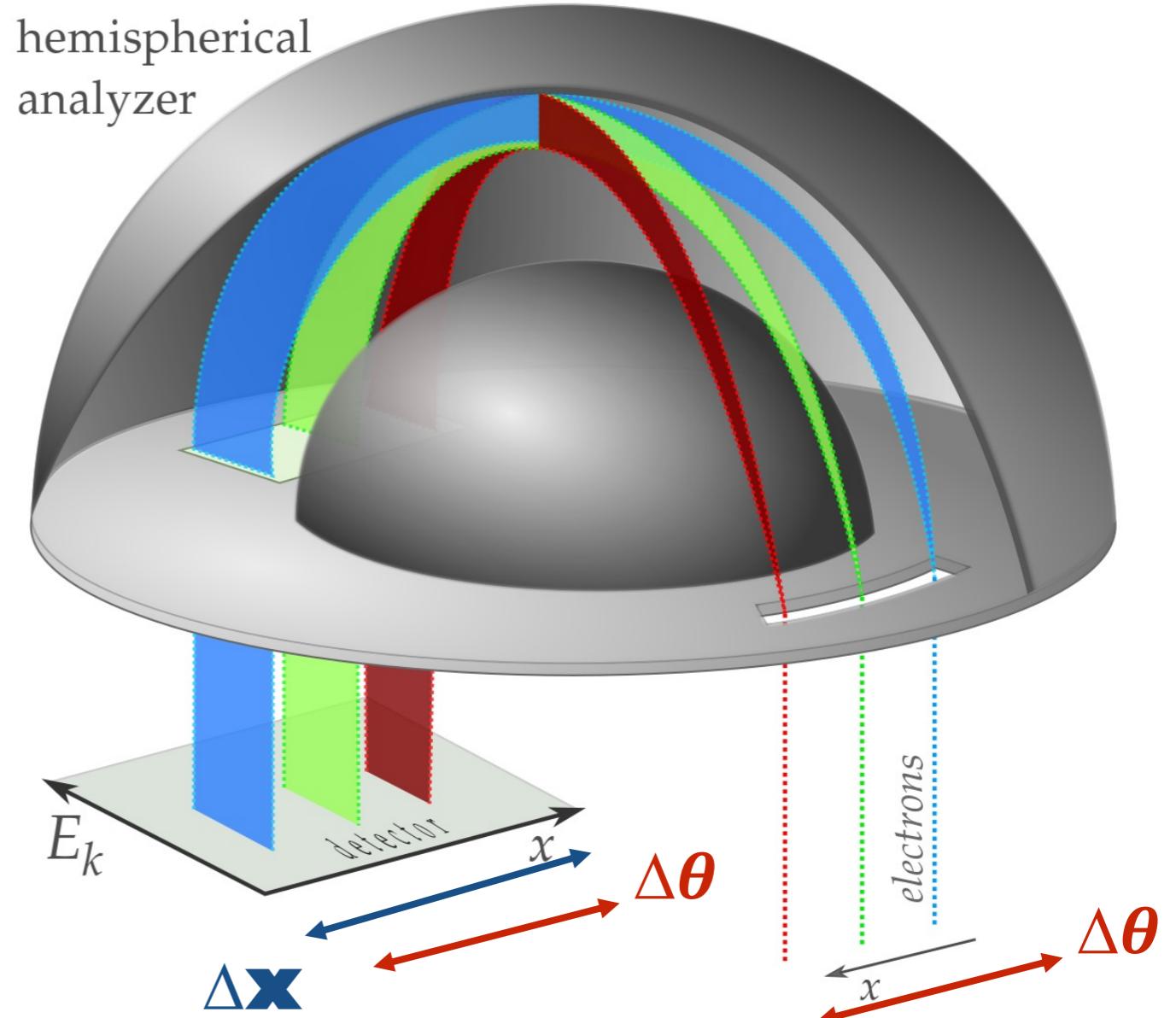
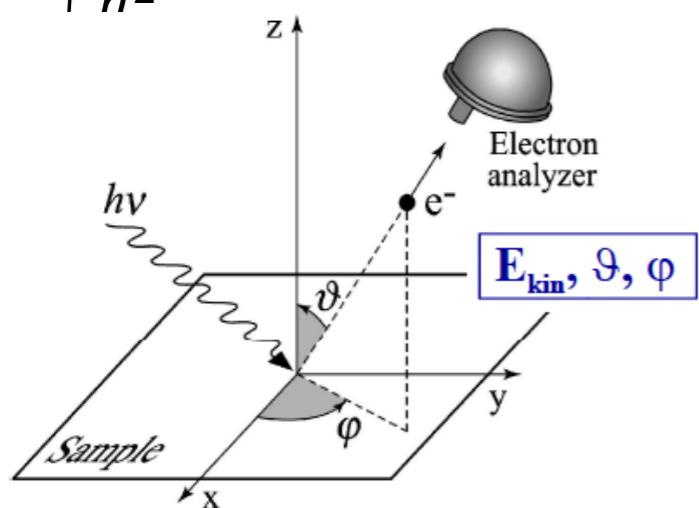
Momentum is ‘vector’ - magnitude & direction (θ, φ)

$$k_f = \sqrt{\frac{2m}{\hbar^2} KE}$$

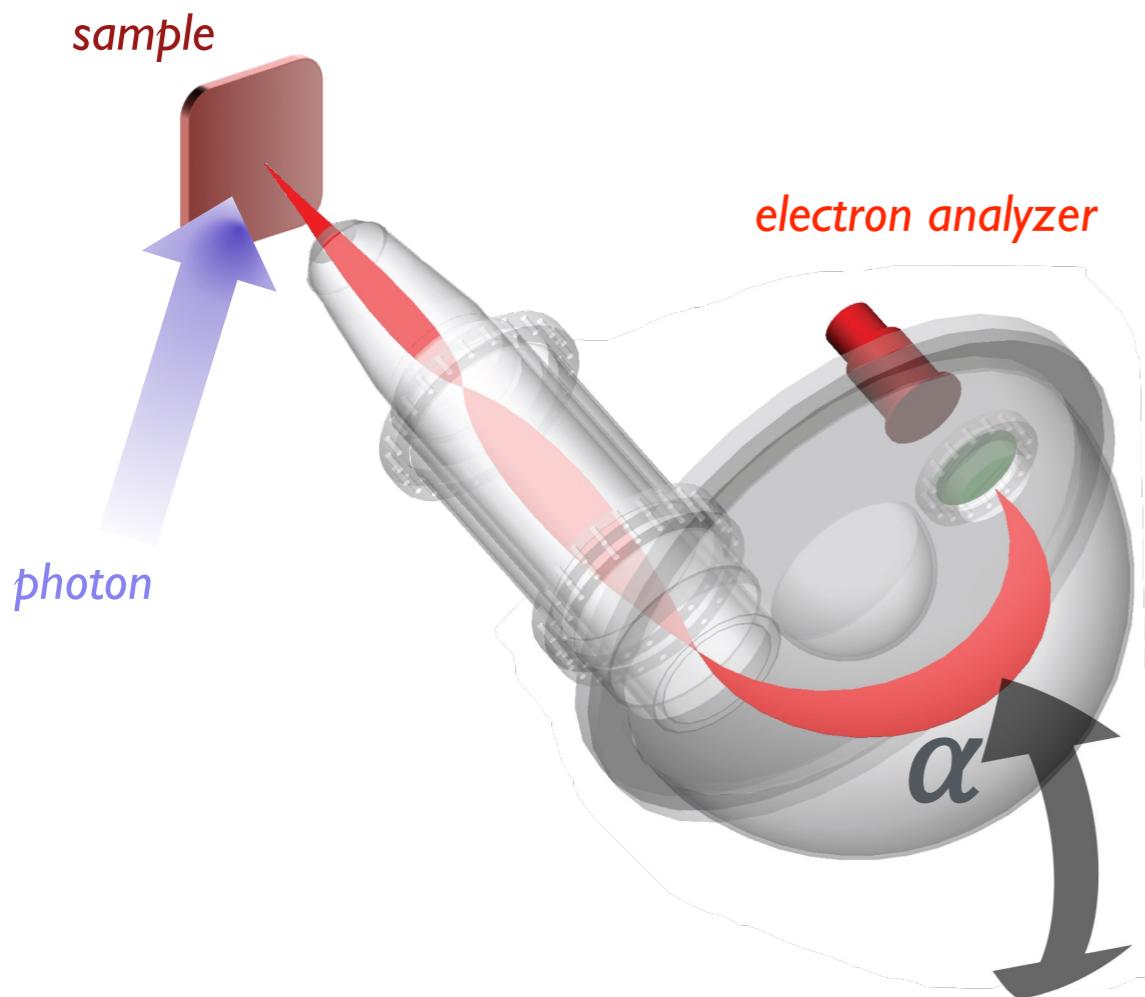
$$k_f^x = \sqrt{\frac{2m}{\hbar^2} KE \sin\theta \cos\phi}$$

$$k_f^y = \sqrt{\frac{2m}{\hbar^2} KE \sin\theta \sin\phi}$$

$$k_f^z = \sqrt{\frac{2m}{\hbar^2} KE \cos\theta}$$

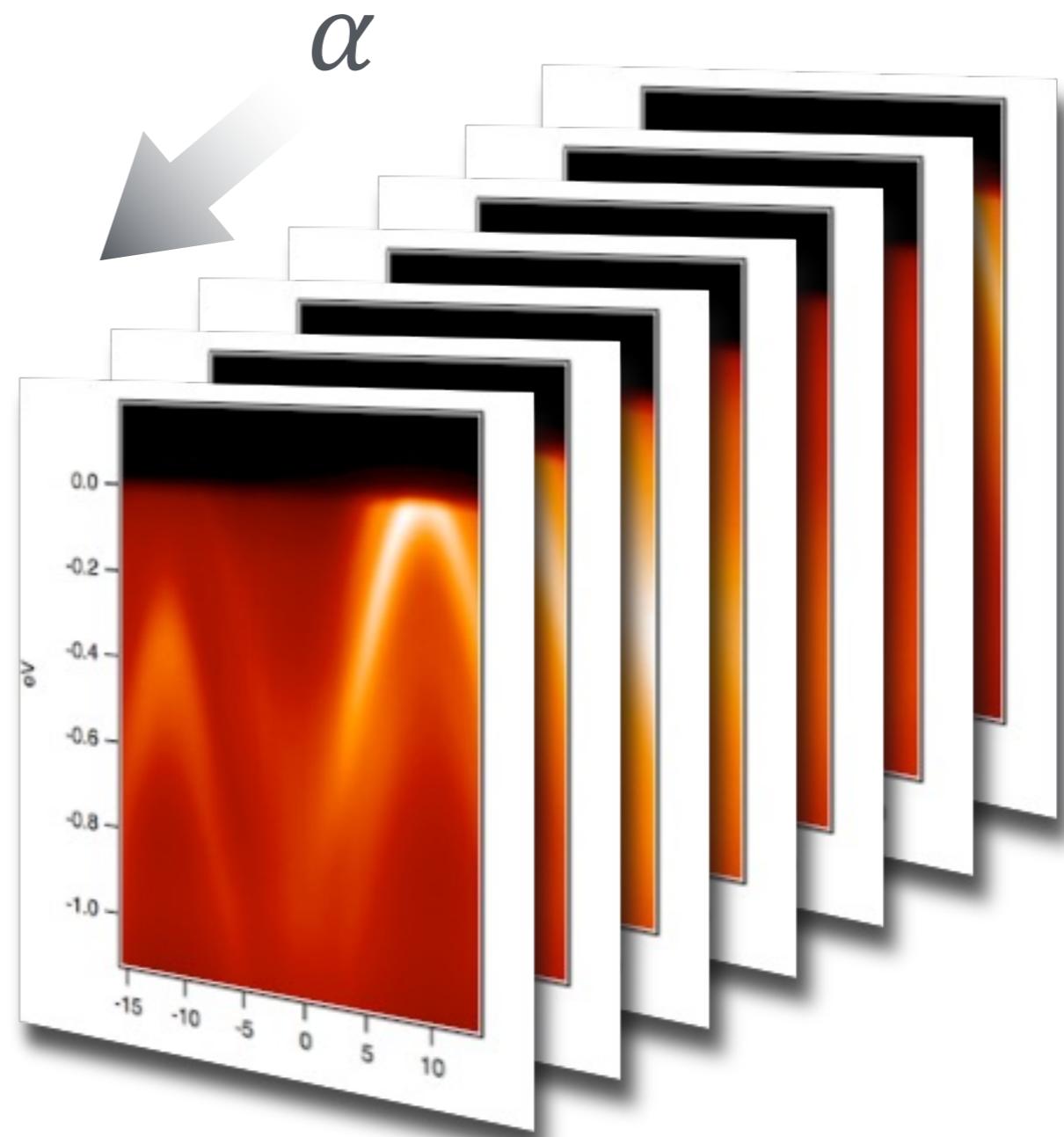


운동량 측정 - angle scan



$$F(\theta, \alpha, KE) \neq F(\theta, \varphi, KE)$$

정확히는 solid angle 정보가 아님!



from Dr. S.-K, Mo's presentation

운동량 측정 - photon energy scan

$$F(\theta, \alpha, KE) \neq F(\theta, \varphi, KE)$$

$$F(\theta, \alpha, \hbar\omega, KE)$$

$$k_f = \sqrt{\frac{2m}{\hbar^2} KE}$$

$$k_f^x = \sqrt{\frac{2m}{\hbar^2} KE \sin \theta}$$

$$k_f^y = \sqrt{\frac{2m}{\hbar^2} KE \cos \theta \sin \alpha}$$

$$k_f^z = \sqrt{(k_f)^2 - (k_f^x)^2 - (k_f^y)^2}$$

$$KE = \hbar\omega - \phi - BE$$

$$k_f^z = \sqrt{(k_f)^2 - (k_f^x)^2 - (k_f^y)^2}$$



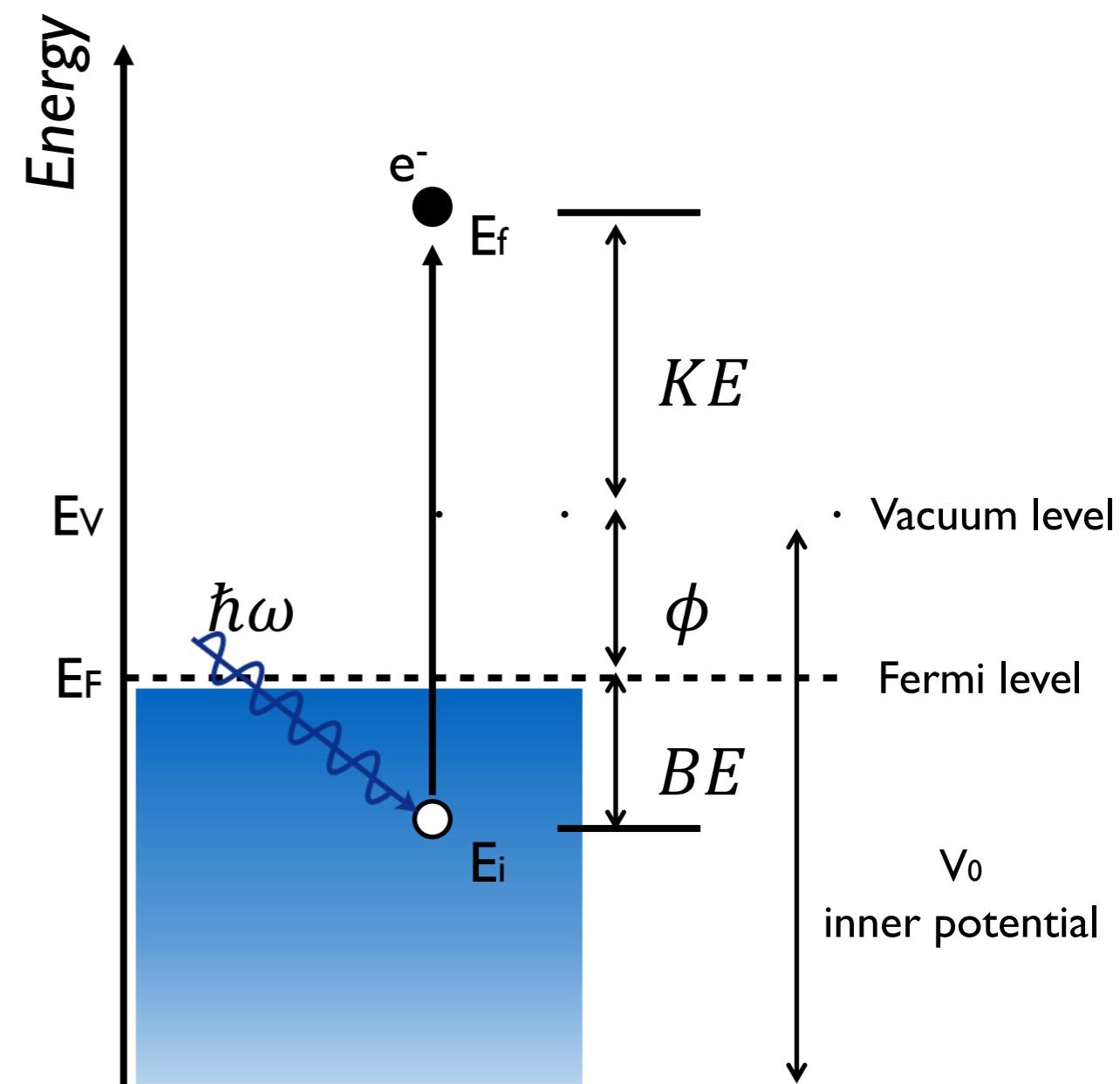
→ $F(k_x, k_y, K.E) @ \text{fixed } k_z$

$F(k_x, k_y, k_z, KE)$

에너지 - 운동량 변환

$|f\rangle F(k_x, k_y, k_z \text{ & } K.E) \longrightarrow |i\rangle B(k_x, k_y, k_z \text{ & } B.E)$

$$\text{에너지 보존} KE = \hbar\omega - \phi - BE$$



운동량 변화

$$|f\rangle F(k_x, k_y, k_z \text{ & } K.E) \longrightarrow |i\rangle B(k_x, k_y, k_z \text{ & } B.E)$$

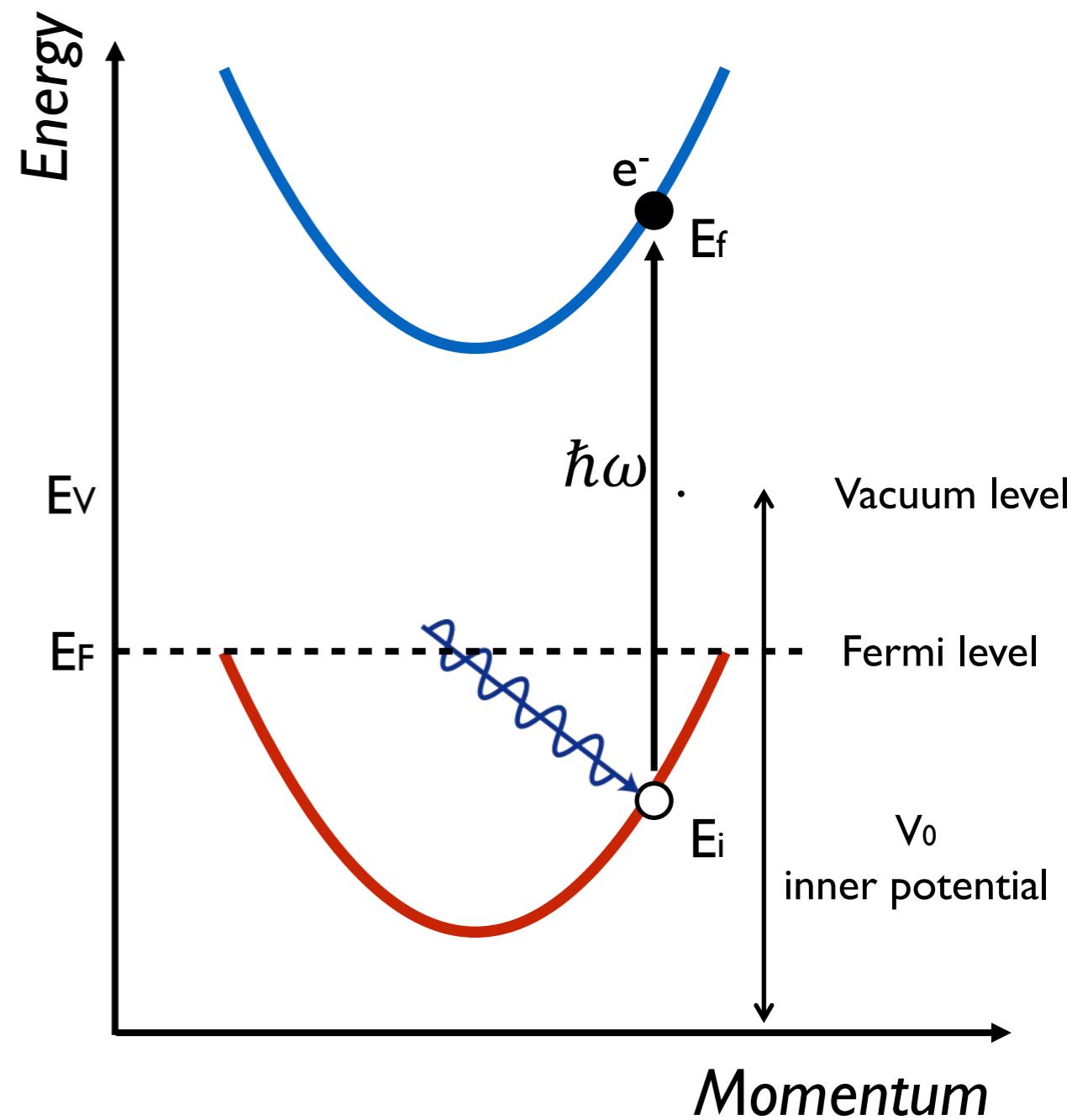
에너지 보존 $KE = \hbar\omega - \phi - BE$

운동량 보존 $k_i + \cancel{k_{photon}} = k_f$

$$E_{ph} = pc = \hbar c k_{ph} \sim 0.01 \text{ \AA}^{-1} @ 20 \text{ eV}$$

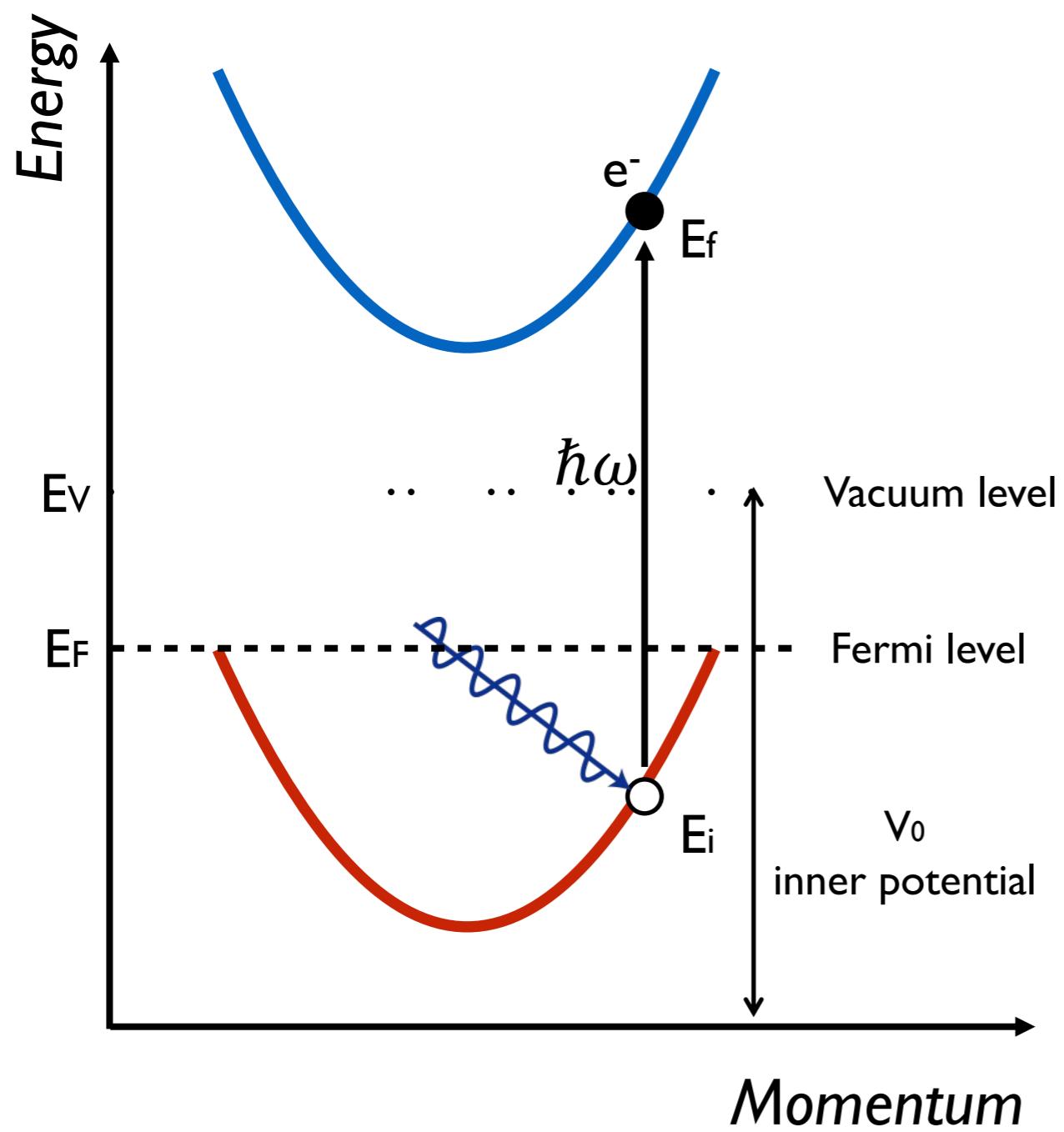
$$E_e = (\hbar k_e)^2 / 2m \sim 2 \text{ \AA}^{-1} @ 16 \text{ eV}$$

Vertical transition!

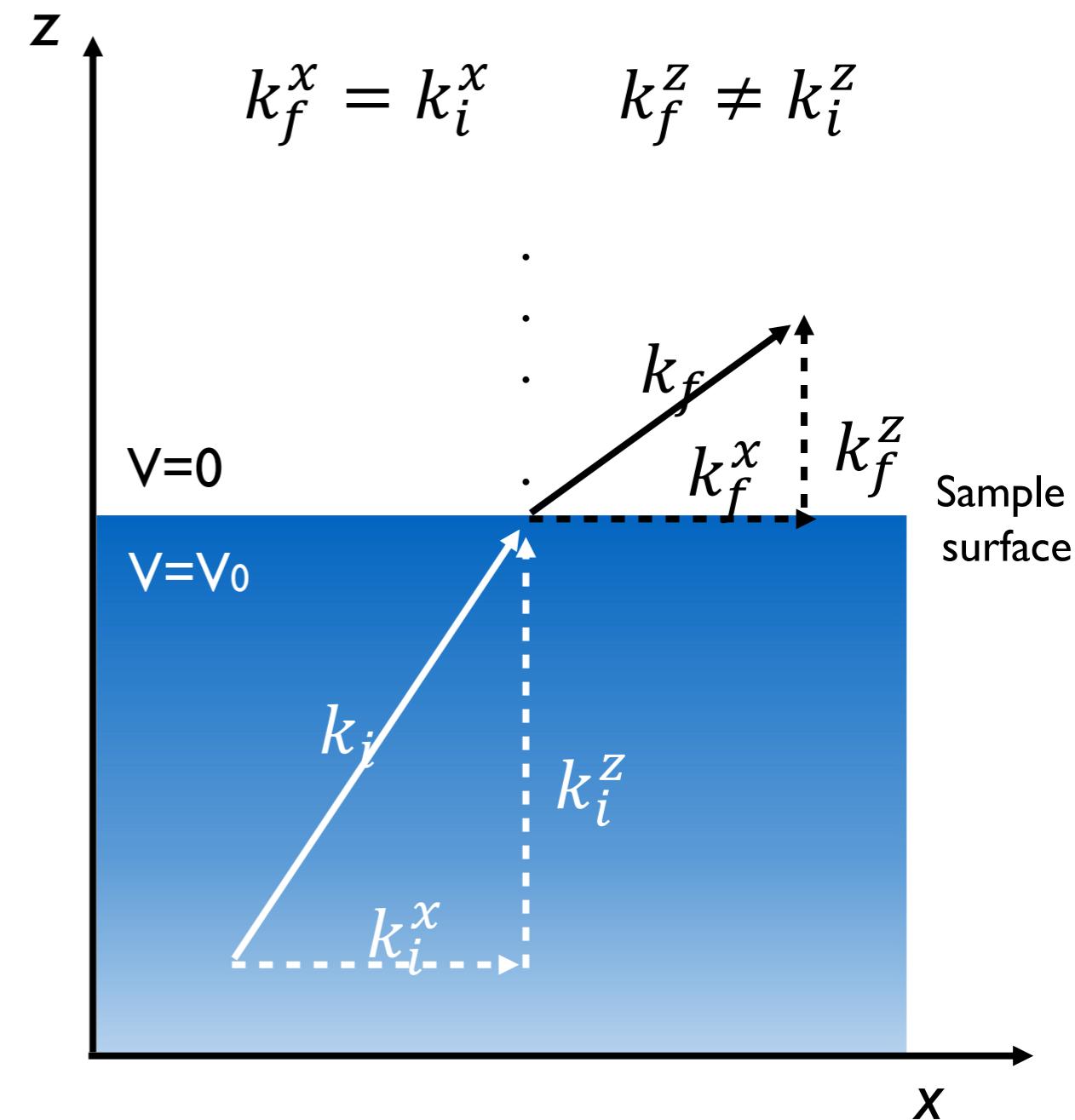


표면 전자 회절

Energy-momentum space

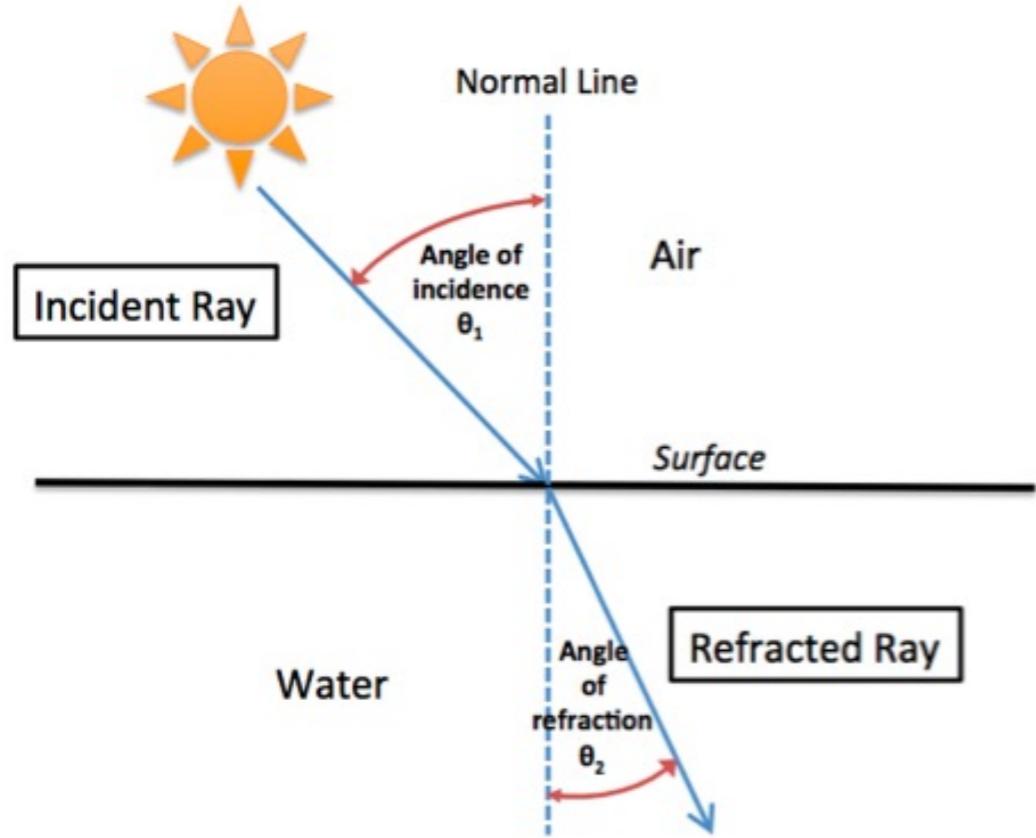


Real space



표면 전자 회절

스넬의 법칙



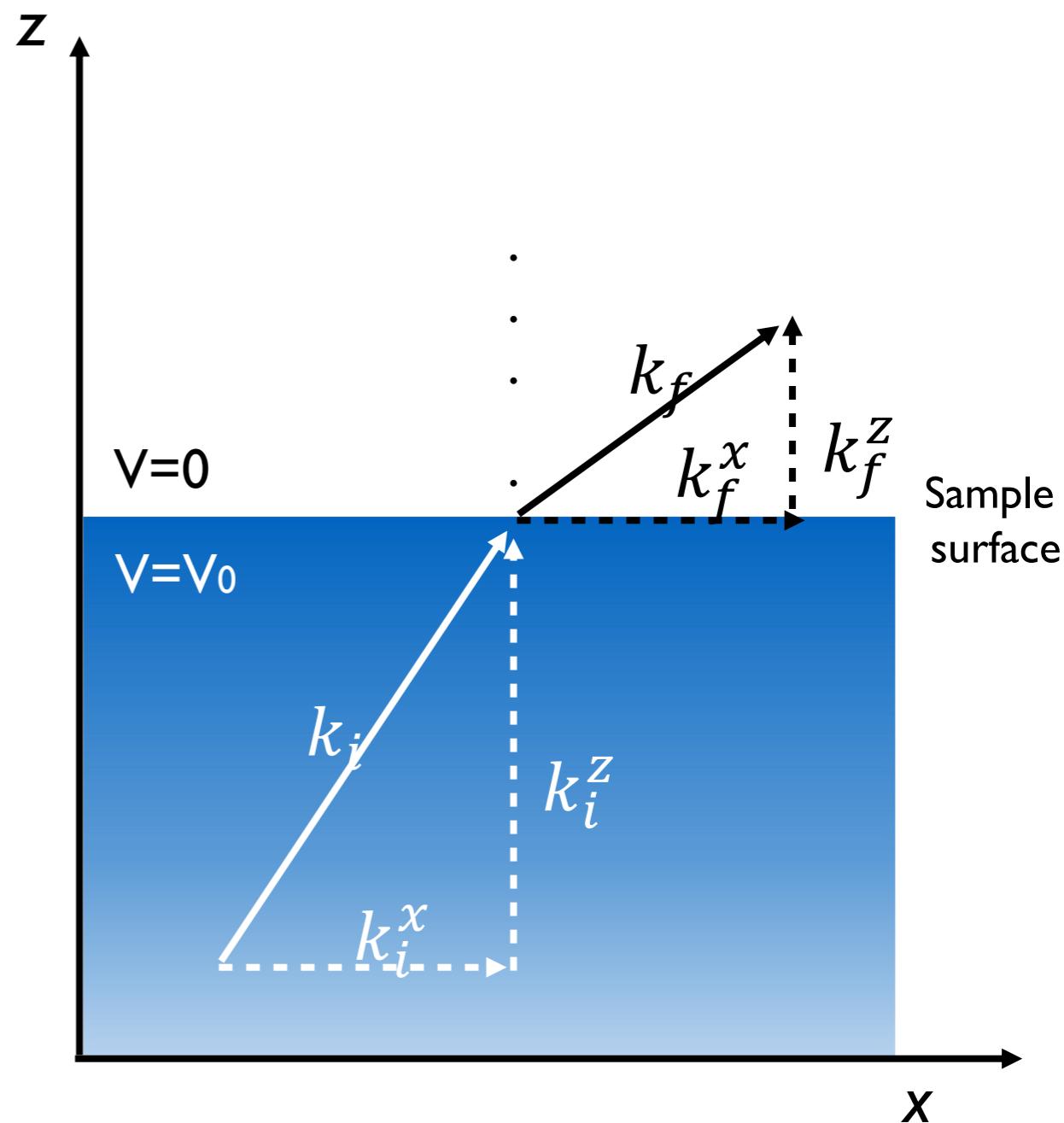
In-plane direction

$$k_f^x = k_i^x \text{ OK!}$$

Out of plane direction

$$k_f^z \neq k_i^z \text{ ??}$$

Real space



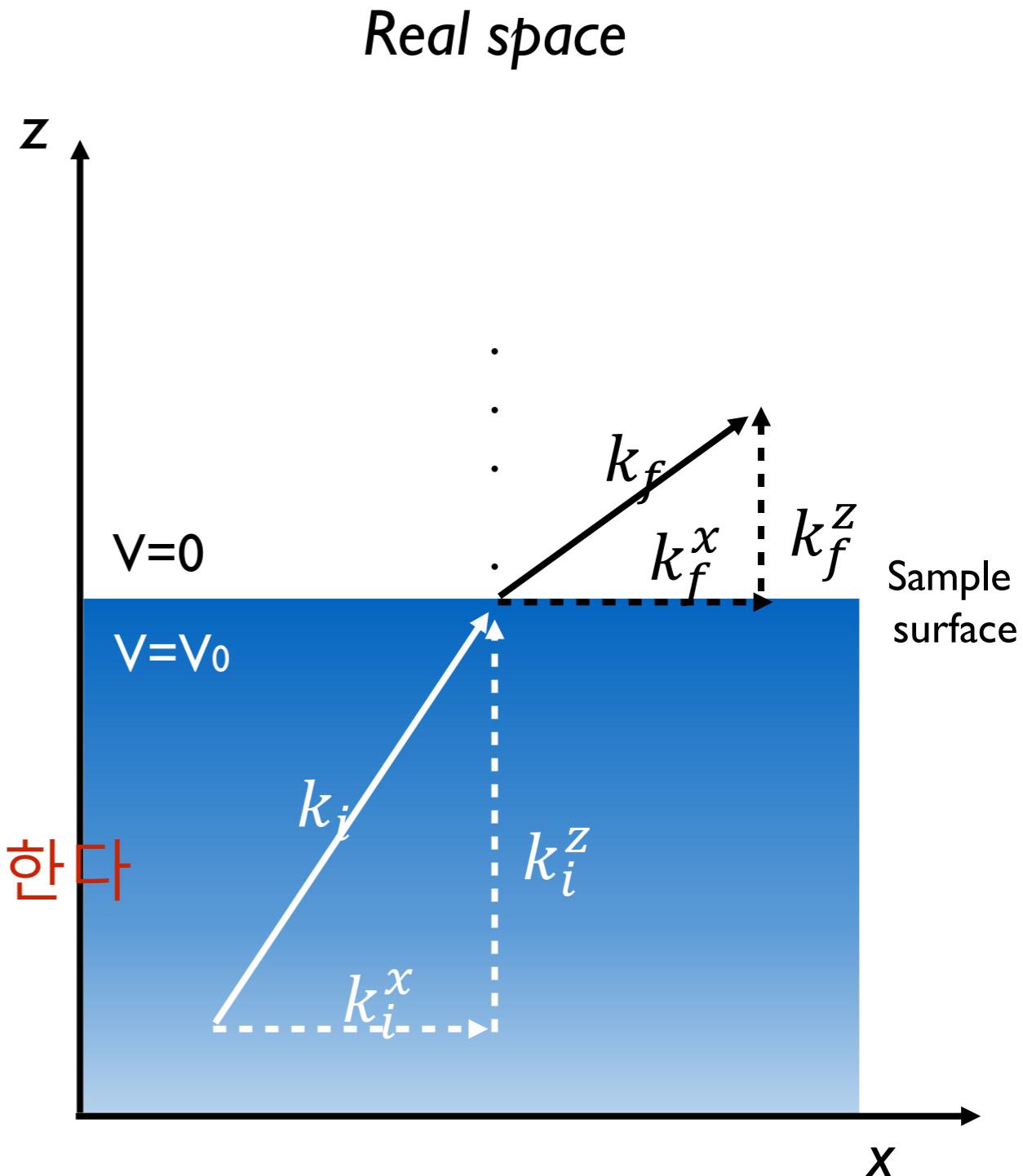
그럼 k_z 정보는 어떻게 아는가?

$$k_f = \sqrt{\frac{2m}{\hbar^2} KE} \quad k_i = \sqrt{\frac{2m}{\hbar^2} (KE + V_0)}$$

??

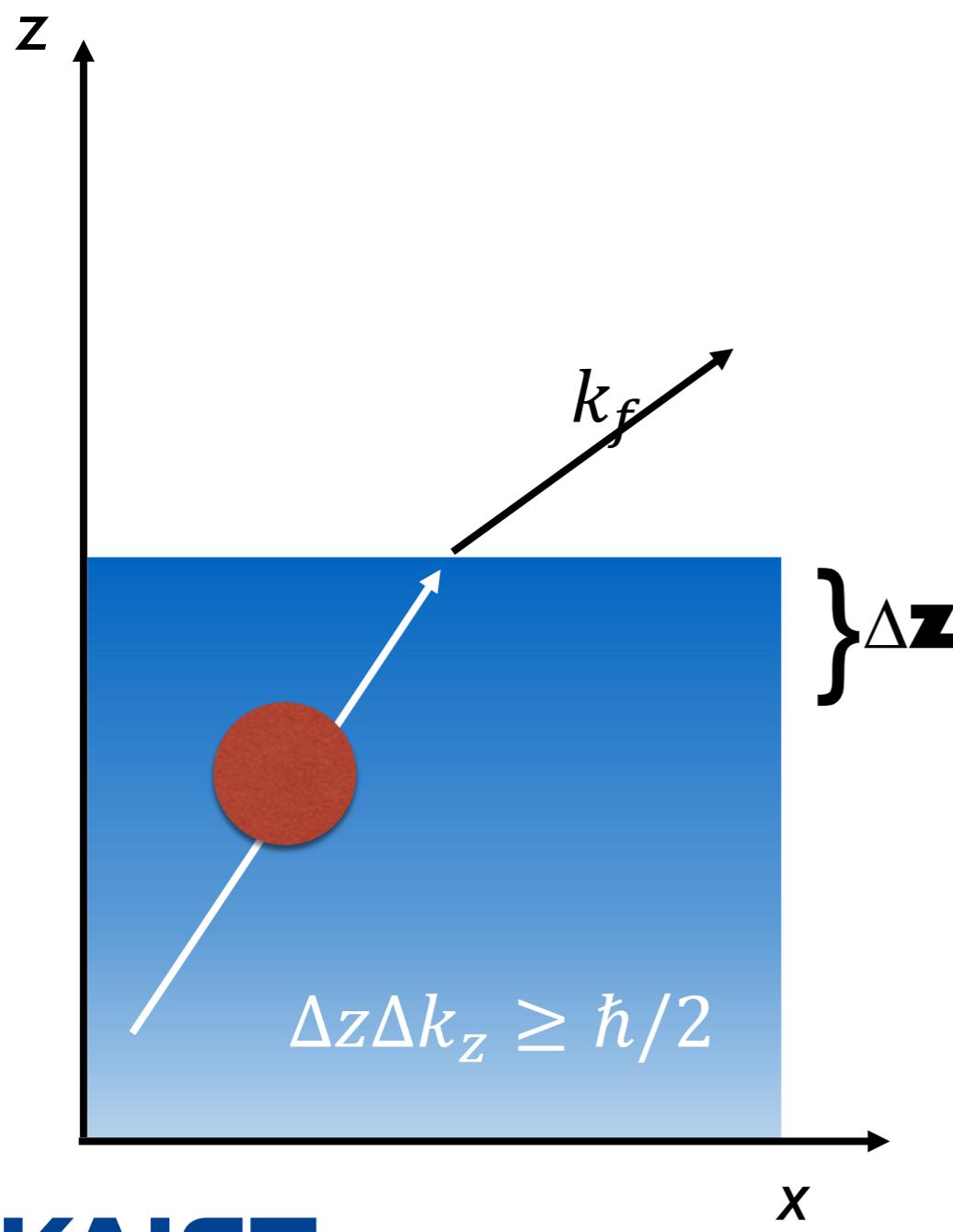
$F(\theta, \alpha, \hbar\omega, KE) \longrightarrow F(k_x, k_y, k_z, KE)$

전자구조의 주기성을 확인하여 V_0 를 정한다

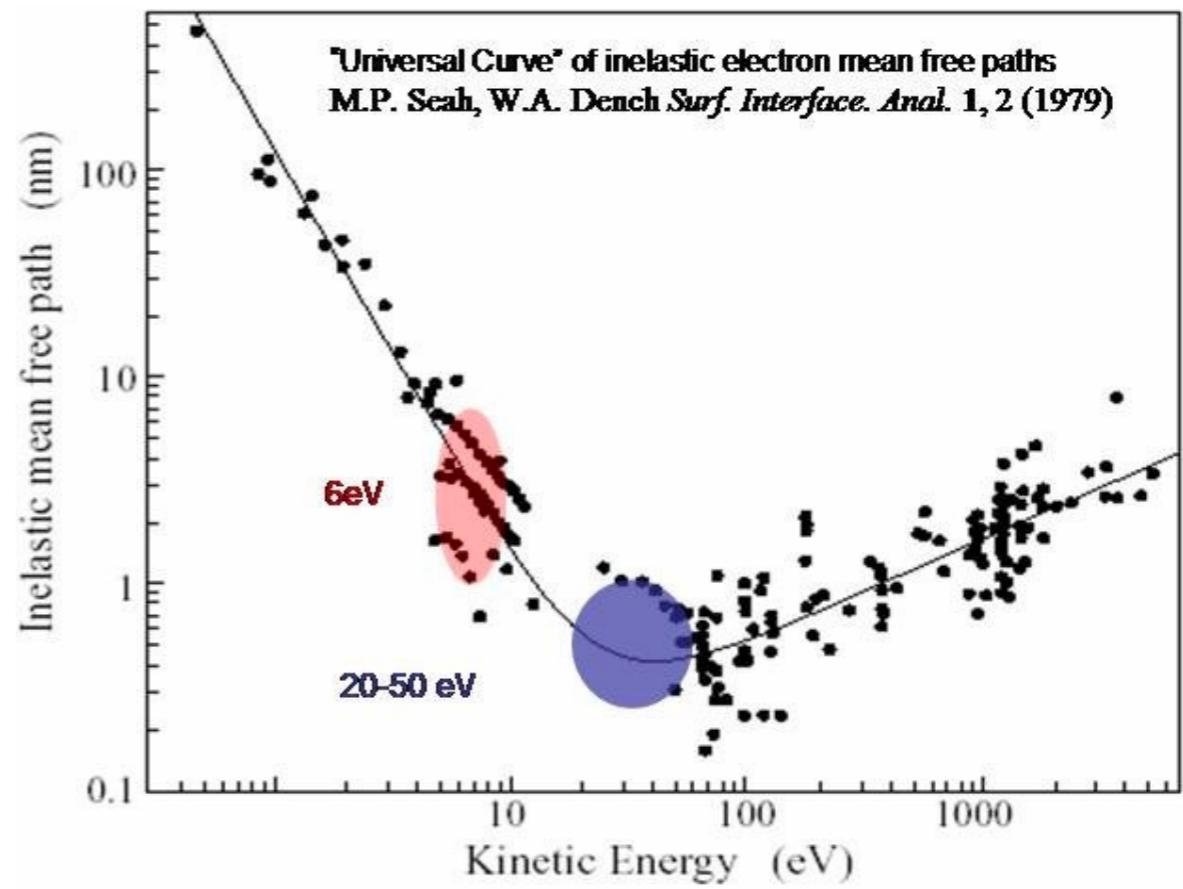


k_z 정의에 있어 다른 어려운 점

$$|f\rangle F(k_x, k_y, k_z \text{ & } K.E) \longrightarrow |i\rangle B(k_x, k_y, k_z \text{ & } B.E)$$

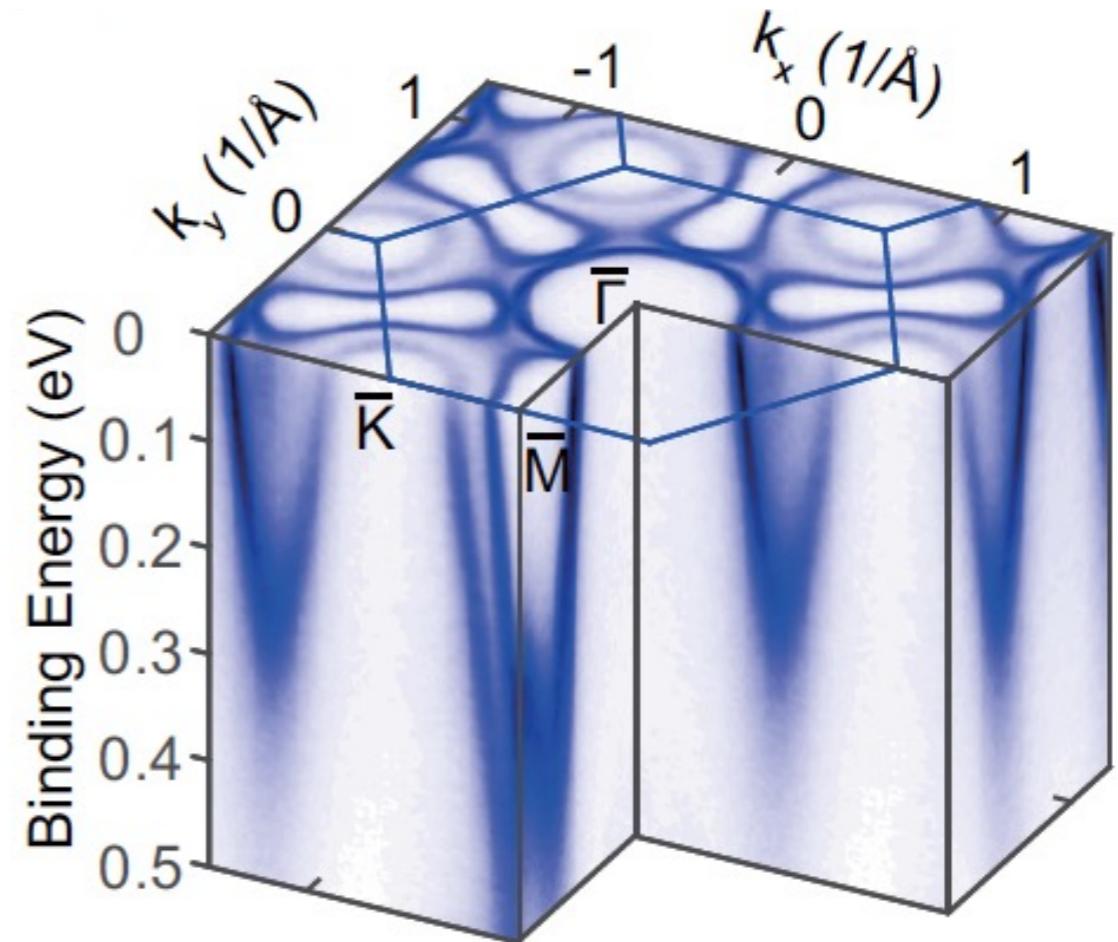
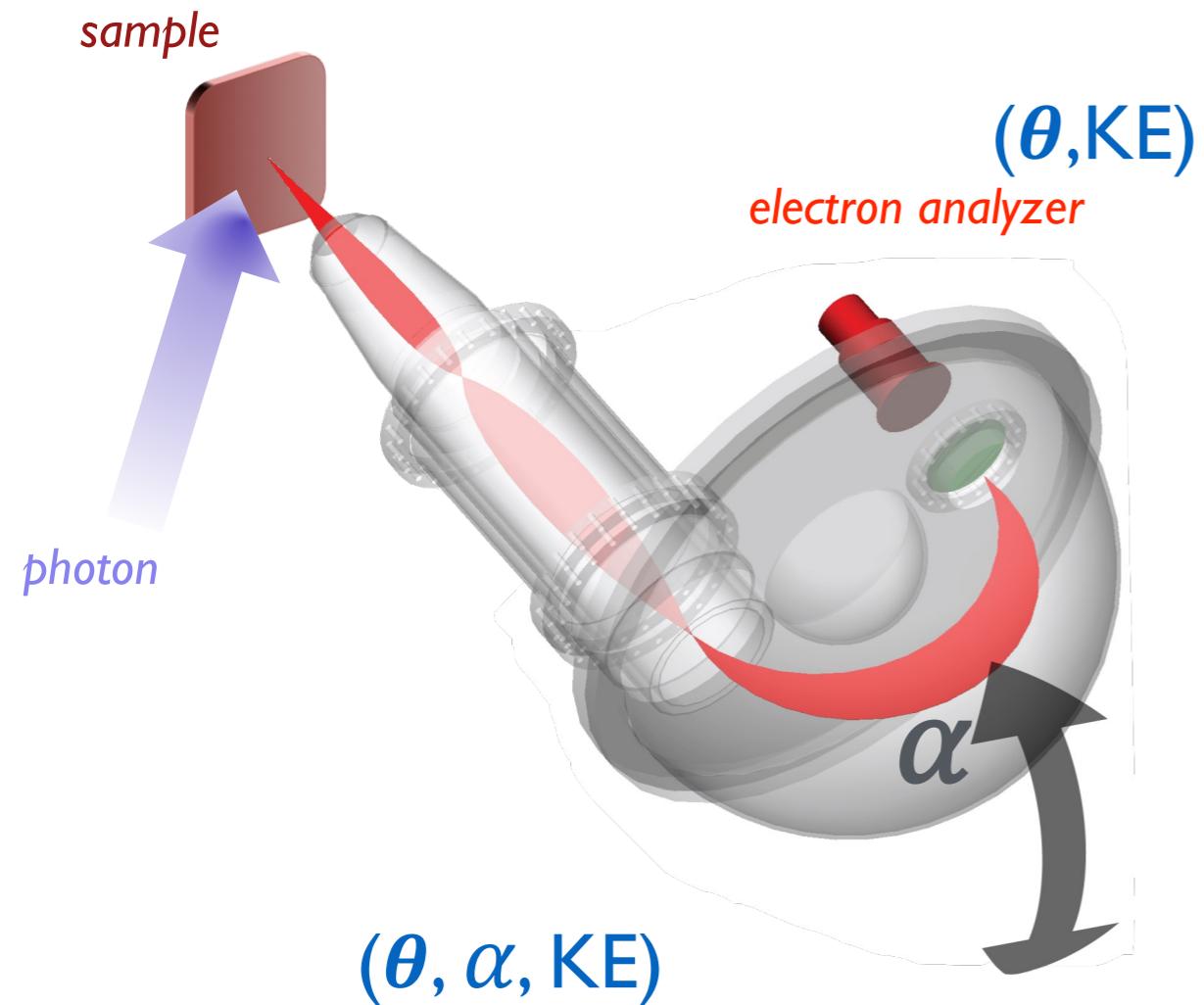


k_z 는 정확히 알 수 없다!
 Δk_z 만큼 합쳐서 보고 있다!

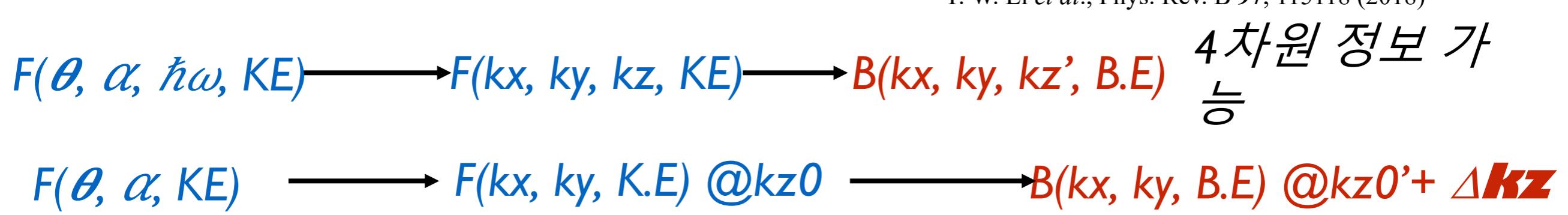


ARPES는 surface sensitive technique이다!

전자구조 매핑 요약



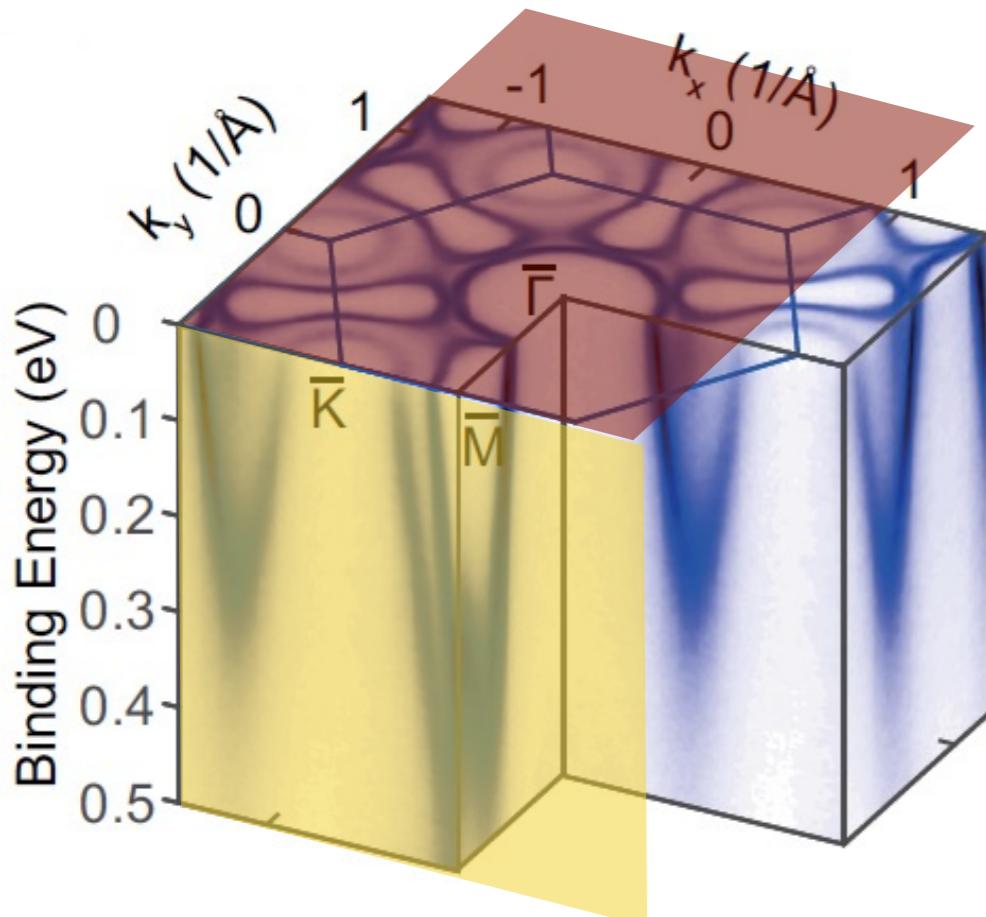
Y. W. Li *et al.*, Phys. Rev. B 97, 115118 (2018)



ARPES data plot 종류

$I(k_x, k_y, BE) @k_z 0' + \Delta k_z$

3 차원 data

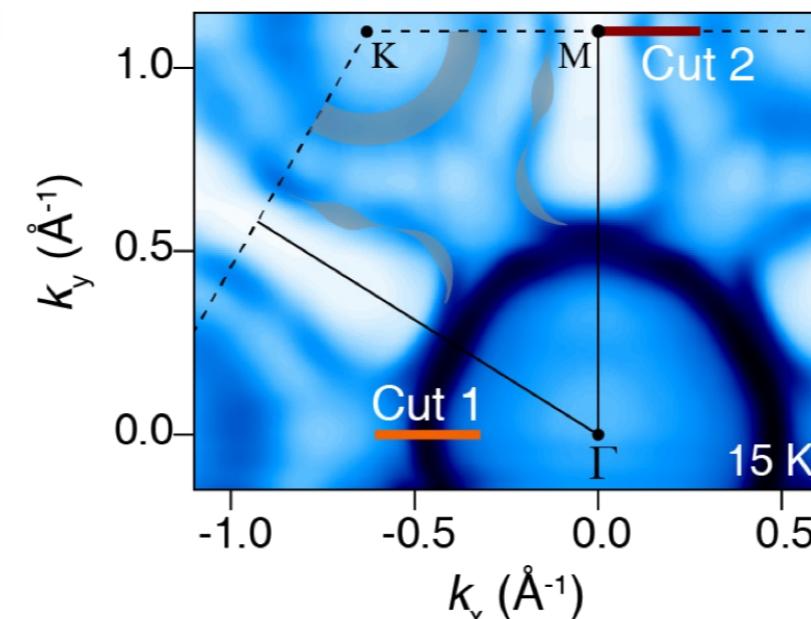


논문 지면 또는 화면은 2
차원

2 차원 Plot

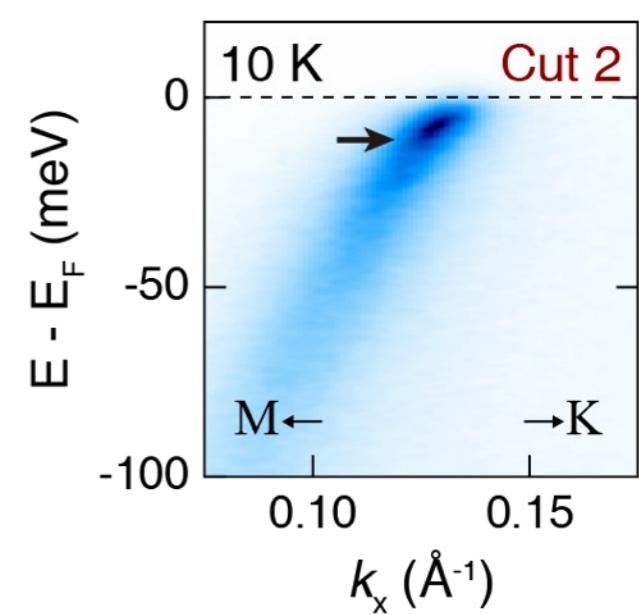
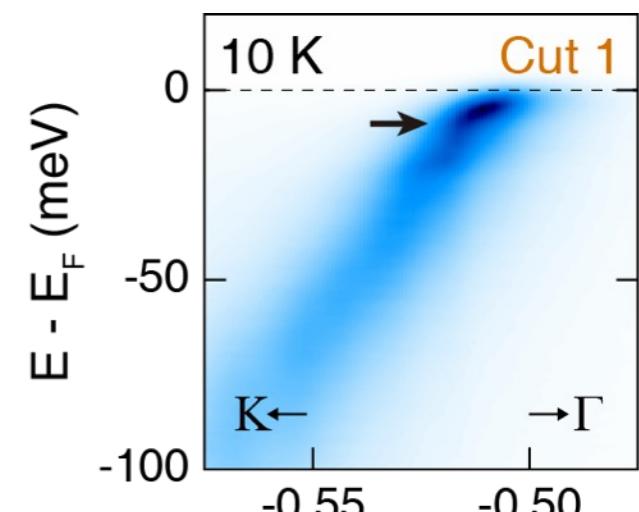
$I(k_x, k_y)$
@fixed k_z , BE

Constant energy map
(Fermi surface map)



$I(BE, k_x)$
@fixed k_y , k_z

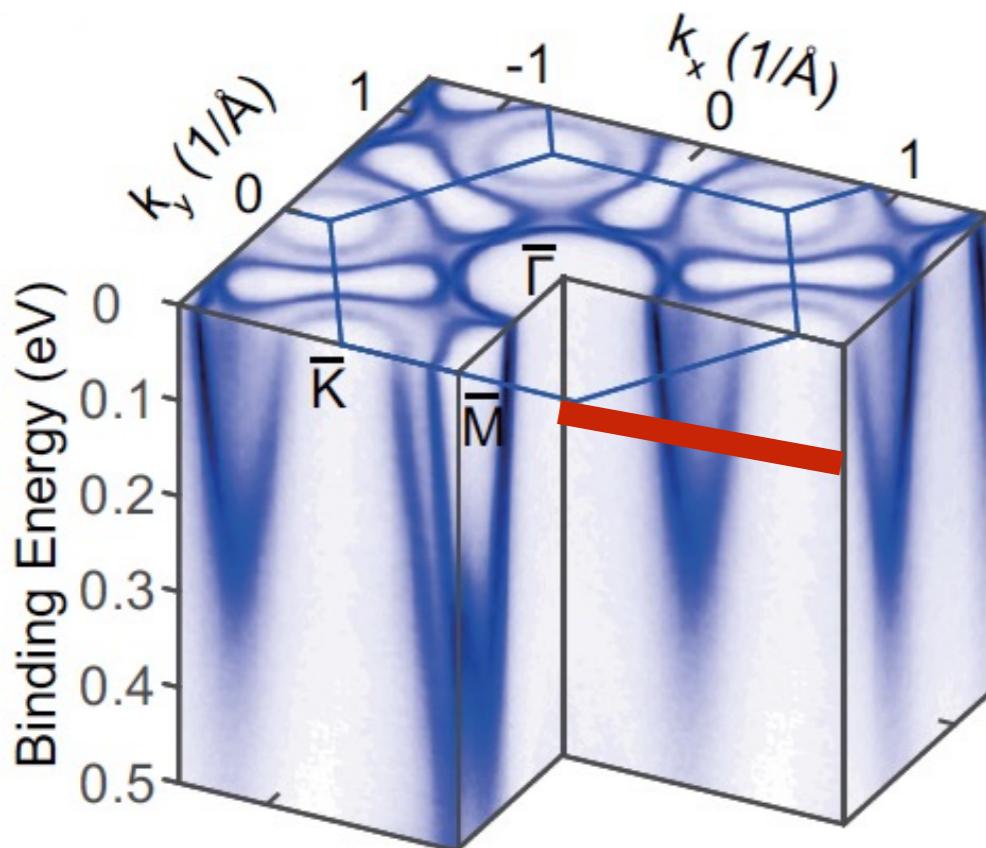
High symmetry cut



ARPES data plot 종류

$I(k_x, k_y, BE) @k_z 0' + \Delta k_z$

3 차원 data

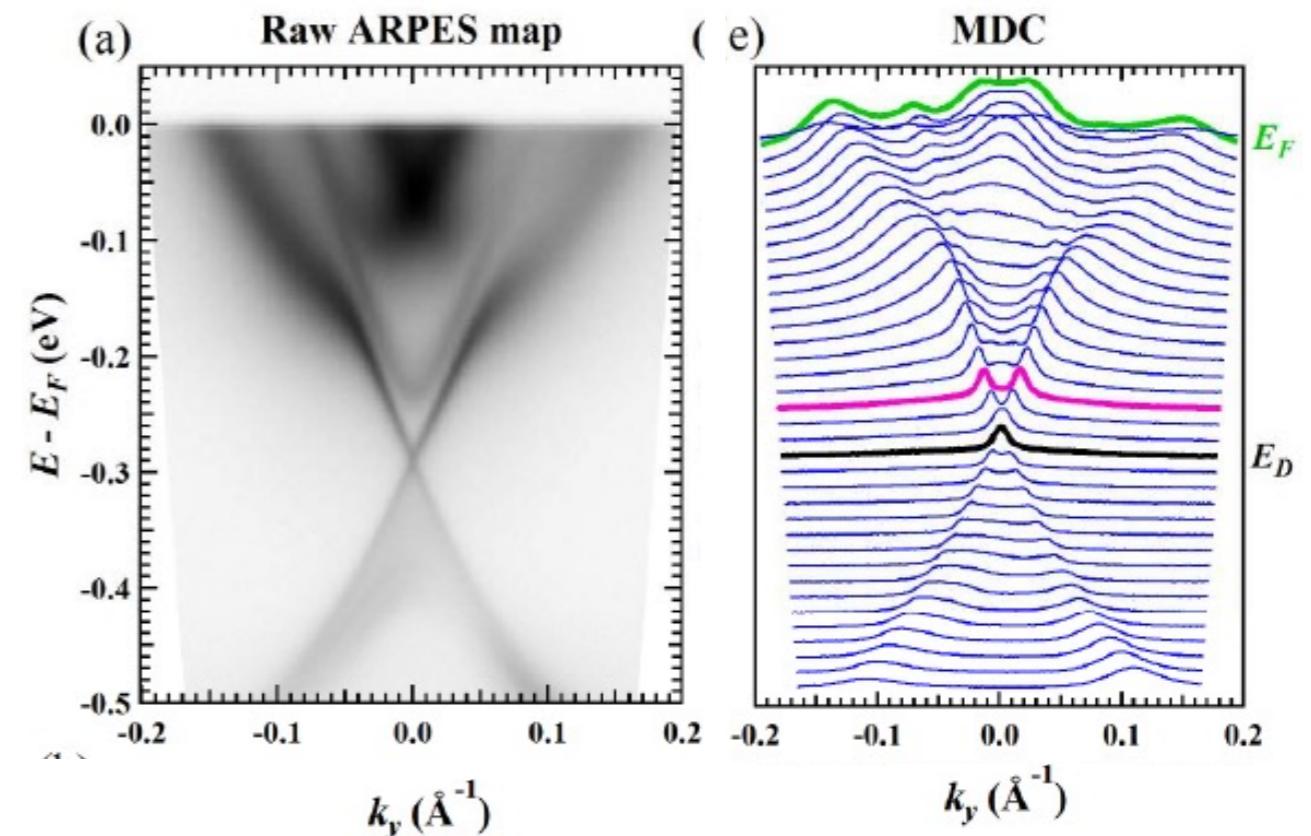


논문 지면 또는 화면은 2
차원

1 차원 Plot

$I(k_x)$
@fixed k_y, k_z, BE

Momentum Distribution Curve
(MDC)

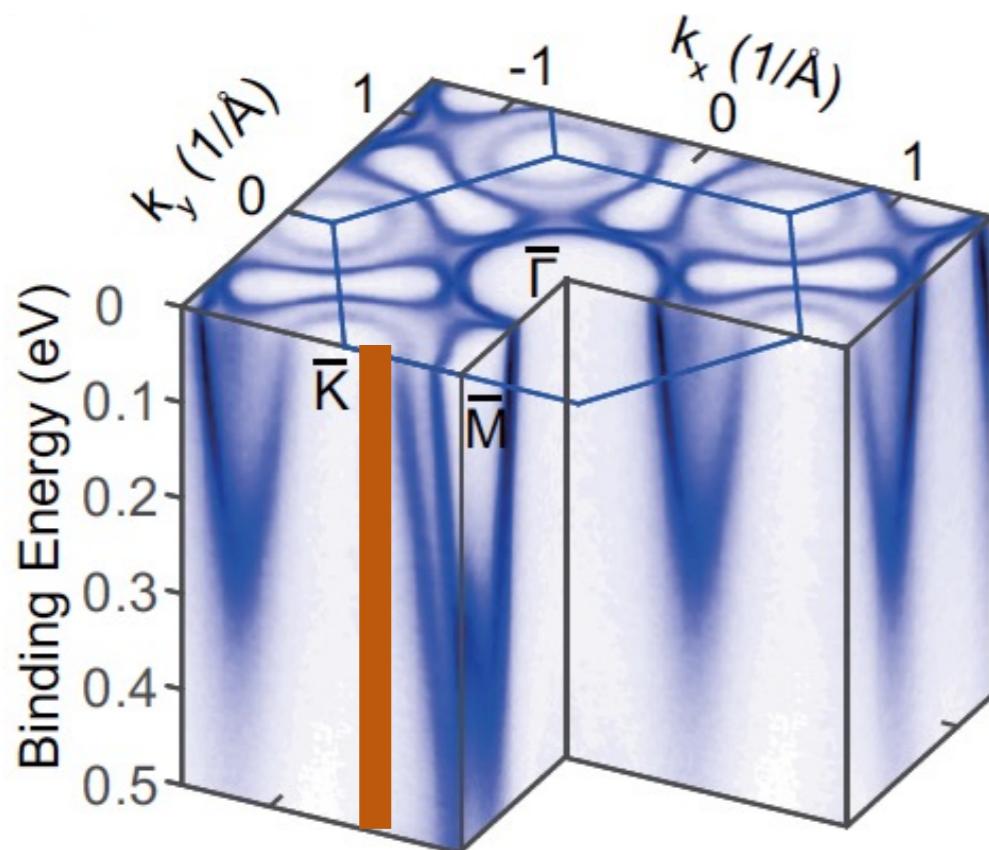


Y. Hao *et al.*, PRX 9, 041038 (2019)

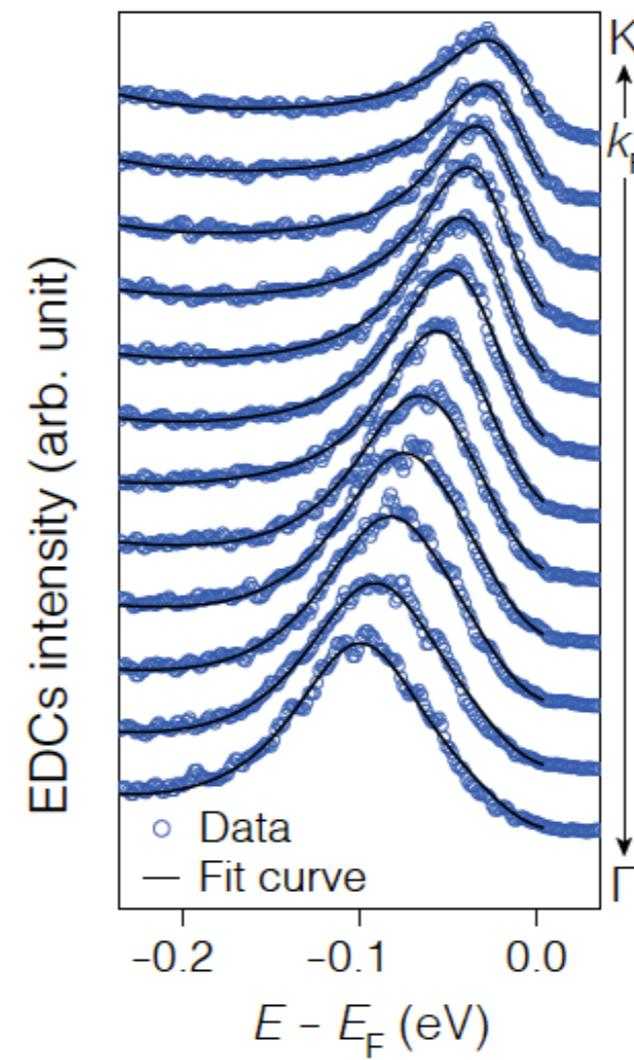
ARPES data plot 종류

$I(k_x, k_y, BE) @k_z 0' + \Delta k_z$

3 차원 data

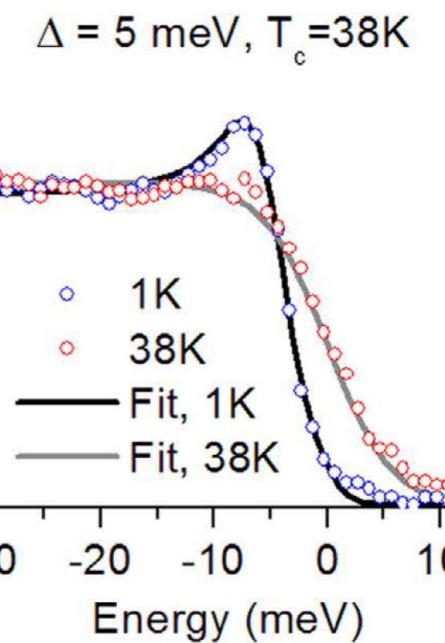


$I(BE)$
@fixed k_x, k_y, k_z



I 차원 Plot

Energy Distribution Curve
(EDC)



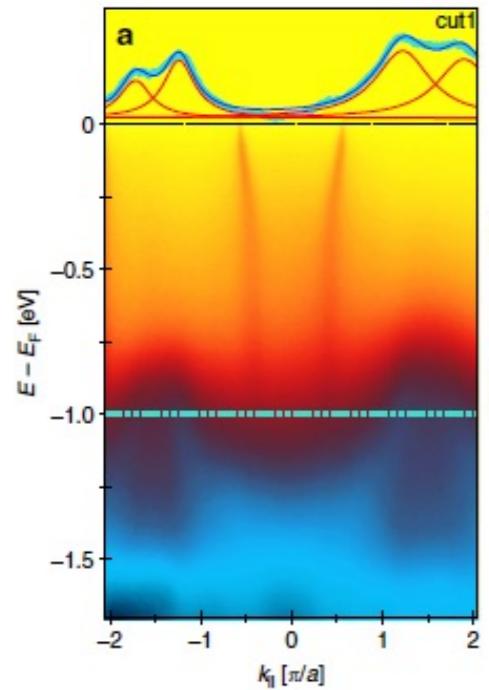
W. S. Lee et al., Nature (2007)

목차

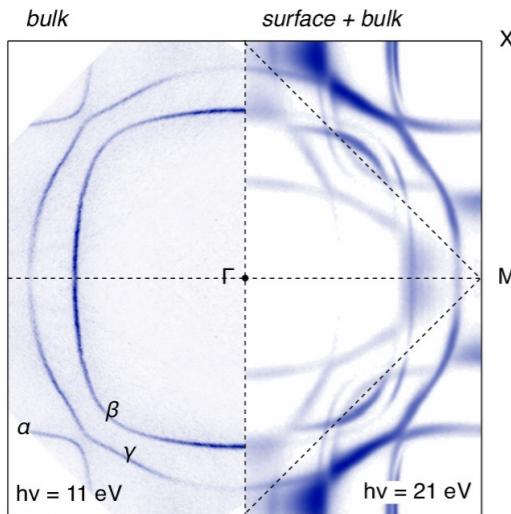
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ARPES as a k -space microscope

Correlated system

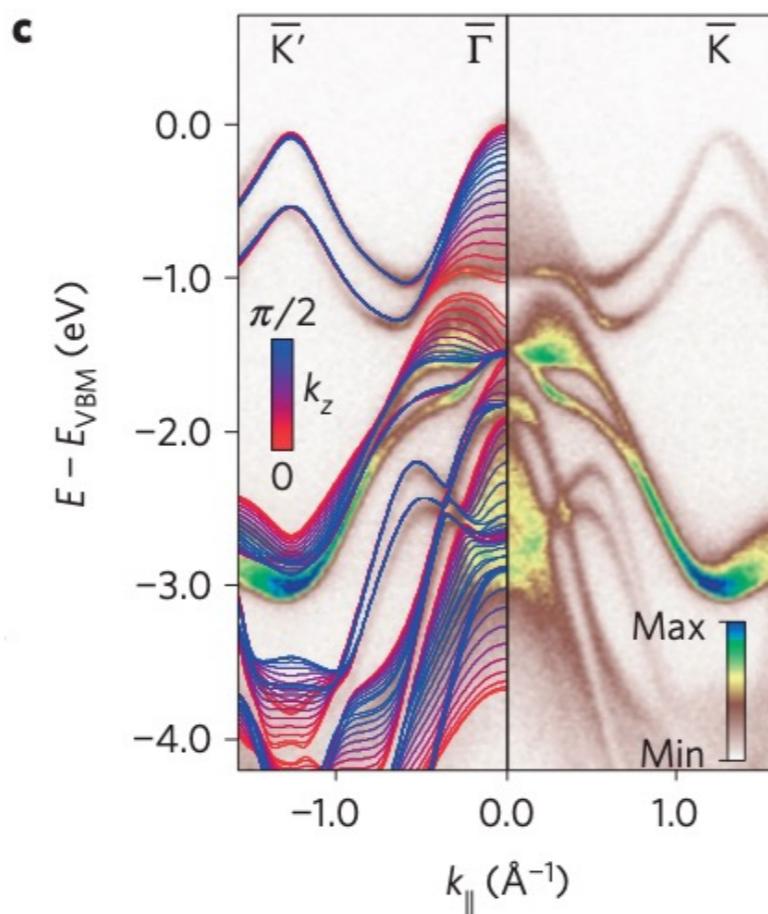


C. E. Matt *et al.*, *Nat. Comm.* (2018)



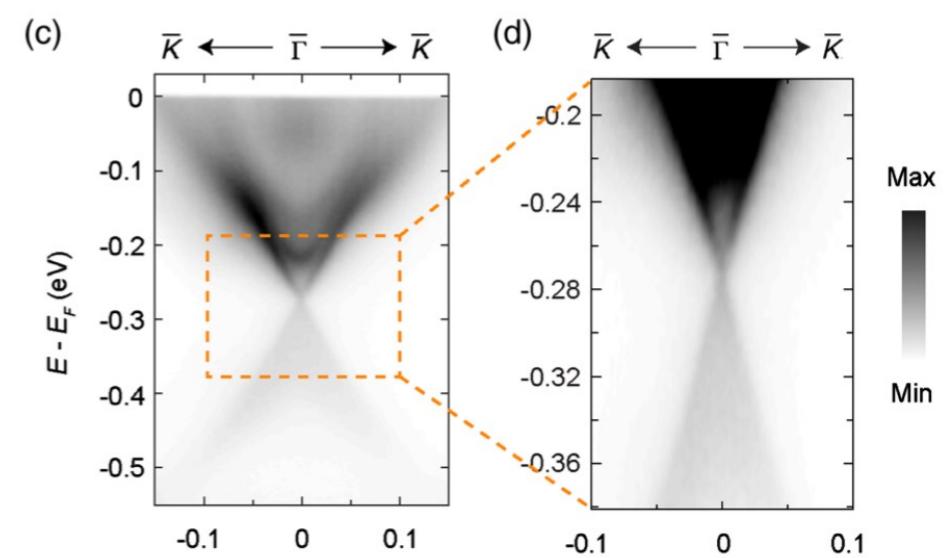
A. Tamai *et al.*, *PRX* (2019)

2D materials

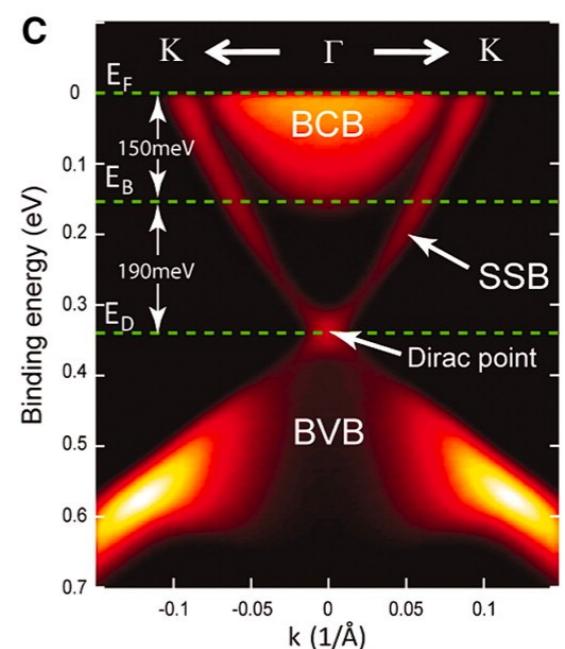


J. M. Riley, *et al.*, *Nat. Phys.* (2014)

Topological materials



Y. J. Chen, *et al.*, *PRX* (2019)



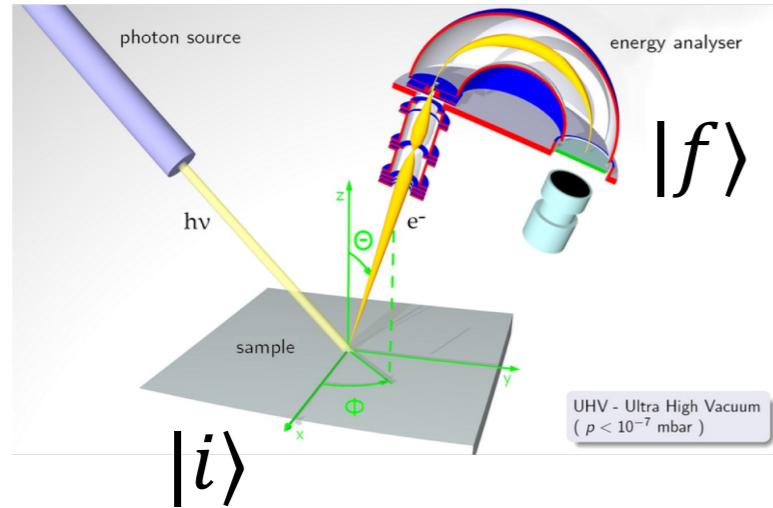
Y. Chen *et al.*, *Science* (2010)

ARPES는 밴드만 보여 준다?

No!

밴드 뿐만 아니라 전자가 고체 안에서 어떻게 살고 있는지 알고 준다!

Photoelectric effect in terms of quantum mechanics



$$|i\rangle \longrightarrow |f\rangle$$

dipole transition by $H' = -\frac{e}{mc} \mathbf{A} \cdot \mathbf{p}$

transition rate

$$\omega_{fi} = \frac{2\pi}{\hbar} \left| \langle f | \vec{A} \cdot \vec{p} | i \rangle \right|^2 \delta(E_f - E_i - h\nu)$$

실제로는 N particle system에서 전자를 뽑아 본다

Transition rate $w_{fi} = \frac{2\pi}{\hbar} |\langle \Psi_f^N | H_{int} | \Psi_i^N \rangle|^2 \delta(E_f^N - E_i^N - h\nu)$

Sudden approximation $\Psi_f^N \rightarrow \Psi_f^N = A\phi_f^k \Psi_f^{N-1} \quad \Psi_i^N \rightarrow \Psi_i^N = A\phi_i^k \Psi_i^{N-1}$

$$w_{fi} \propto \sum_{f,i} \left| M_{f,i}^k \right|^2 \sum_m \left| c_{m,i} \right|^2 \delta(E_{kin} + E_m^{N-1} - E_i^N - h\nu)$$

$$\left| M_{f,i}^k \right|^2 \equiv \left| \langle \phi_f^k | \mathbf{A} \cdot \mathbf{p} | \phi_i^k \rangle \right|^2 \quad A^\pm(\mathbf{k}, \omega) = \sum_m \left| \langle \Psi_m^{N\pm 1} | c_{\mathbf{k}}^\pm | \Psi_i^N \rangle \right|^2 \delta(\omega - E_m^{N\pm 1} + E_i^N)$$

$$I(\mathbf{k}, E_{kin}) = \sum_{f,i} w_{f,i} \approx \underline{|M(k)|^2} \underline{A^-(k, \omega)} f(\omega)$$

Matrix element *Spectral weight: how electron moves*
: symmetry info

M(\mathbf{k})에서 알 수 있는 정보

$$I(\mathbf{k}, E_{kin}) = \sum_{f,i} w_{f,i} \approx \underline{|M(k)|^2 A^-(k, \omega) f(\omega)}$$

$$M(k) = \langle \vec{f} | \vec{A} \cdot \vec{p} | i \rangle = \langle \hat{f} | \vec{e} \cdot \vec{r} | i \rangle \quad \hat{e} \cdot \vec{r} = x \quad \text{light polarization}$$

dipole approx.

양자역학에서 배운
것

$$M(k) = \langle \underset{\text{even}}{2s} | x | \underset{\text{odd}}{1s} \rangle = 0$$

Matrix element로부터 파동함수의
symmetry 정보를 알 수 있다.

$$M(k) = \langle \underset{\text{odd}}{2p_x} | x | \underset{\text{even}}{1s} \rangle \neq 0$$

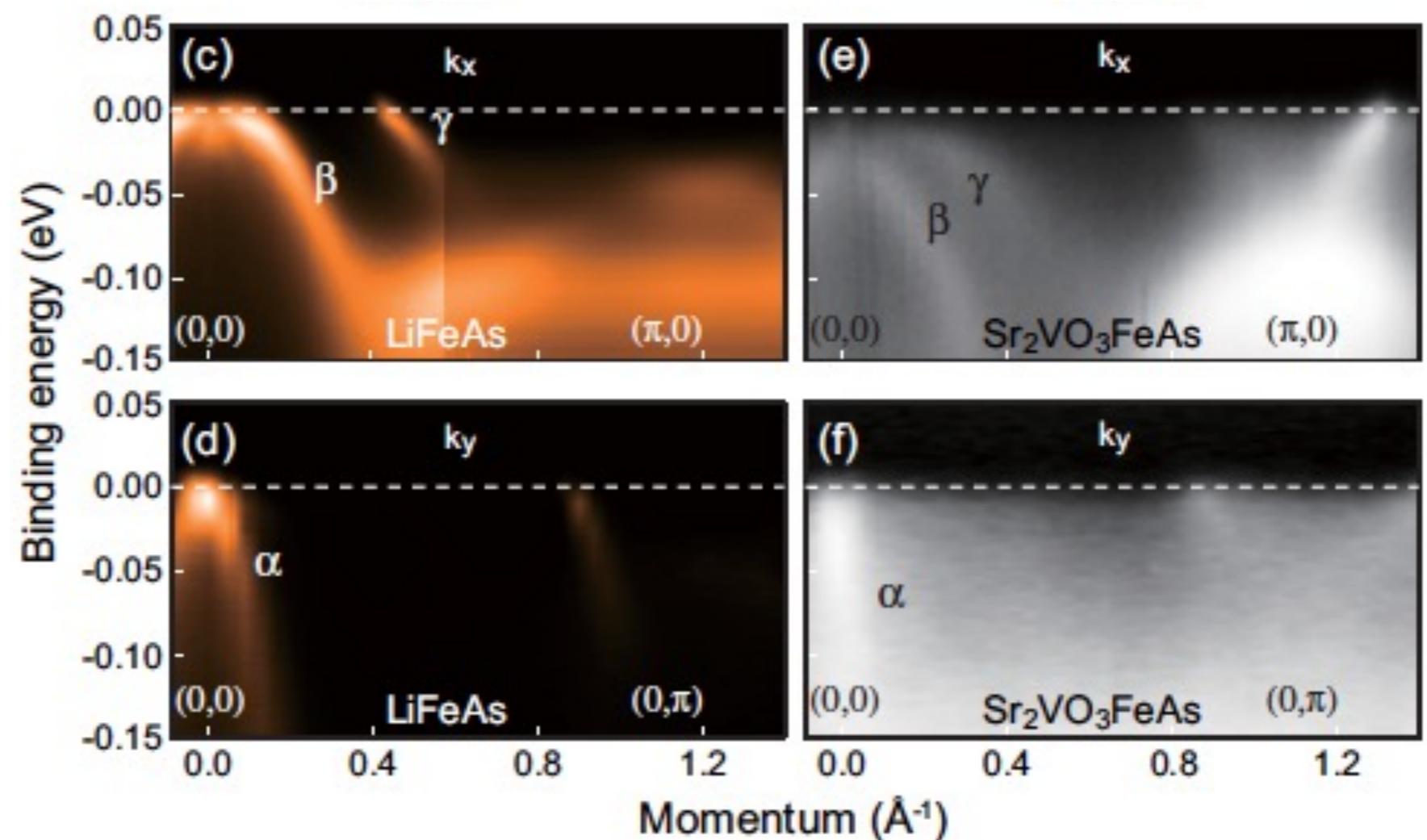
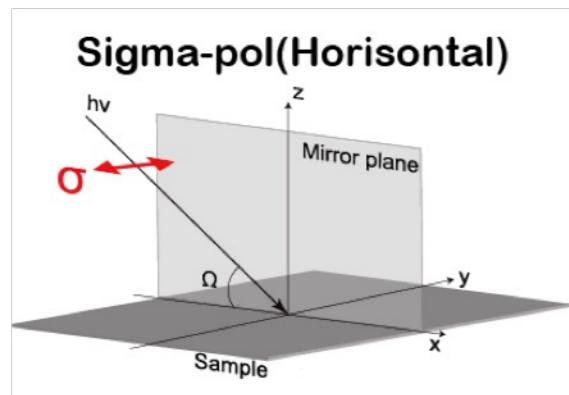
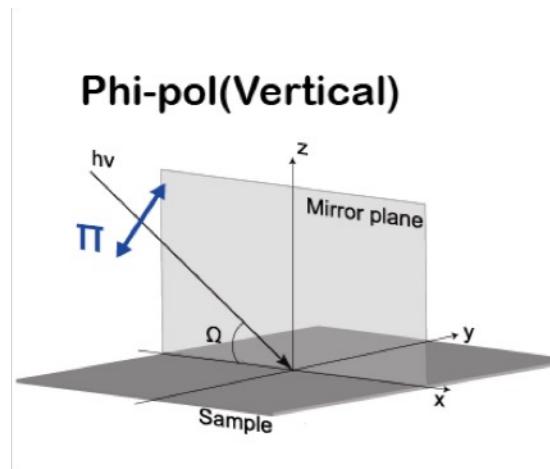
선편광 사용의 경우

with linear polarization,

parity information of initial state

$\hat{e} \cdot \vec{r}$

$$\hat{e} \cdot \vec{r} = x, y, z$$



d_{xy}

d_{yz}

d_{zx}

원편광 사용의 경우

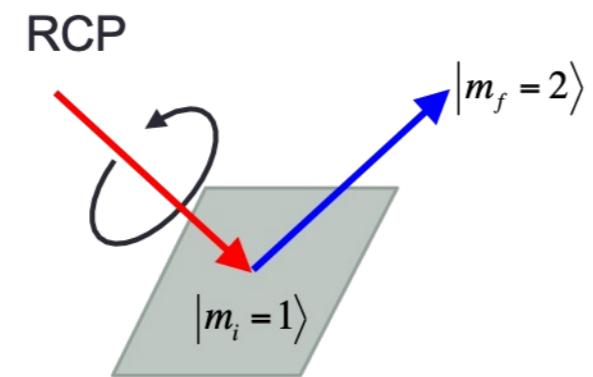
with circular polarization,

quantity related to inversion or time-reversal symmetry

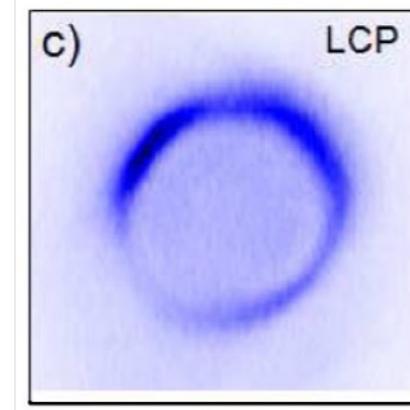
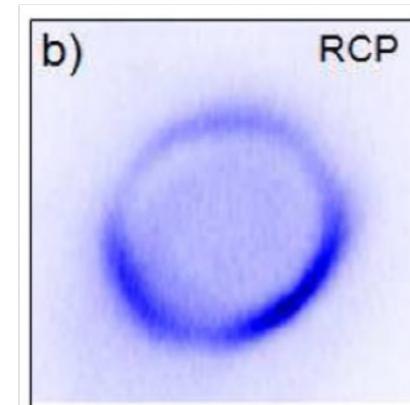
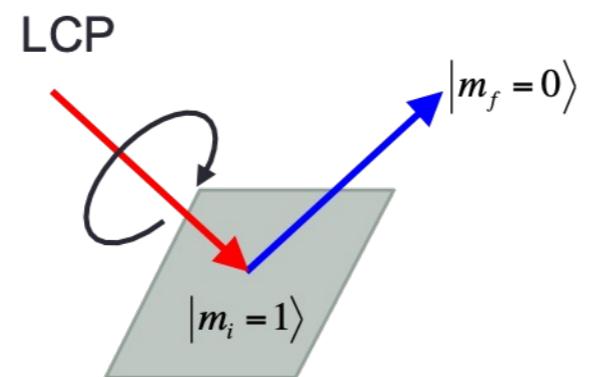
$\hat{e} \cdot \vec{r}$

$$\hat{e} \cdot \vec{r} = x \pm iy$$

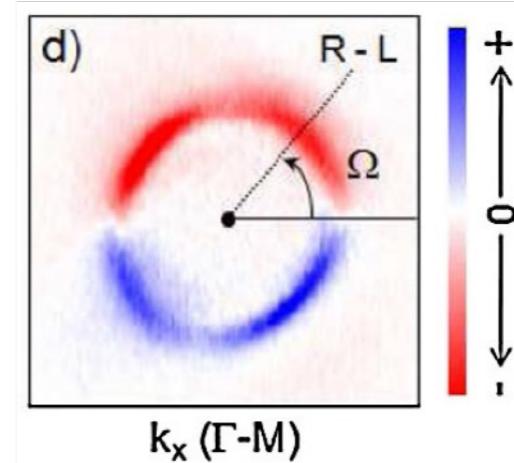
RCP
 Right CP
 $\rightarrow m_f = m_i + 1$



LCP
 Left CP
 $\rightarrow m_f = m_i - 1$



$$I_{CD} = I_{RCP} - I_{LCP}$$



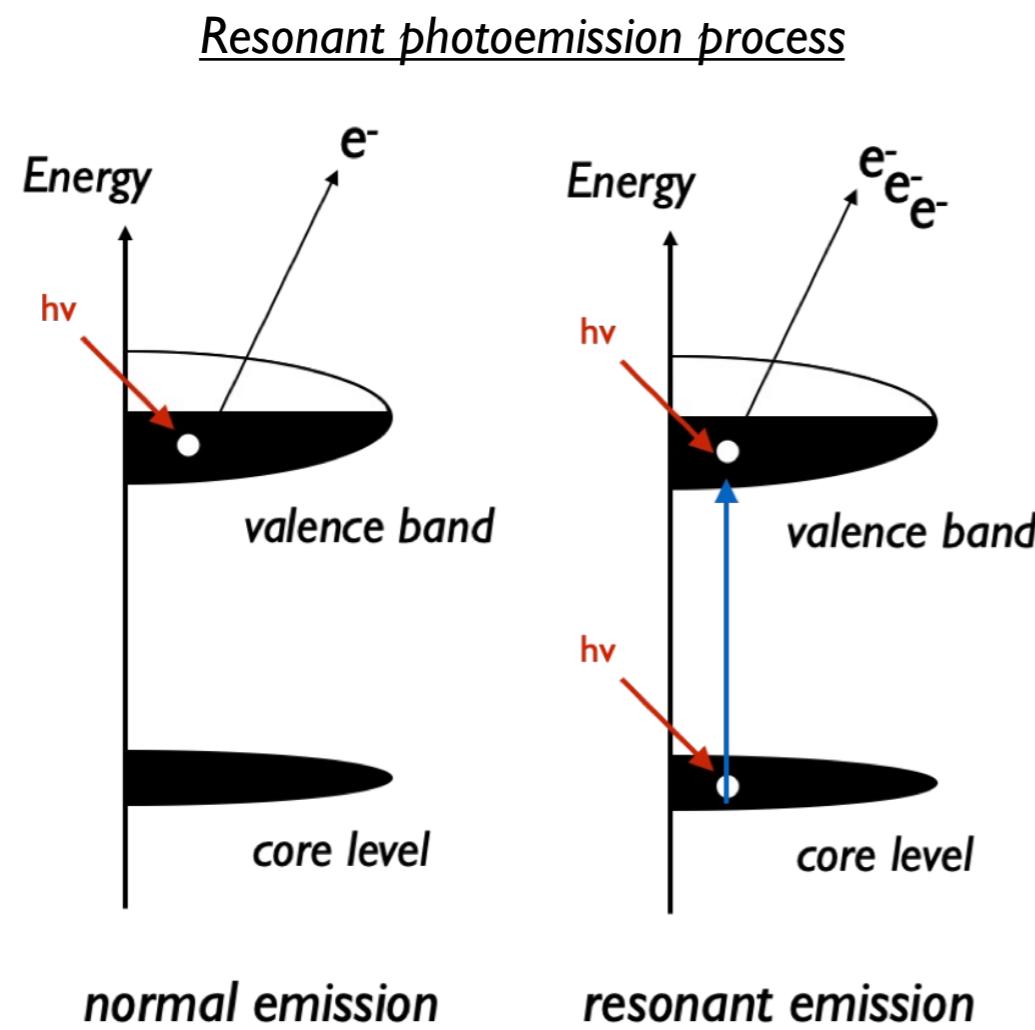
Sign : relative direction
 Size : relative OAM size

- S. R. Park, et al. Phys. Rev. Lett. **108**, 046805 (2012)

Circular dichroism \rightarrow OAM in the initial state

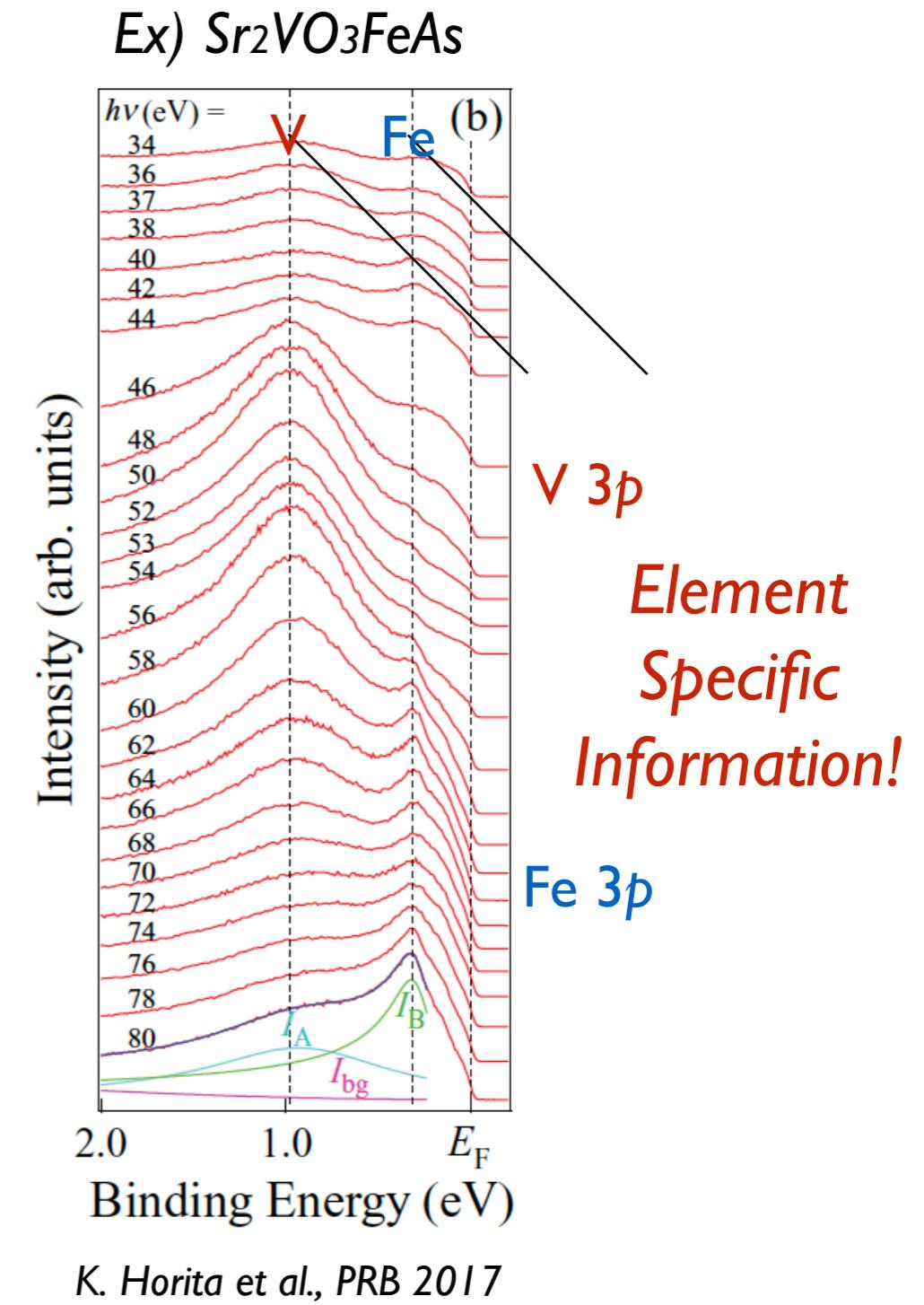
from Dr. S. Cho's presentation

More on $M(k)$: Resonant photoemission



$$I(\mathbf{k}, E_{kin}) \approx |M(k)|^2$$

$$M(k) = \langle f | \hat{e} \cdot \hat{r} | i \rangle + \langle f | \hat{e} \cdot \hat{r} | m \rangle \langle m | \hat{e} \cdot \hat{r} | core \rangle$$

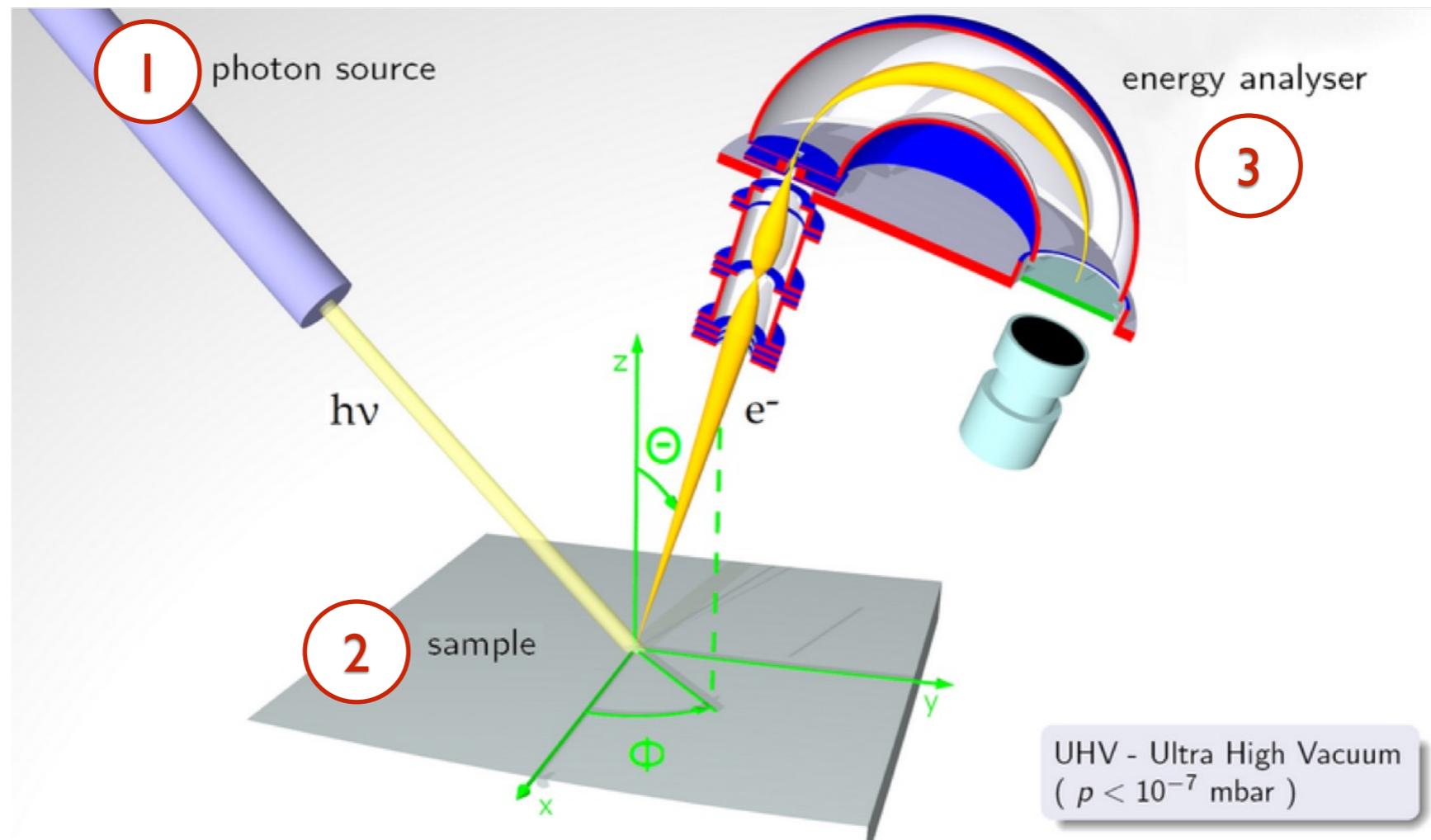


K. Horita et al., PRB 2017

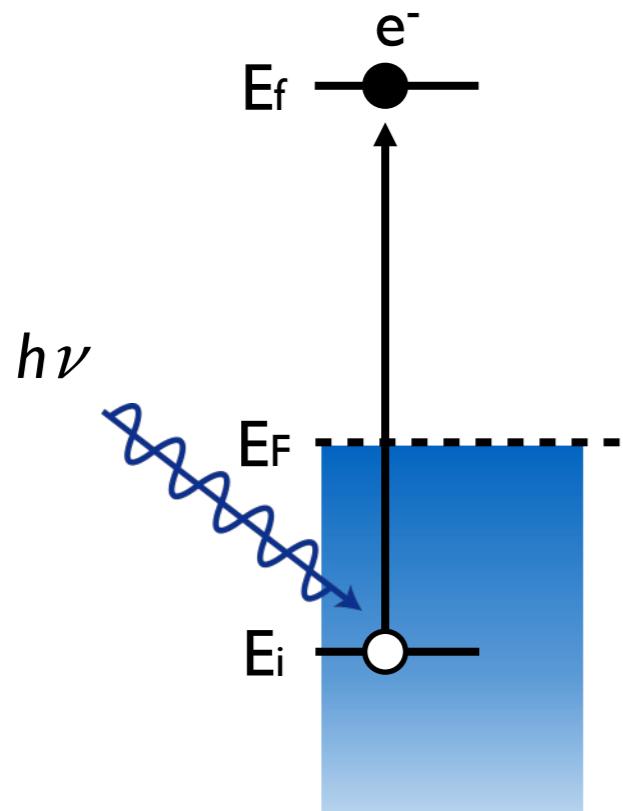
목차

- ✓ 각분해능 광전자 분광의 기초
 - ✓ 광전효과- 각분해능?
 - ✓ 관측법 및 관측결과를 전자구조로 매팅 하는 법
 - ✓ 기본 데이터 읽는 법
- ✓ 심화- ARPES로 얻을 수 있는 정보 / Intensity에 숨겨진 정보
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- ✓ 심화- ARPES 기법 리뷰
 - ✓ 빛
 - ✓ 샘플
 - ✓ 전자 분광 및 검출

심화 - ARPES technique 2/3



광원의 요구 조건

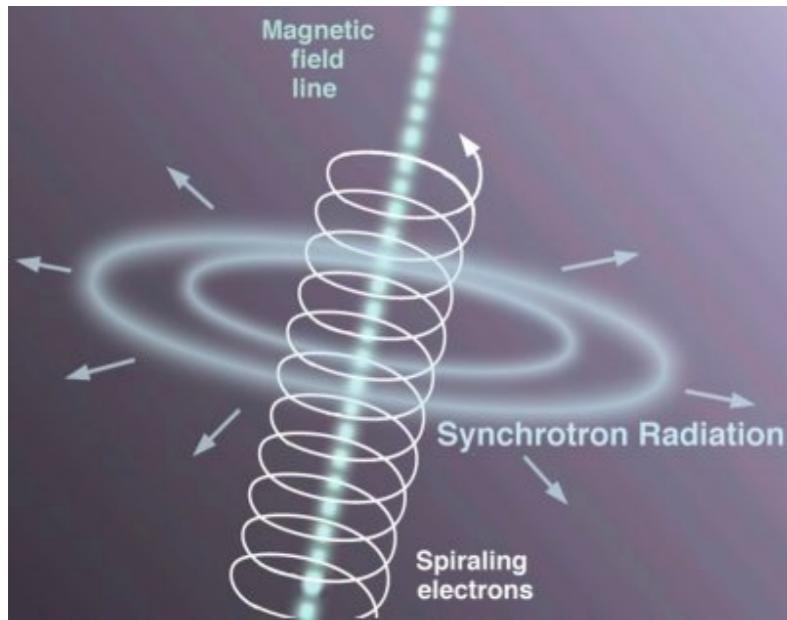


- ✓ 일함 수 (~ 4.5 eV)보다 에너지가 높아야 함
- ✓ 단파장 이여야 함 - 측정 KE로 부터 유일한 BE가 정의됨
- ✓ 센 빛이 필요함 - 측정 효율
- ✓ 에너지를 연속적으로 조절하면 좋음 - k_z 정보 취합
- ✓ 크기가 작으면 작을수록 좋음 - 에너지/운동량 분해능

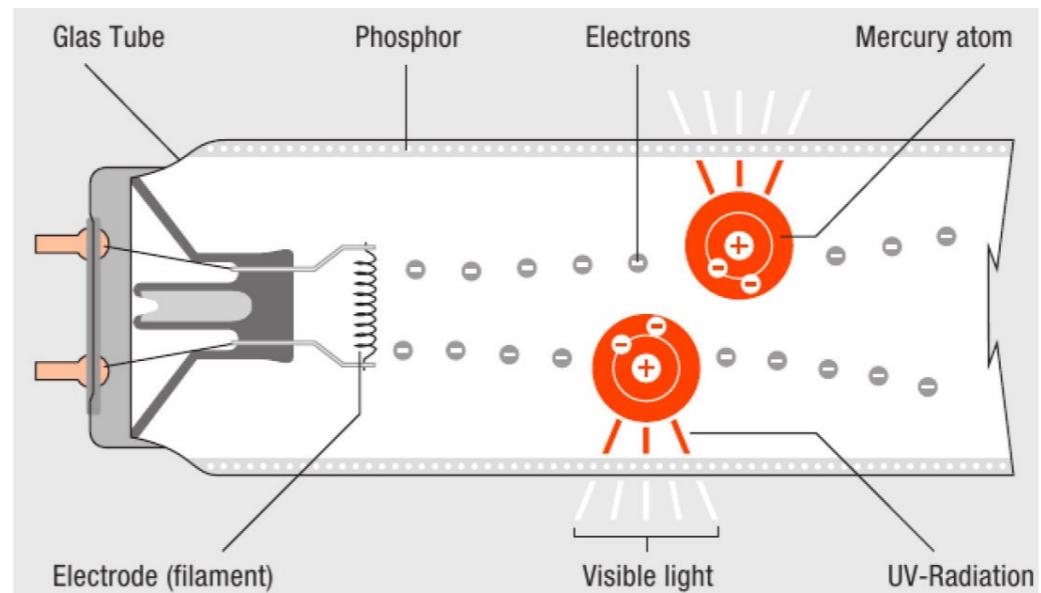
$$KE = \hbar\omega - \phi - BE$$

광원의 종류

Synchrotron radiation



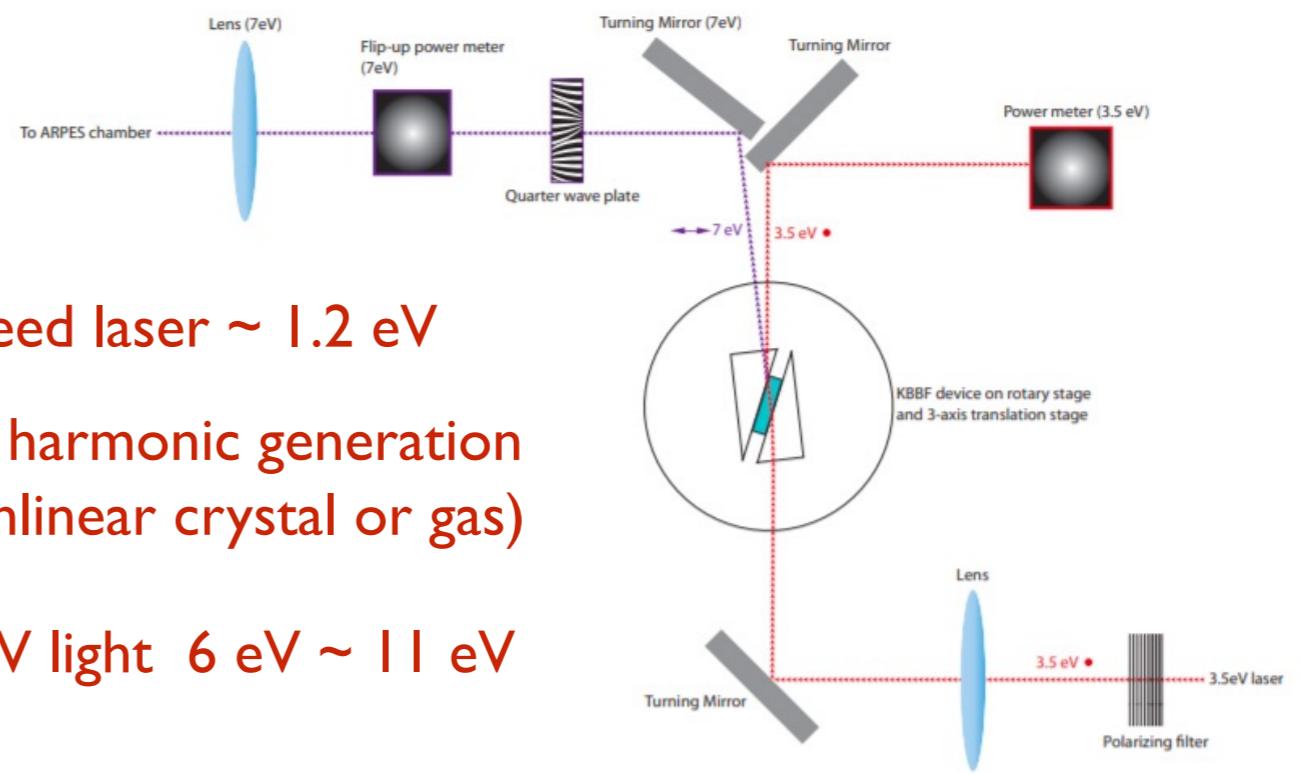
Gas discharge lamp (He)



VUV laser

Seed laser ~ 1.2 eV
high harmonic generation
(nonlinear crystal or gas)

VUV light 6 eV ~ 11 eV



광원들의 특징

	VUV Laser	Gas discharge lamp (He)	Synchrotron radiation
에너지	6, 7, 11 eV	21.2 eV	10 eV ~ 150 eV
세기 (flux)	$\sim 10^{15}$ photons/s	$\sim 10^{11}$ photons/s	$\sim 10^{13}$ photons/s
Beam size	$\sim 1 \mu\text{m}$	$> 100 \mu\text{m}$	$> 10 \mu\text{m}$
편광조절	○	×	○
Continuous	○	○	○
Pulsed light	○	×	○ (4세대)
Coherency	○	×	×

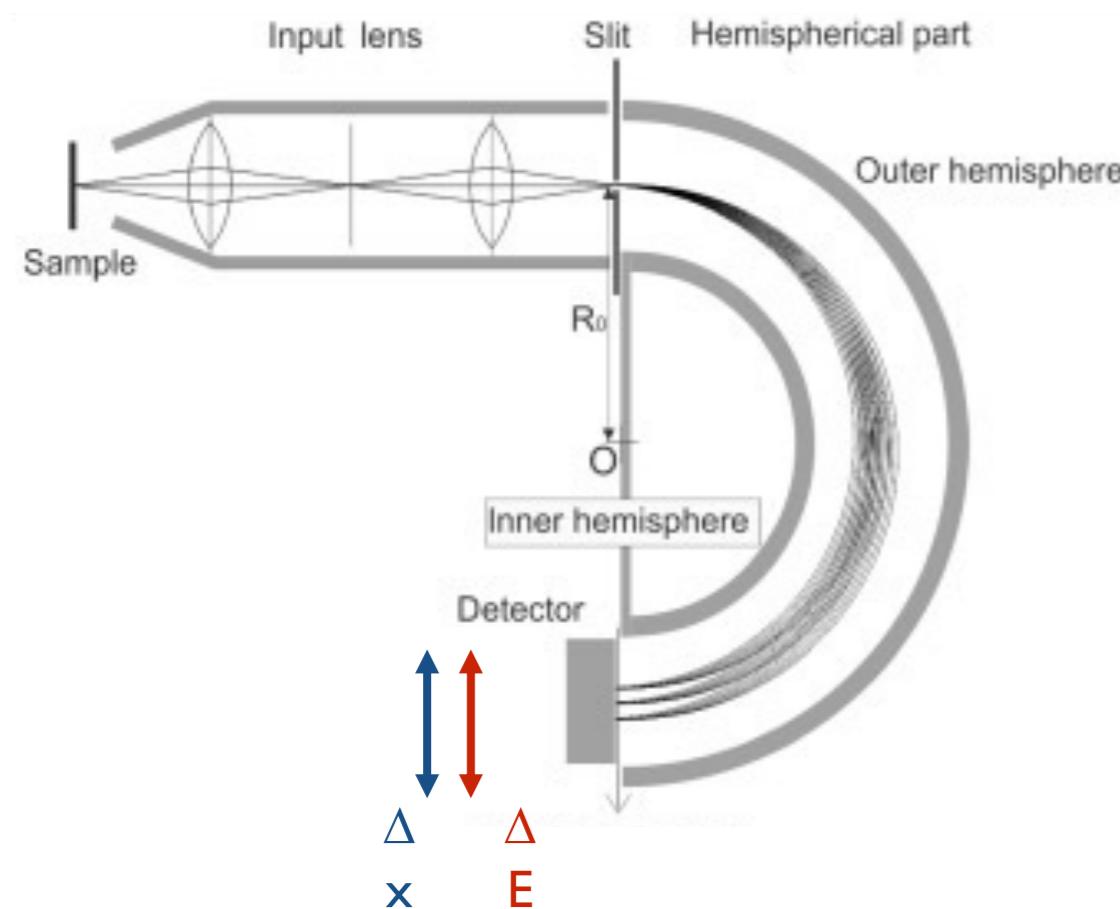
Laser ARPES

결맞음 단파장 작은 빔크기 에너지가 낫다

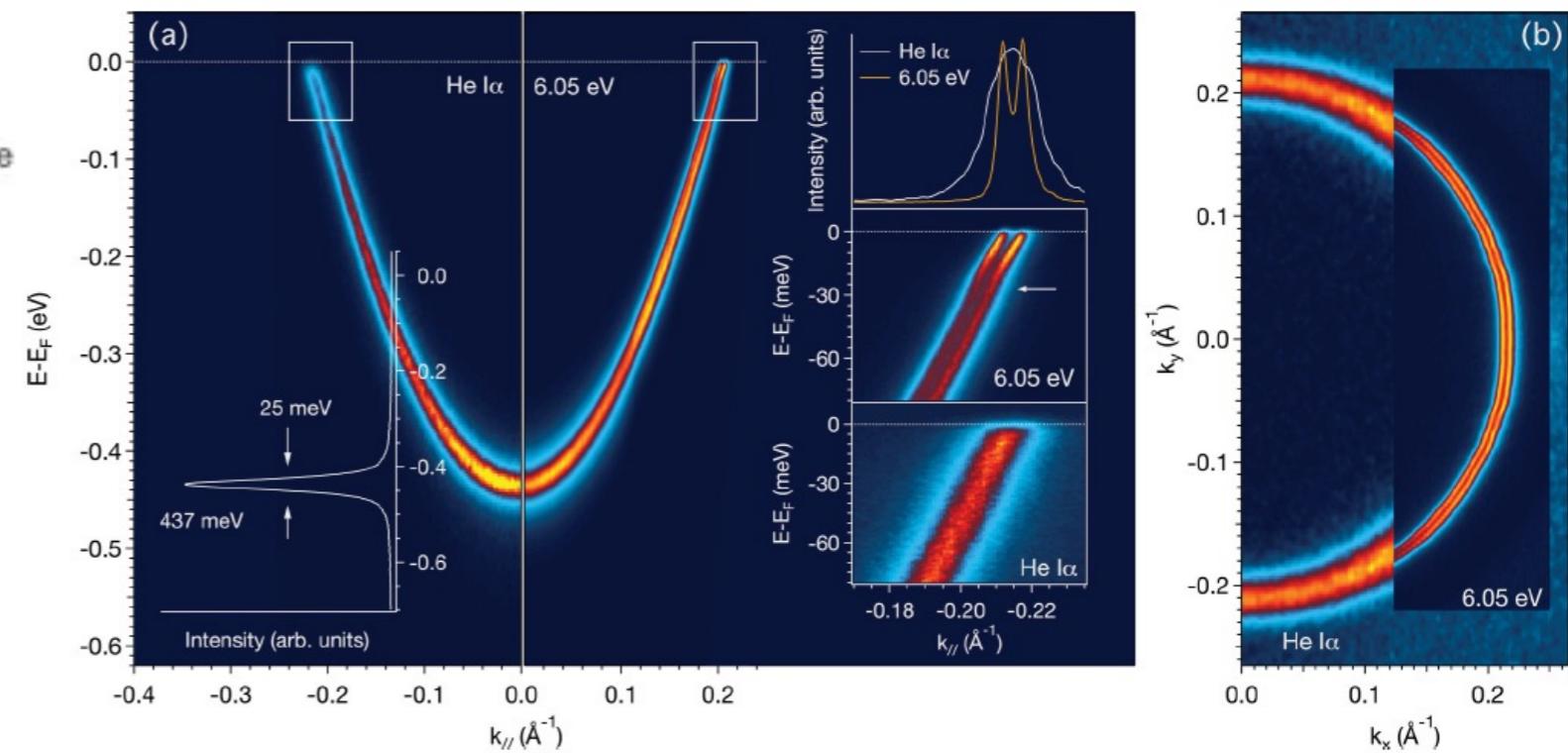
$$KE = \hbar\omega - \phi - BE$$

높은 에너지 & 운동량 해상도
(resolution)

electron lens + electron prism



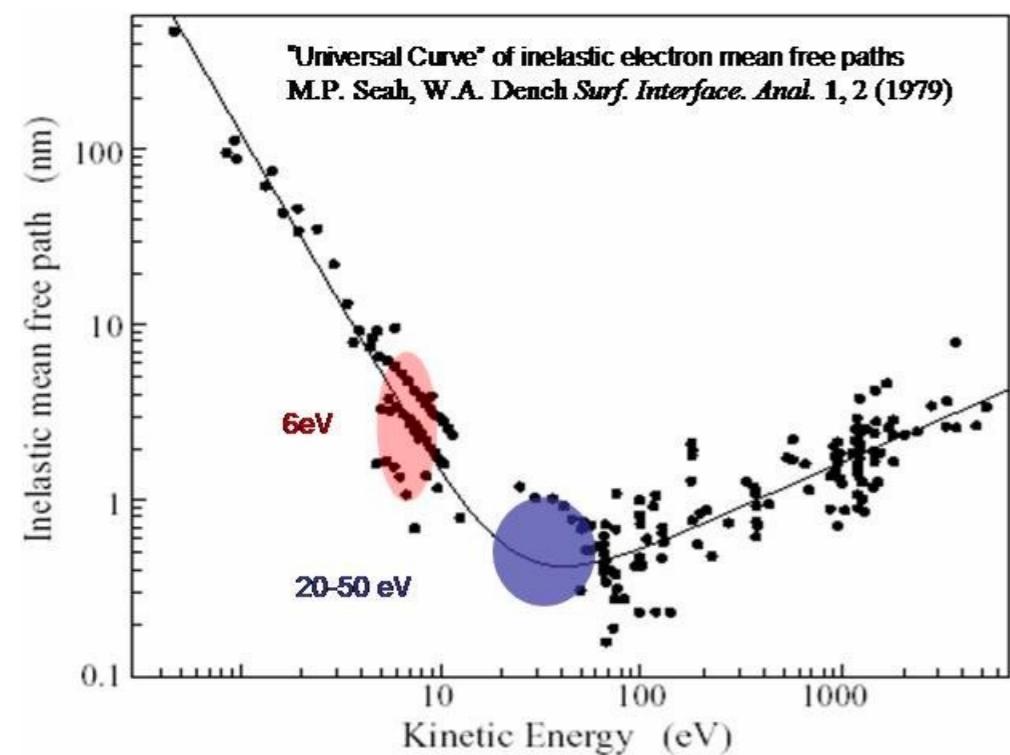
Cu(111) surface state measured by laser & He-lamp



A. Tamai *et al.*, PRB **87**, 075113
(2013)

Laser ARPES

결맞음 단파장 작은 빔크기 에너지가 낮다



Bulk sensitive!!

$$\left| i \right\rangle \xrightarrow{\Delta z} \left| i + \Delta k_z \right\rangle \xrightarrow{\Delta k_z} \left| f \right\rangle$$

저차원 물질만 측정
용이

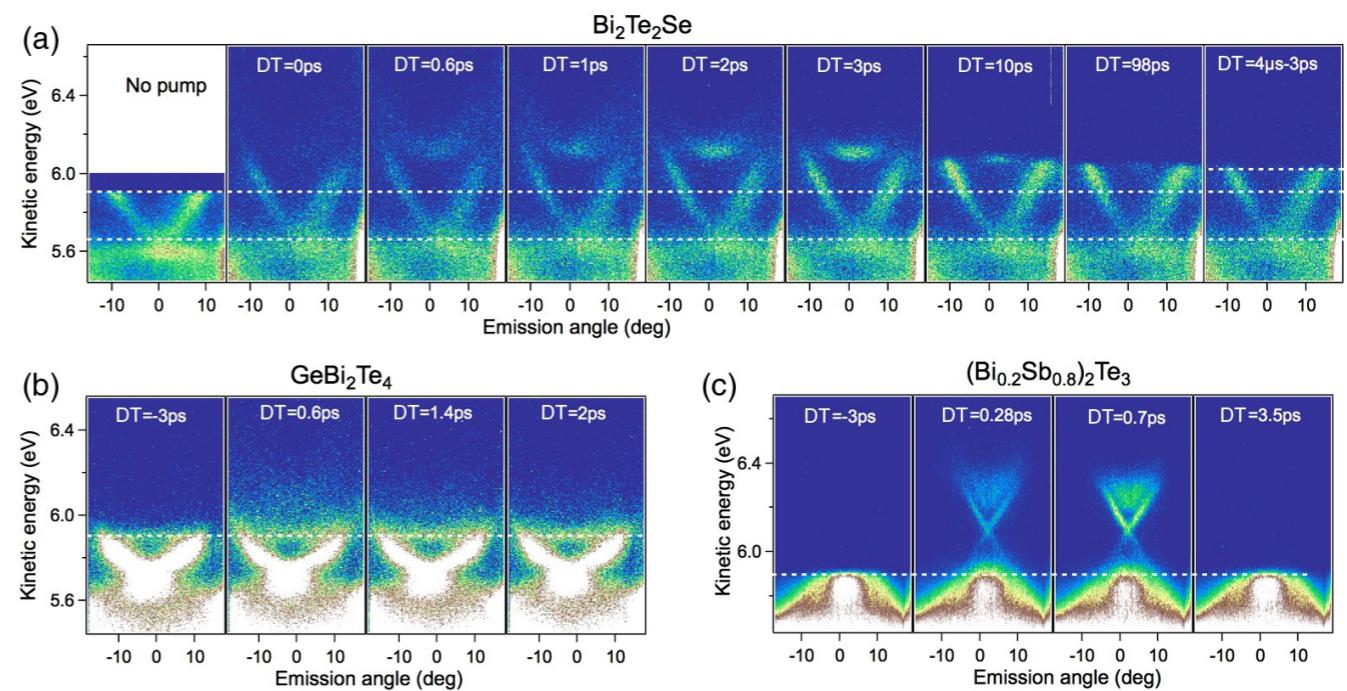
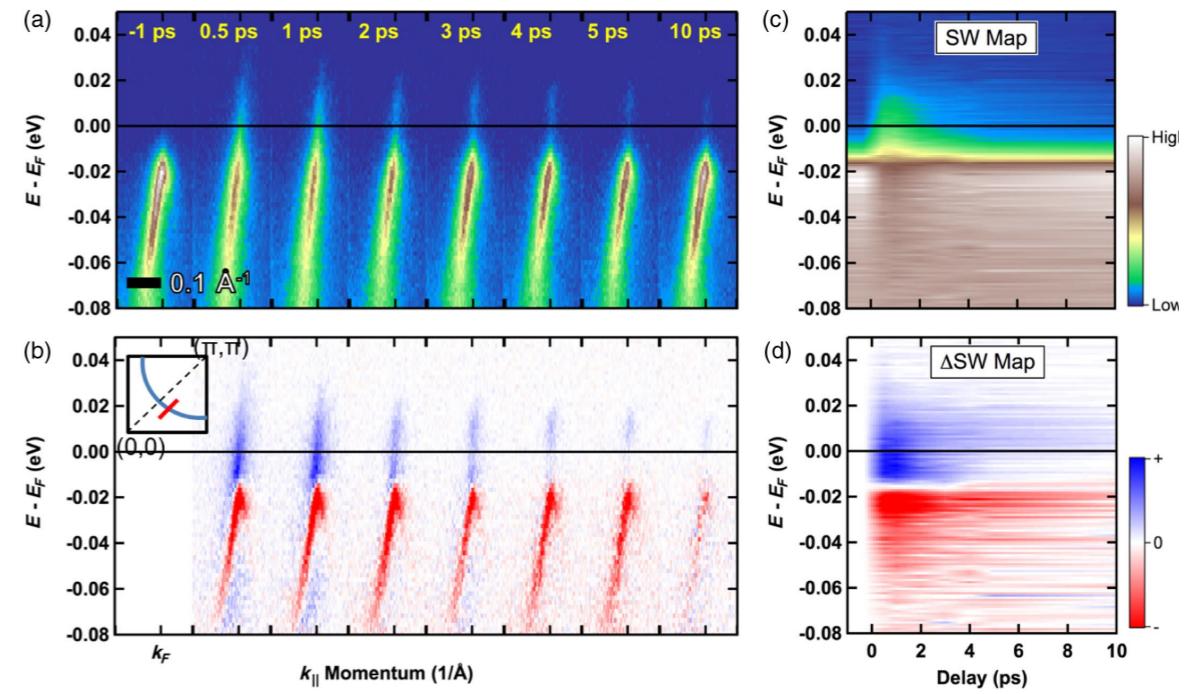
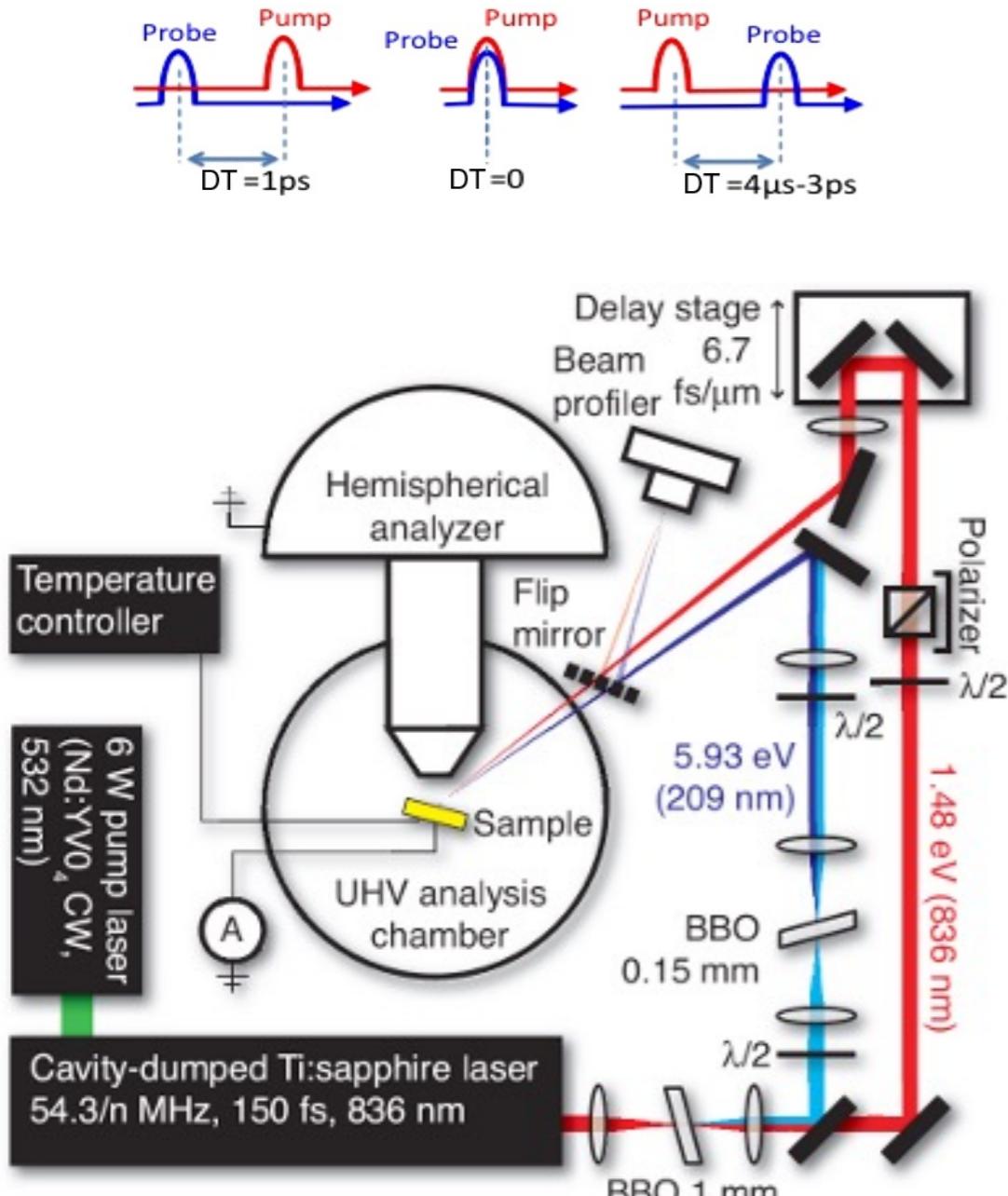
$$k_f = \sqrt{\frac{2m}{\hbar^2} KE}$$

$$k_f^x = \sqrt{\frac{2m}{\hbar^2} KE \sin\theta}$$

$$k_f^y = \sqrt{\frac{2m}{\hbar^2} KE \cos\theta \sin\alpha}$$

Limited momentum
range

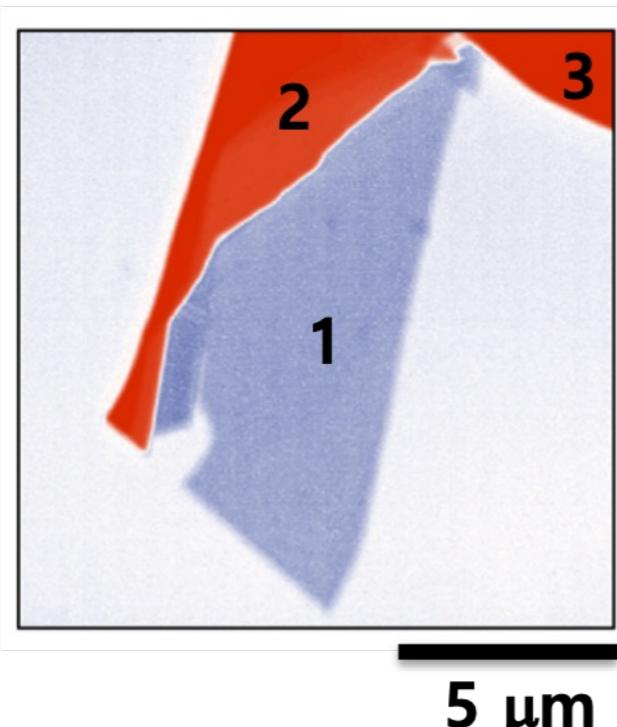
(Laser based) Time resolved ARPES



Nano-ARPES

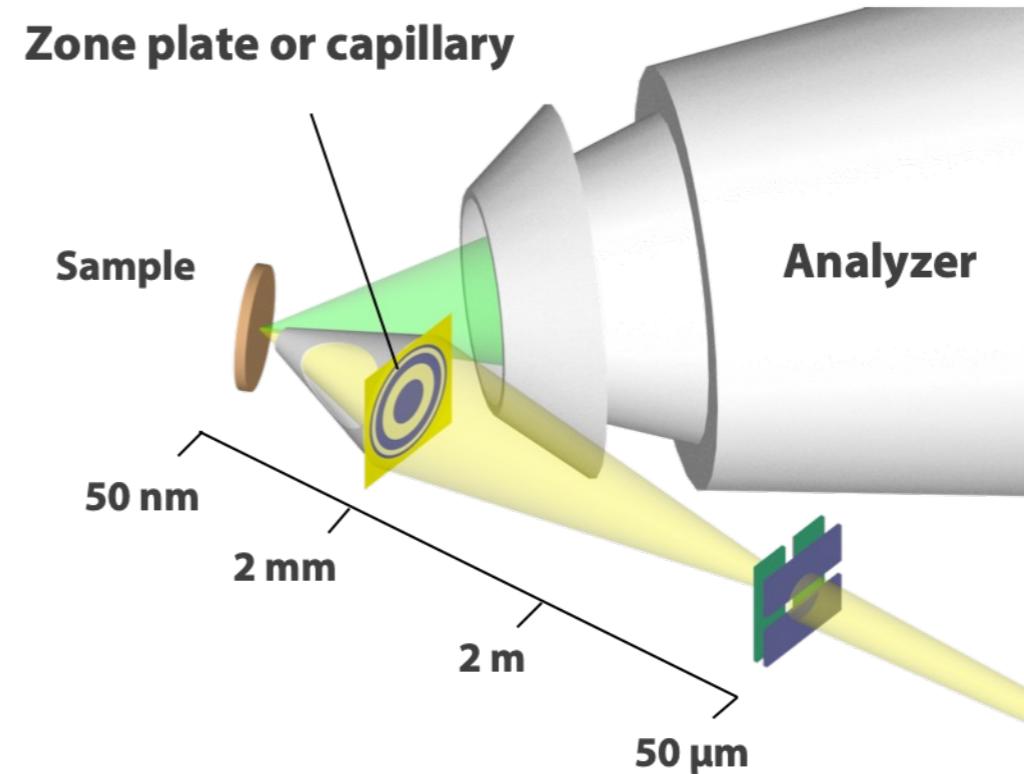
microARPES

beamsize: $30 \sim 200 \mu\text{m}$



nanoARPES

beamsize: $10 \mu\text{m}$ or smaller

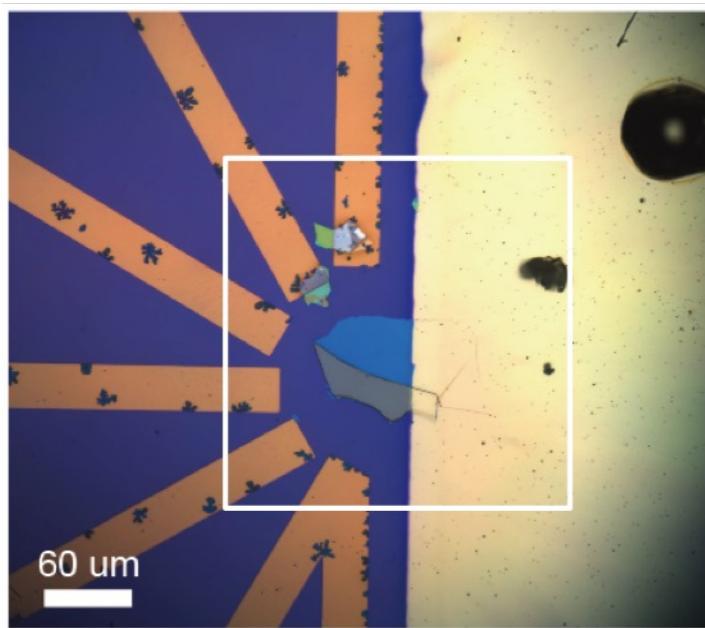


nanoARPES breaks the limit of materials that can be studied by ARPES

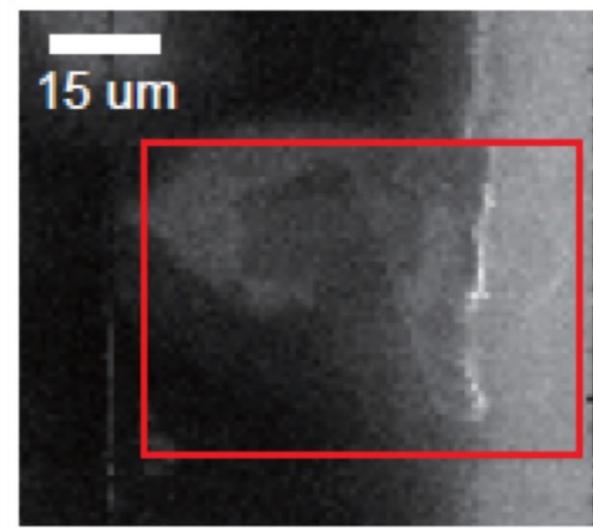
Taken from Prof. K. S. Kim's presentation

Nano-ARPES

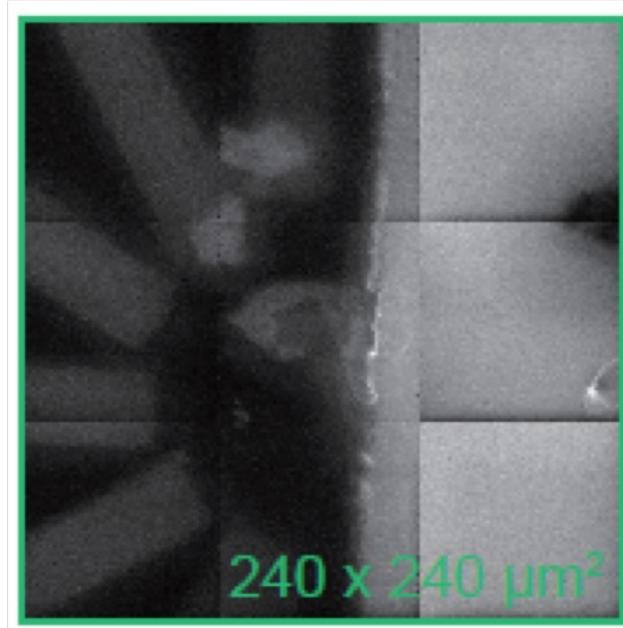
Optical microscope



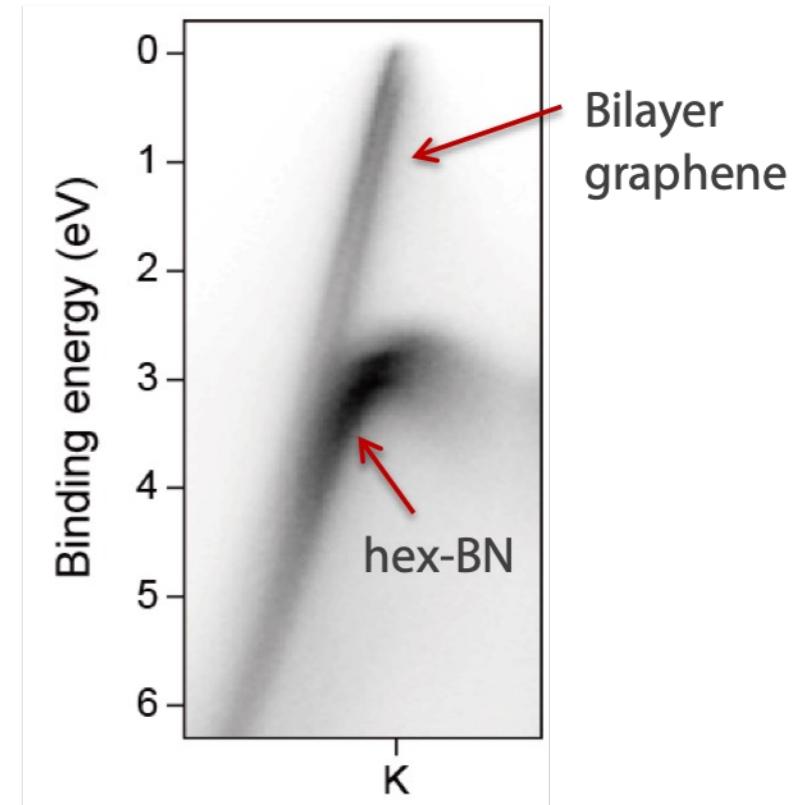
Magnified view



nanoARPES



nanoARPES spectra



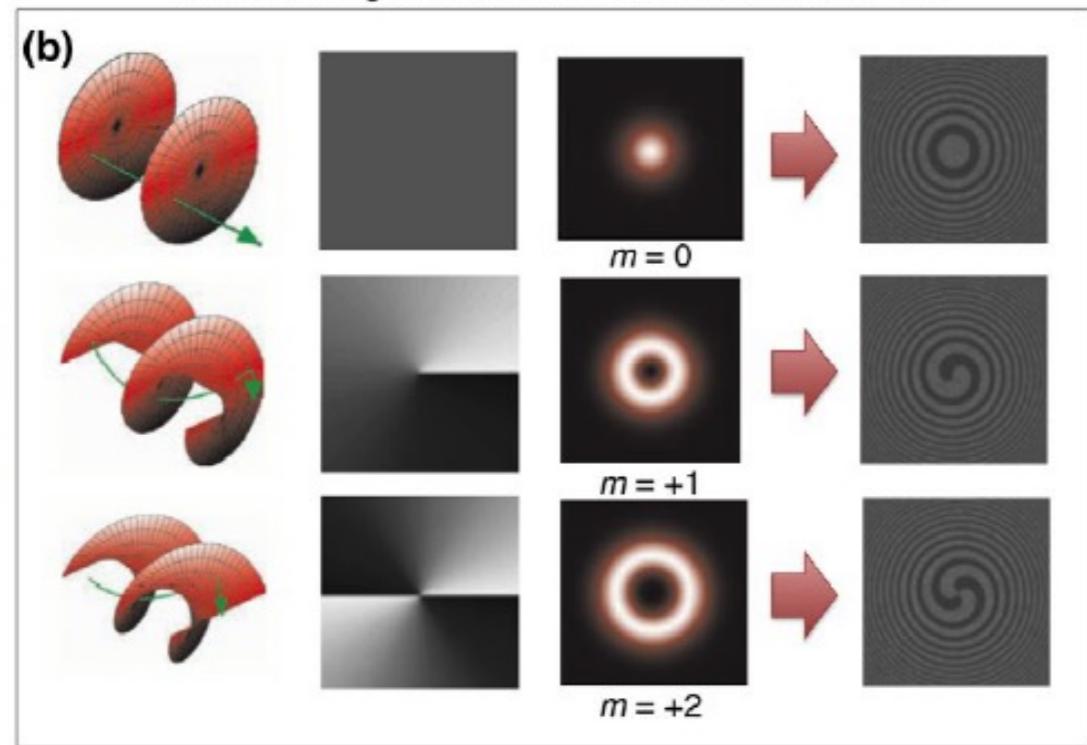
Excellent momentum resolution!

Taken from Prof. K. S. Kim's presentation

light engineering - vortex light

$$\stackrel{\rightarrow}{\rightarrow} \stackrel{\wedge}{\rightarrow} M(k) = \langle f | A \cdot p | i \rangle = \langle f | e \cdot r | i \rangle$$

dipole transition $\Delta m=0, +1, -1$

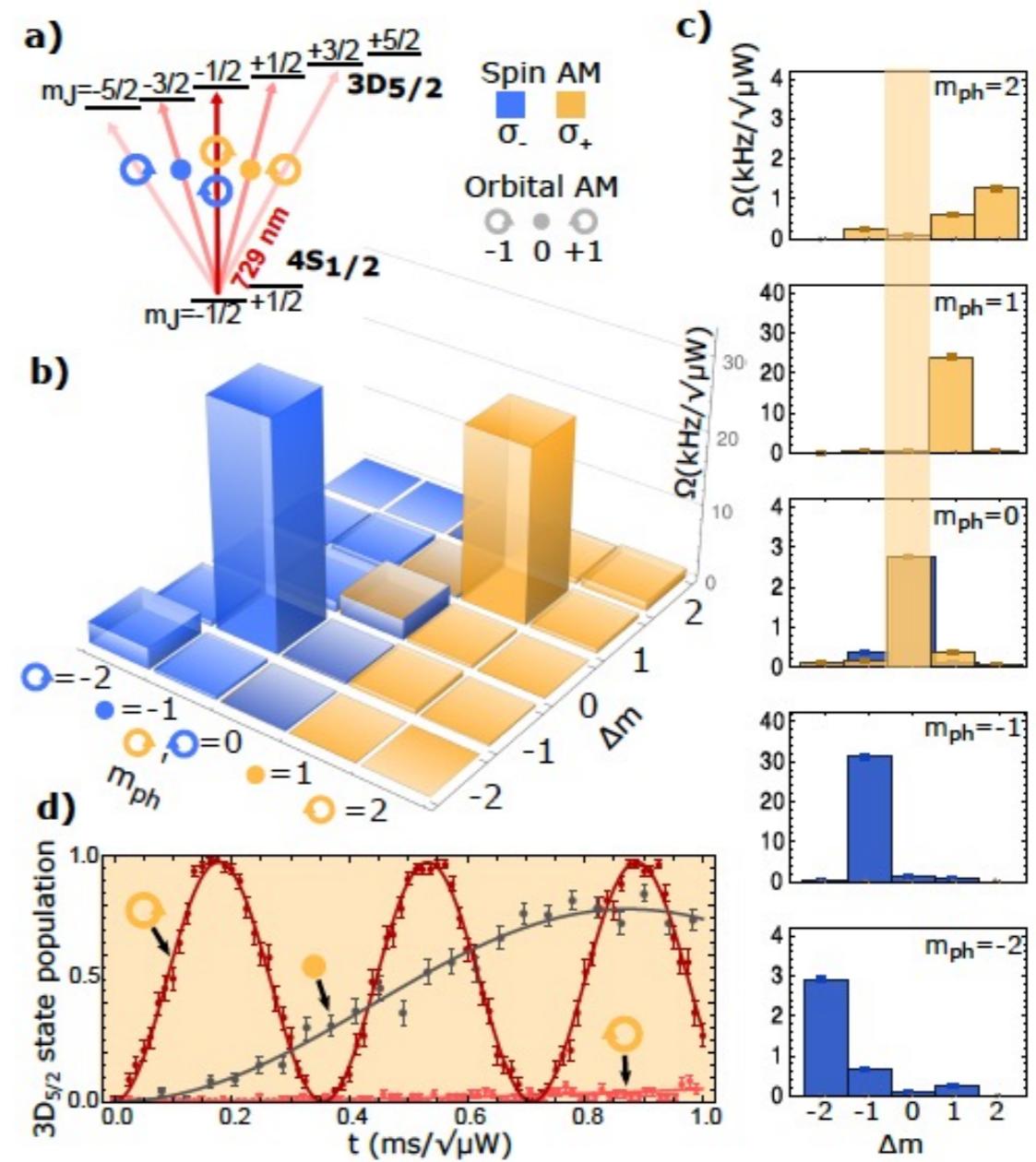


spin angular momentum of light (polarization)

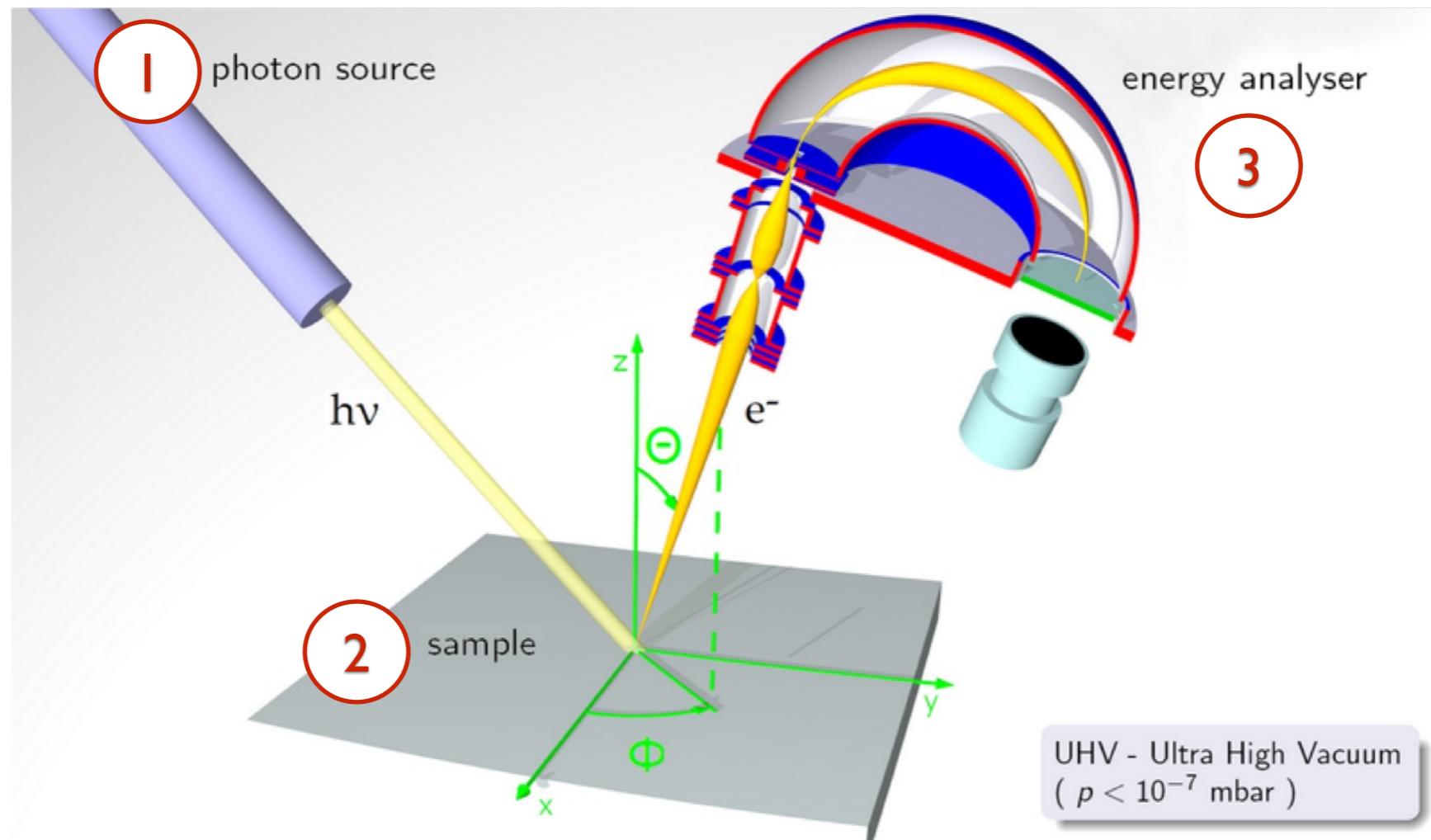
$$m = -1, 0, 1$$

orbital angular momentum of light (chirality of wave front)

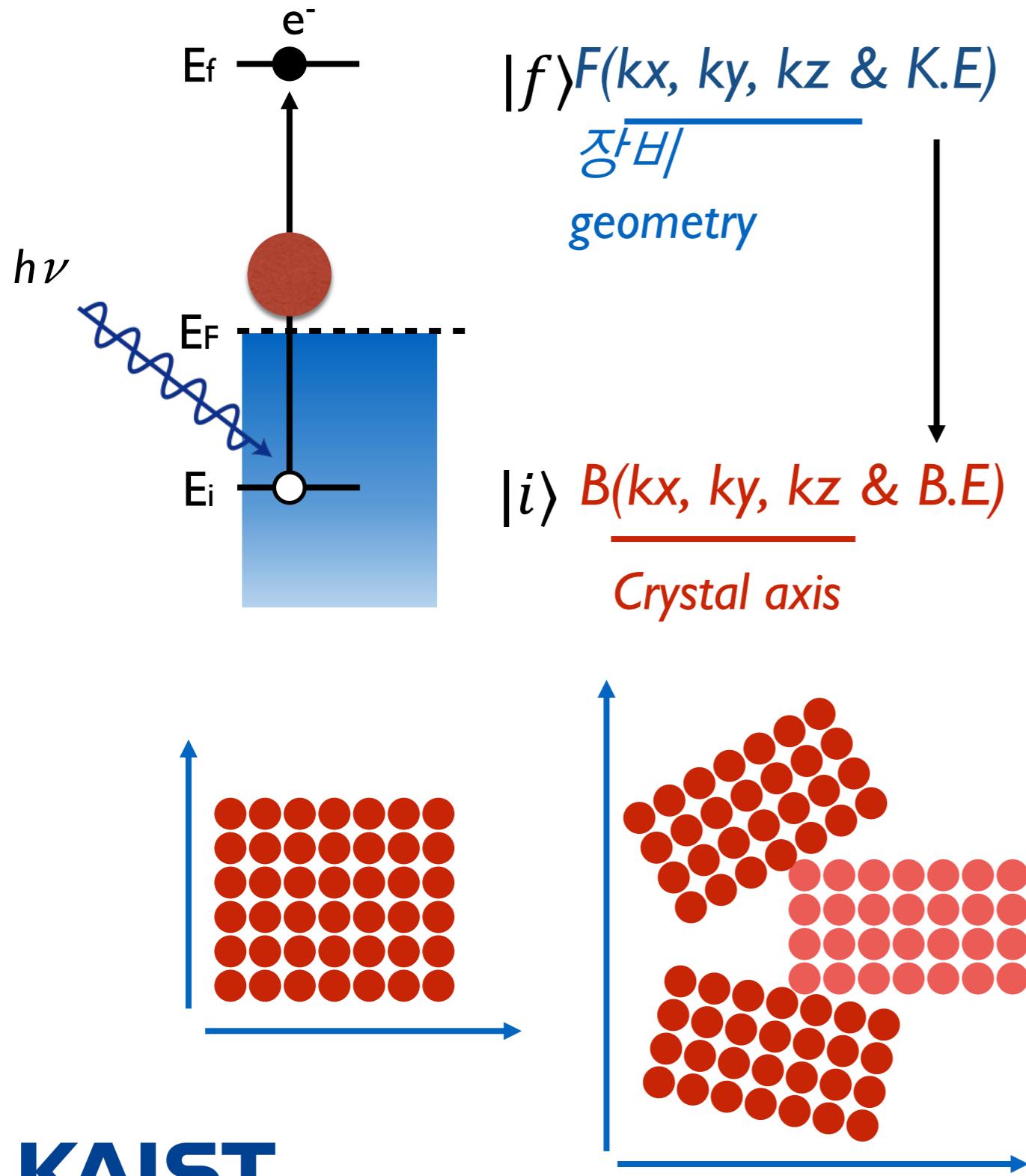
$$m = \dots, -3, -2, 1, 0, 1, 2, 3, \dots$$



심화 - ARPES technique 2/3



시료의 조건, 종류



- ✓ Crystal axis 가 유일하게 정의되어야 함
 - ✓ 단결정 (single crystal),
 - ✓ 에피 박막 (epitaxial thin film)
 - ✓ 2D flake
- ✓ 전기전도도가 있어야 함
 - ✓ Metal (good)
 - ✓ Semiconductor & insulator (possible)
- ✓ 표면이 원자 수준으로 깨끗해야 함
 - ✓ Cleaving
 - ✓ Cleaning (Sputtering, annealing, flashing)

The weakness of ARPES

Unique crystal axis

Must be clean!!!

✓ Number of systems is limited

✓ limited choice of control parameter

✓ ARPES is too much direct

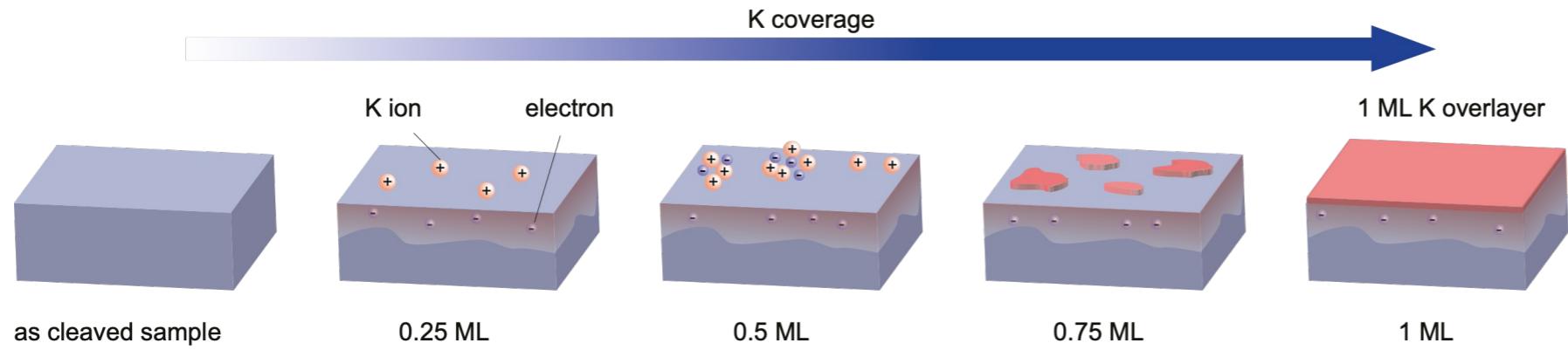
Doping
Pressure
Temperature
Magnetic field
Electric field

Total systems

Single crystal

Clean surface

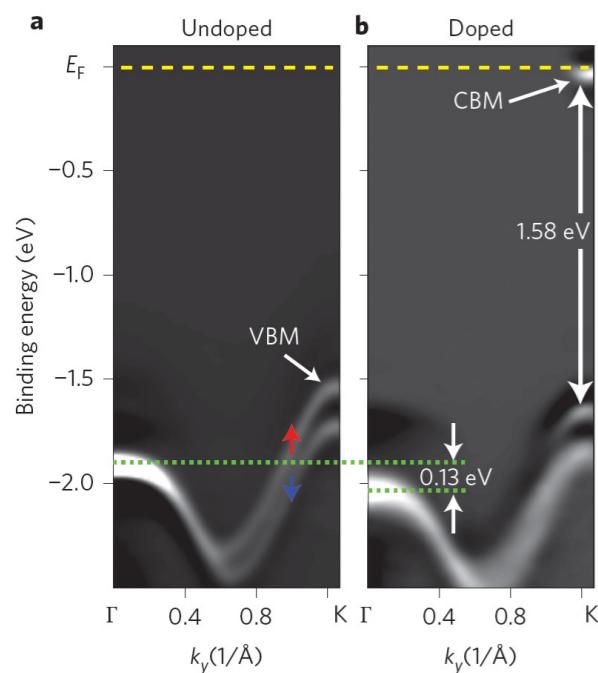
표면 전자 도핑



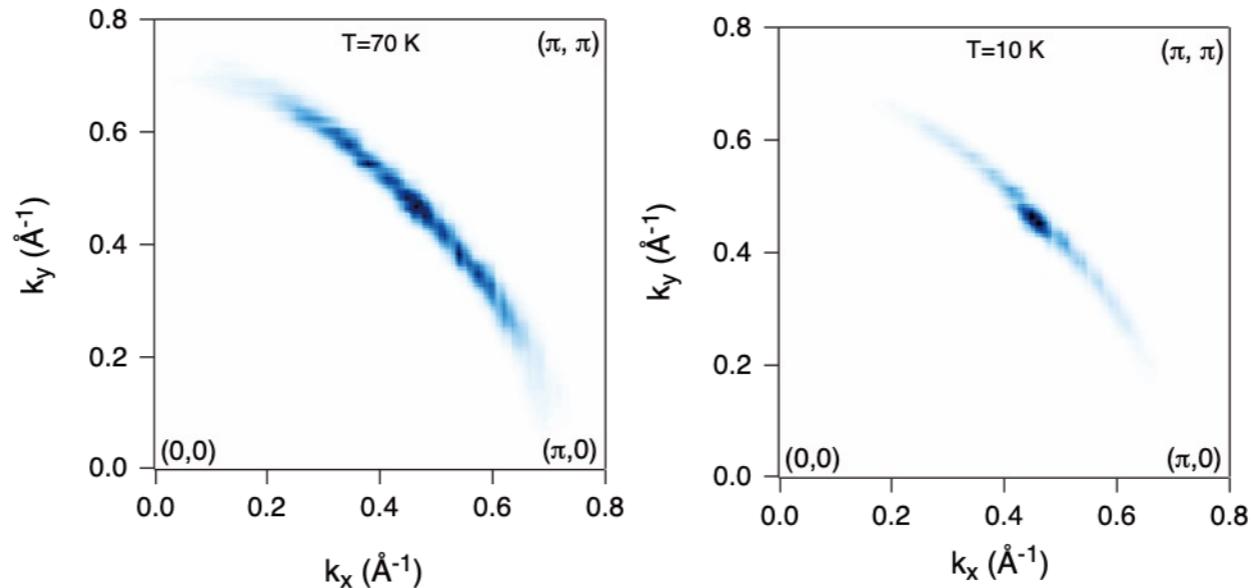
Clean & pure doping
(in lucky case)

No impurity potential
Any or negligible
lattice distortion

Conduction band

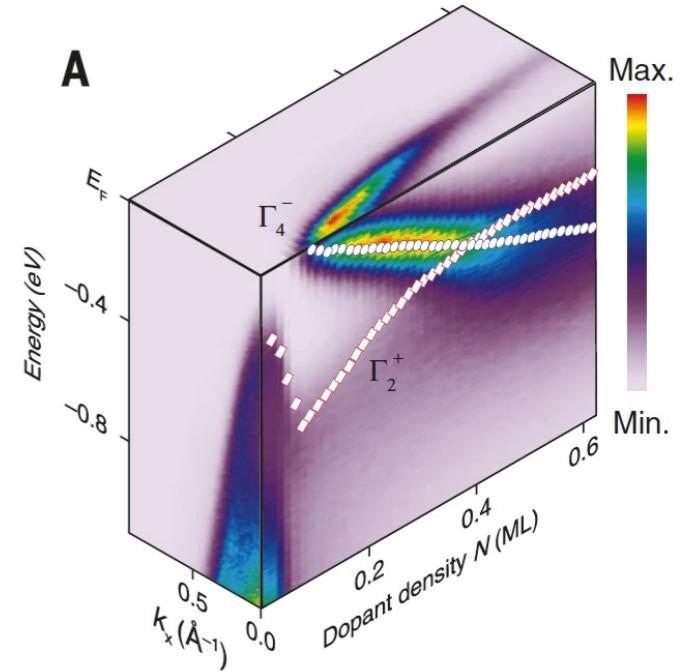


Fermi arc & d-wave node from insulator



Y. K. Kim *et al.*, Nature Phys. **12**, 37-41 (2016)

Band gap tuning

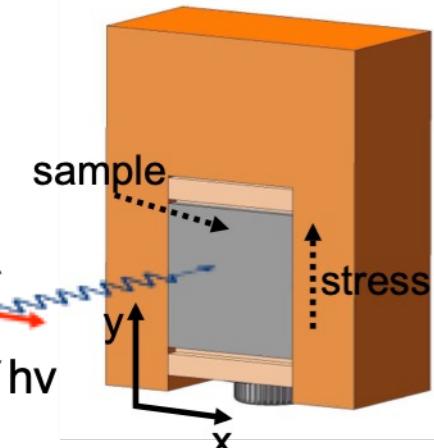
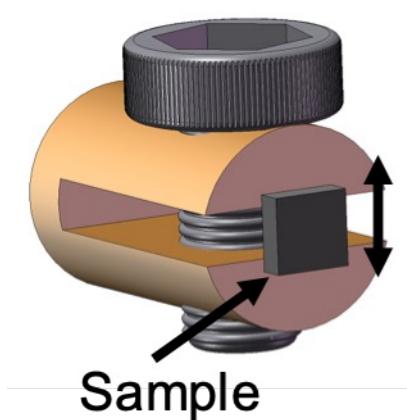


J. Kim *et al.*, Science **349**, 723-726 (2015)

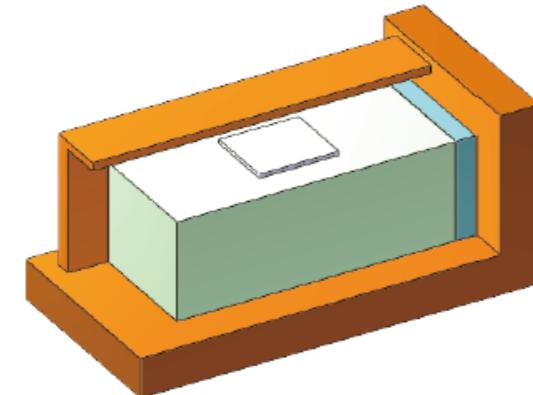
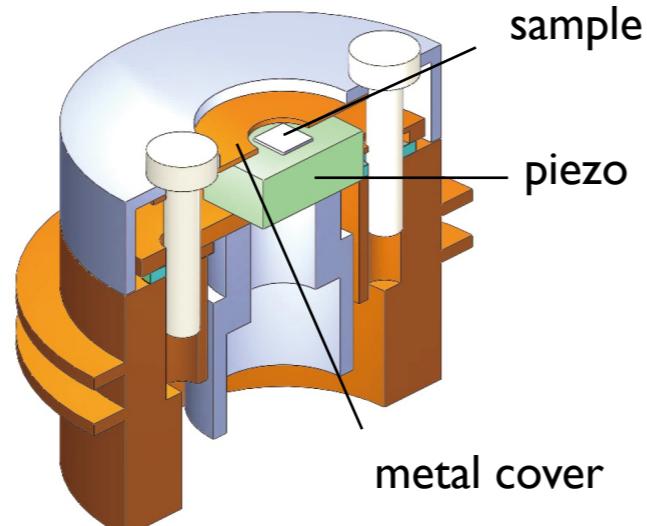
단축 압력 인가

1st type

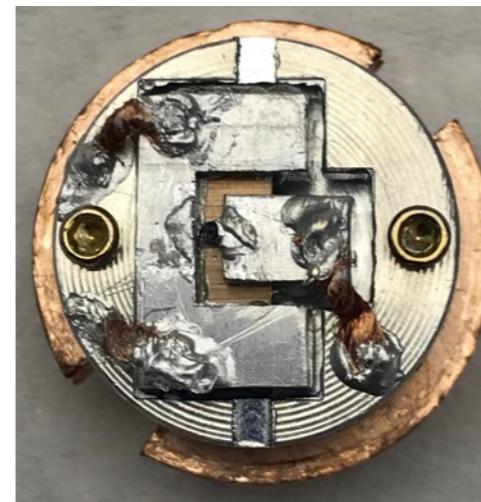
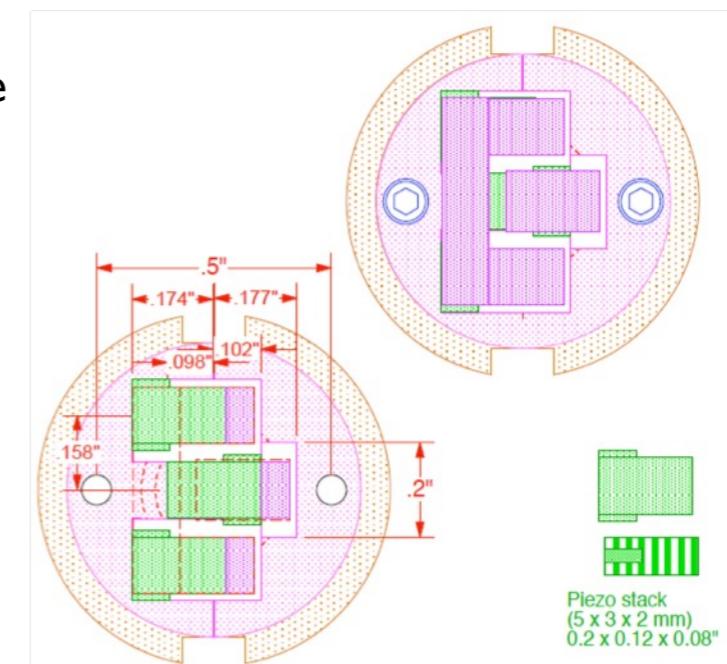
bolt adjustment

2nd type

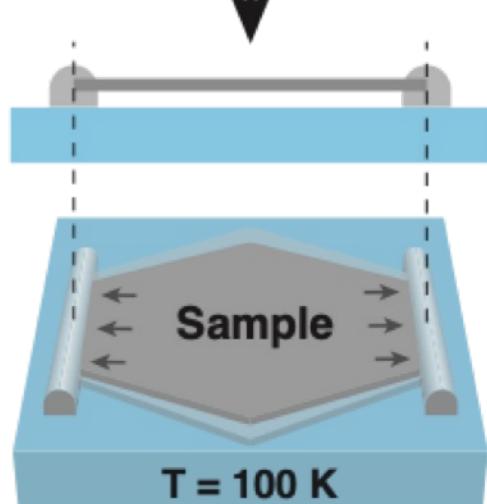
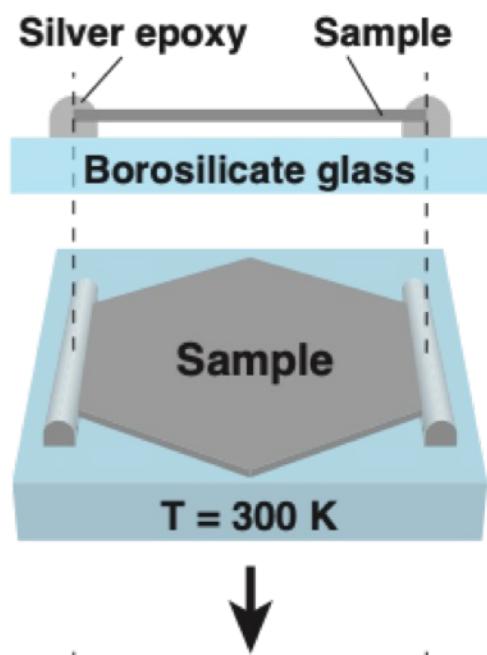
single piezo stack

3rd type

three piezo stack

4th type

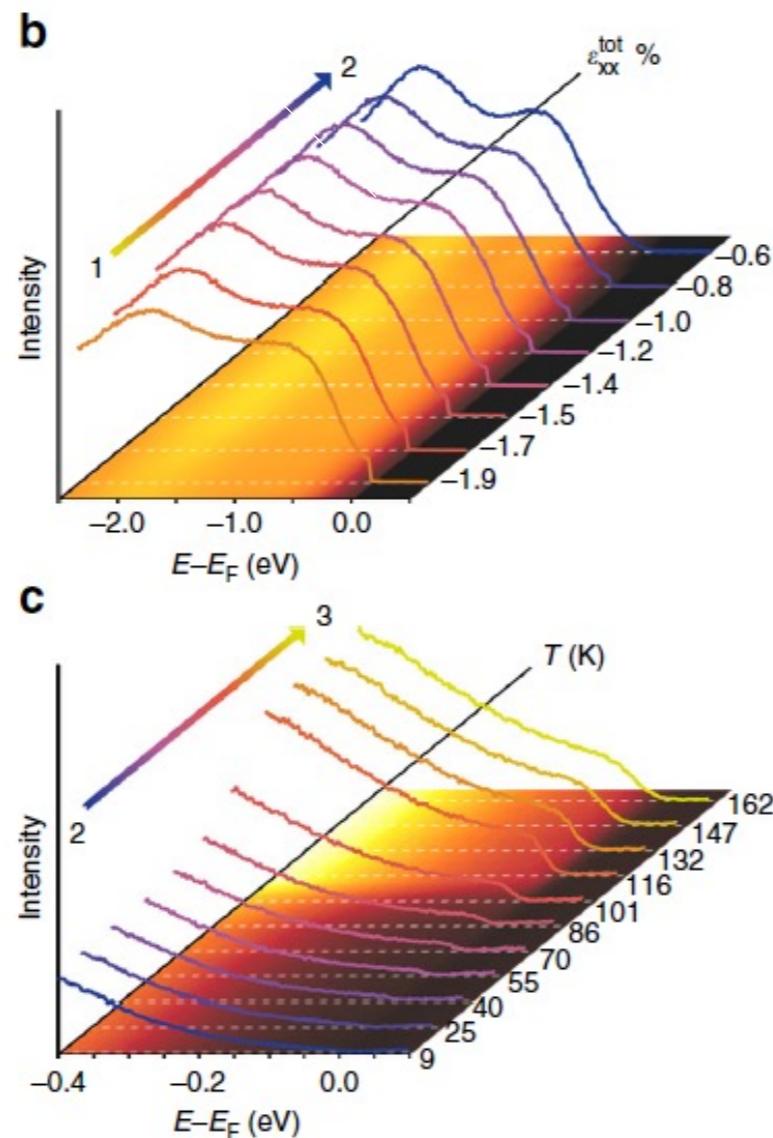
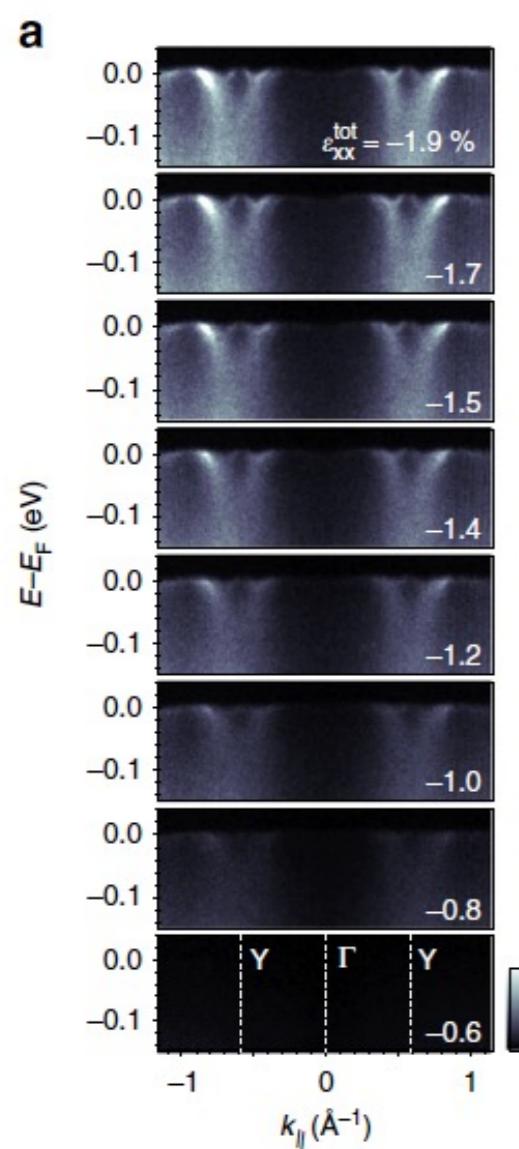
thermal contraction



압력 인가를 활용한 연구 결과

Distorting the local lattice

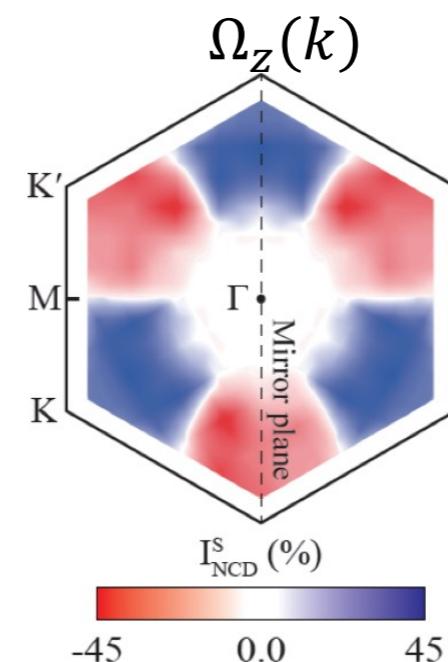
Strain induced metal-insulator transition in Ca_2RuO_4



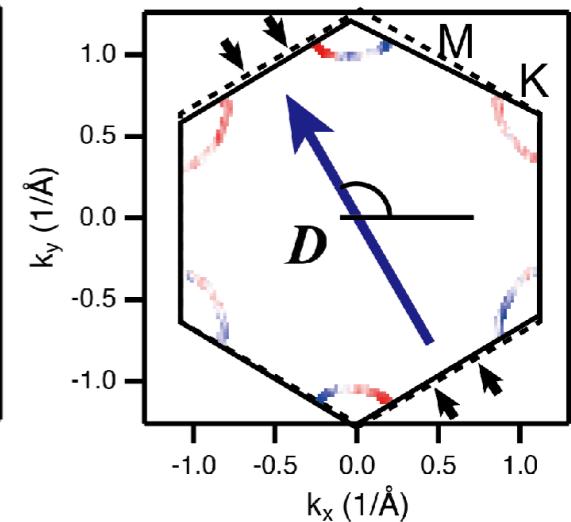
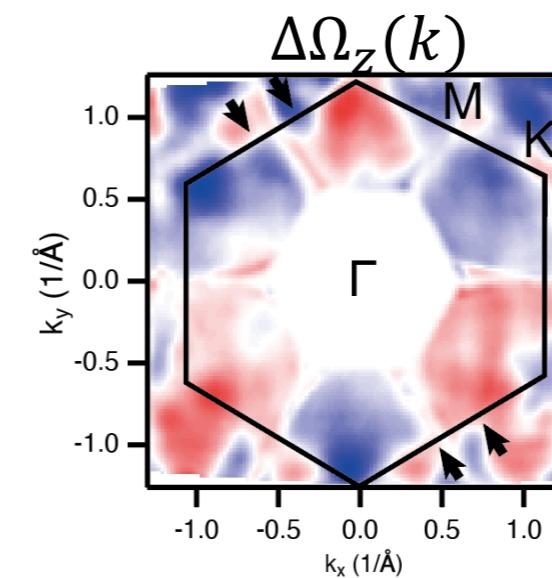
S. Riccò *et al.*, Nat. Comm. **9**, 4535 (2018)

Symmetry breaking

Berry curvature dipole induced by strain

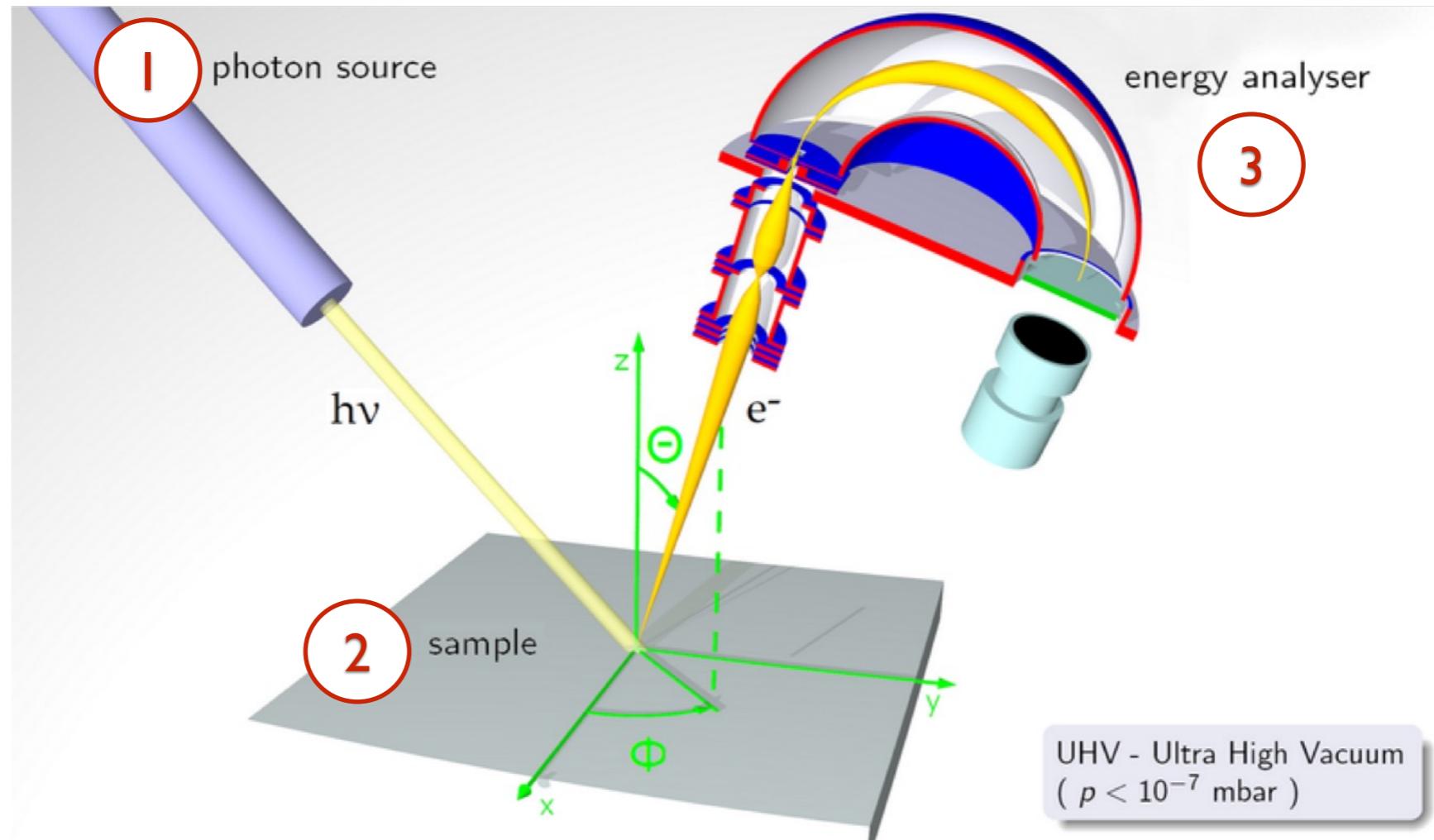


$$D_a = \int_{BZ} \frac{d\mathbf{k}}{(2\pi)^2} f(\mathbf{k}) \partial_{k_a} \Omega_z$$



J. Cha *et al.*, in preparation

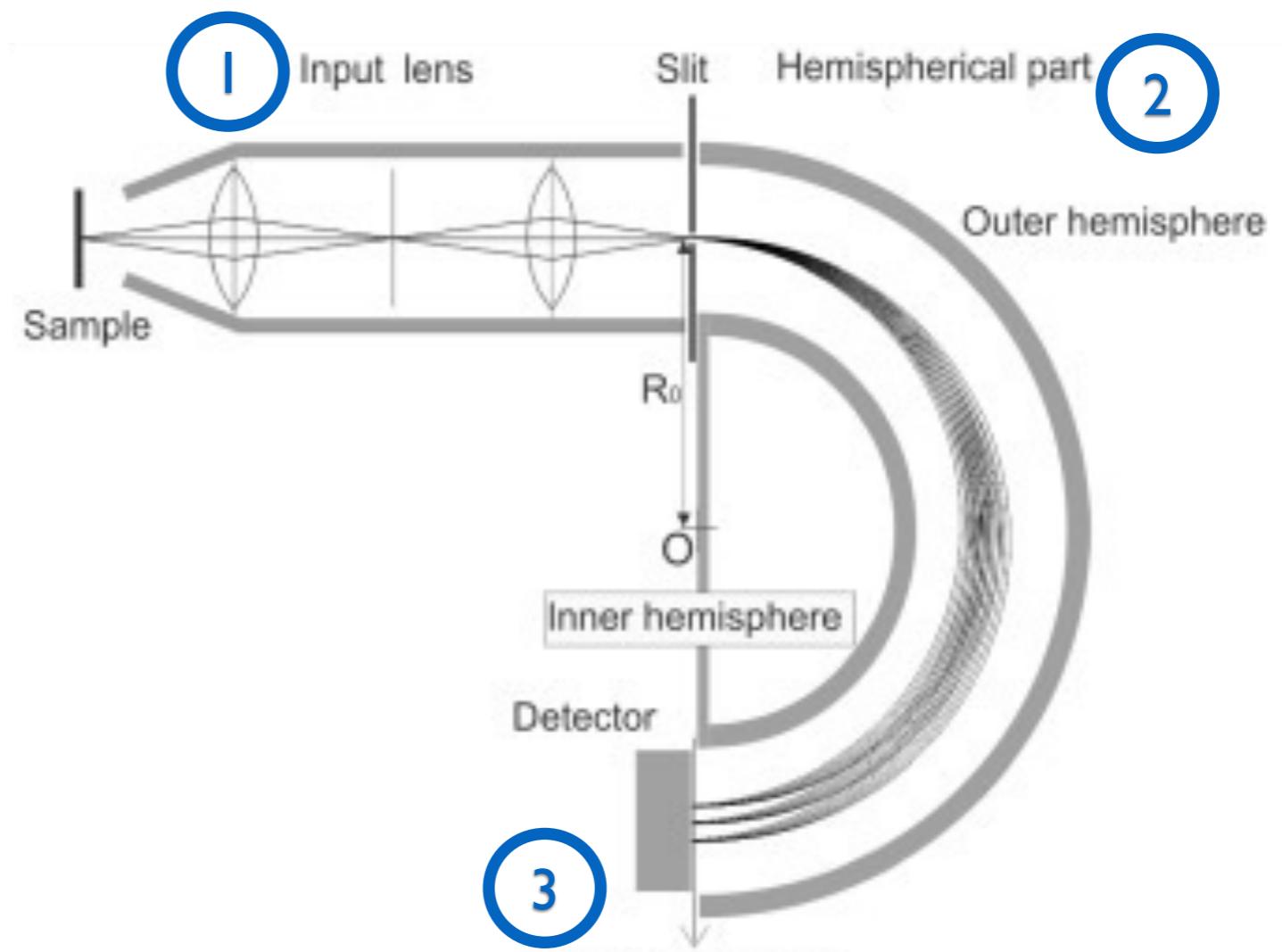
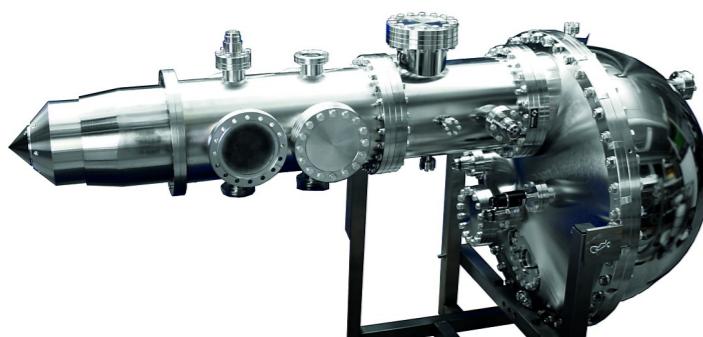
심화 - ARPES technique 2/3



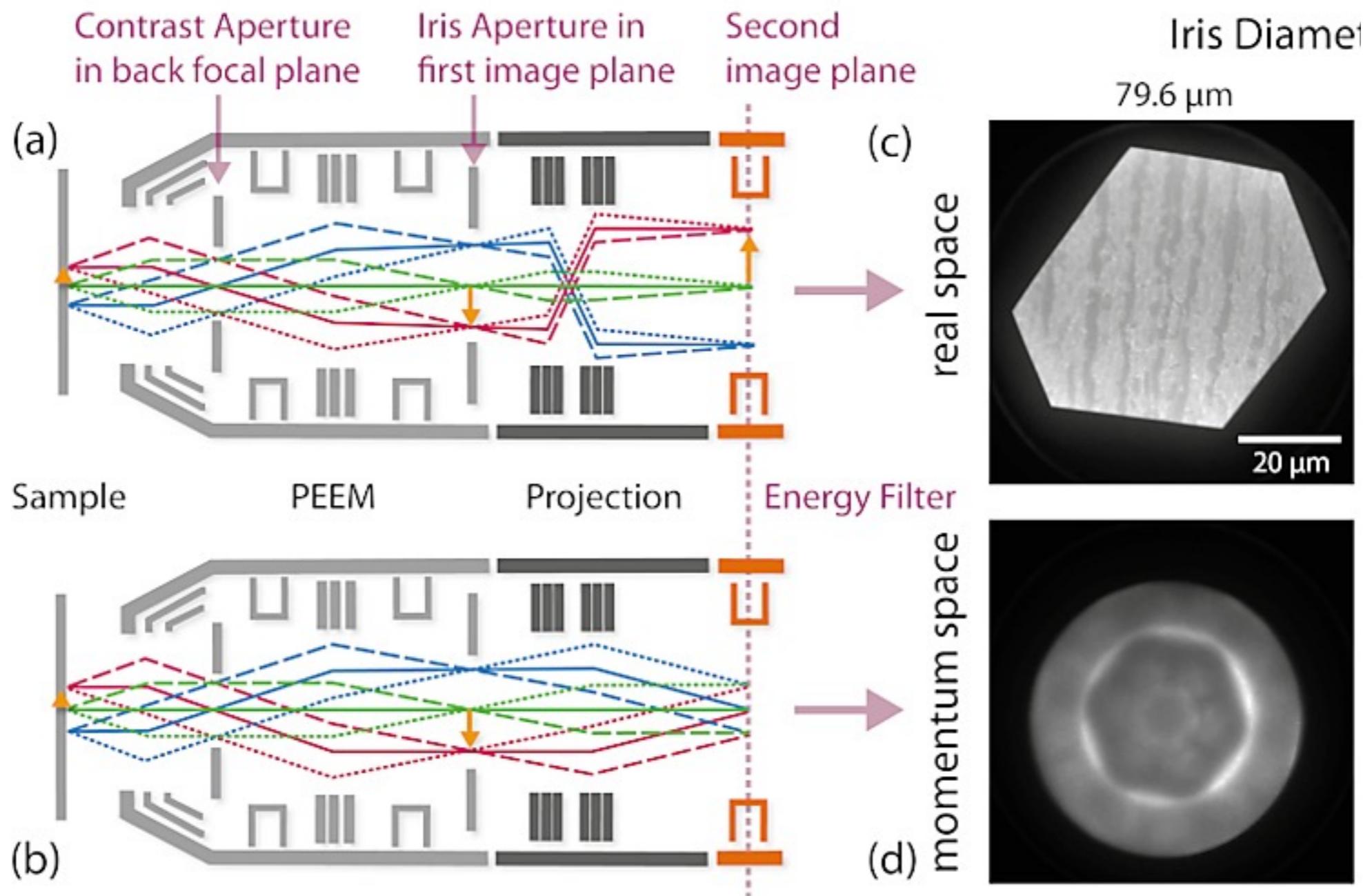
전자 분석기 구성 요소

electron lens + electron prism + electron detector

hemisphere electron analyzer

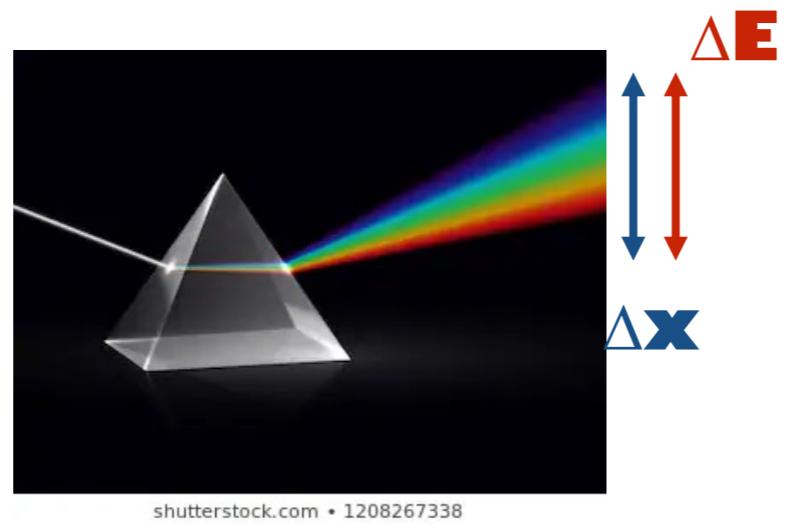


Electron lens - k -PEEM

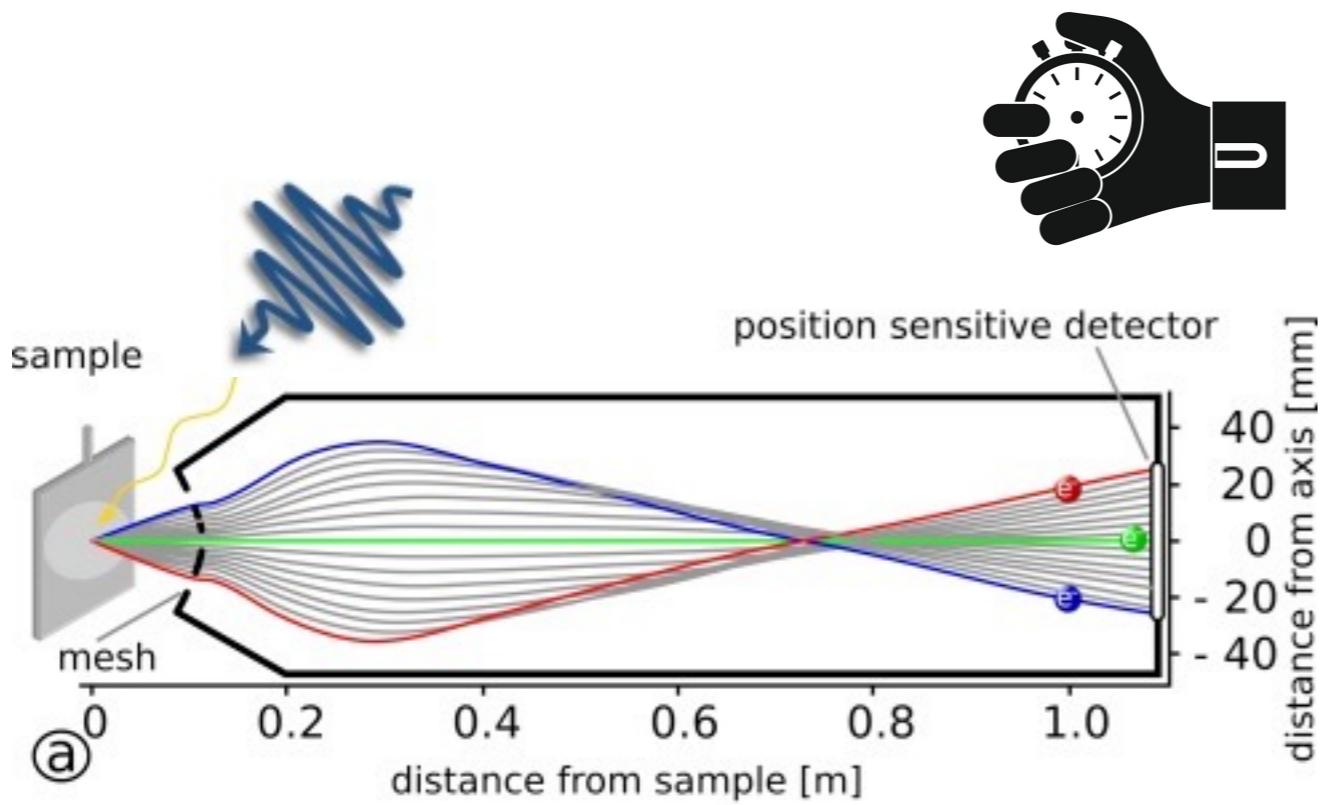
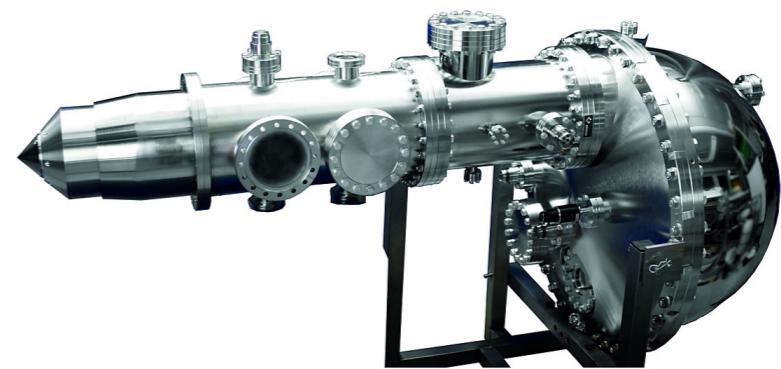


https://www.pro-physik.de/sites/default/files/2019-05/PB_2019_24_27.pdf

Electron Prism - Time of Flight



hemisphere electron analyzer



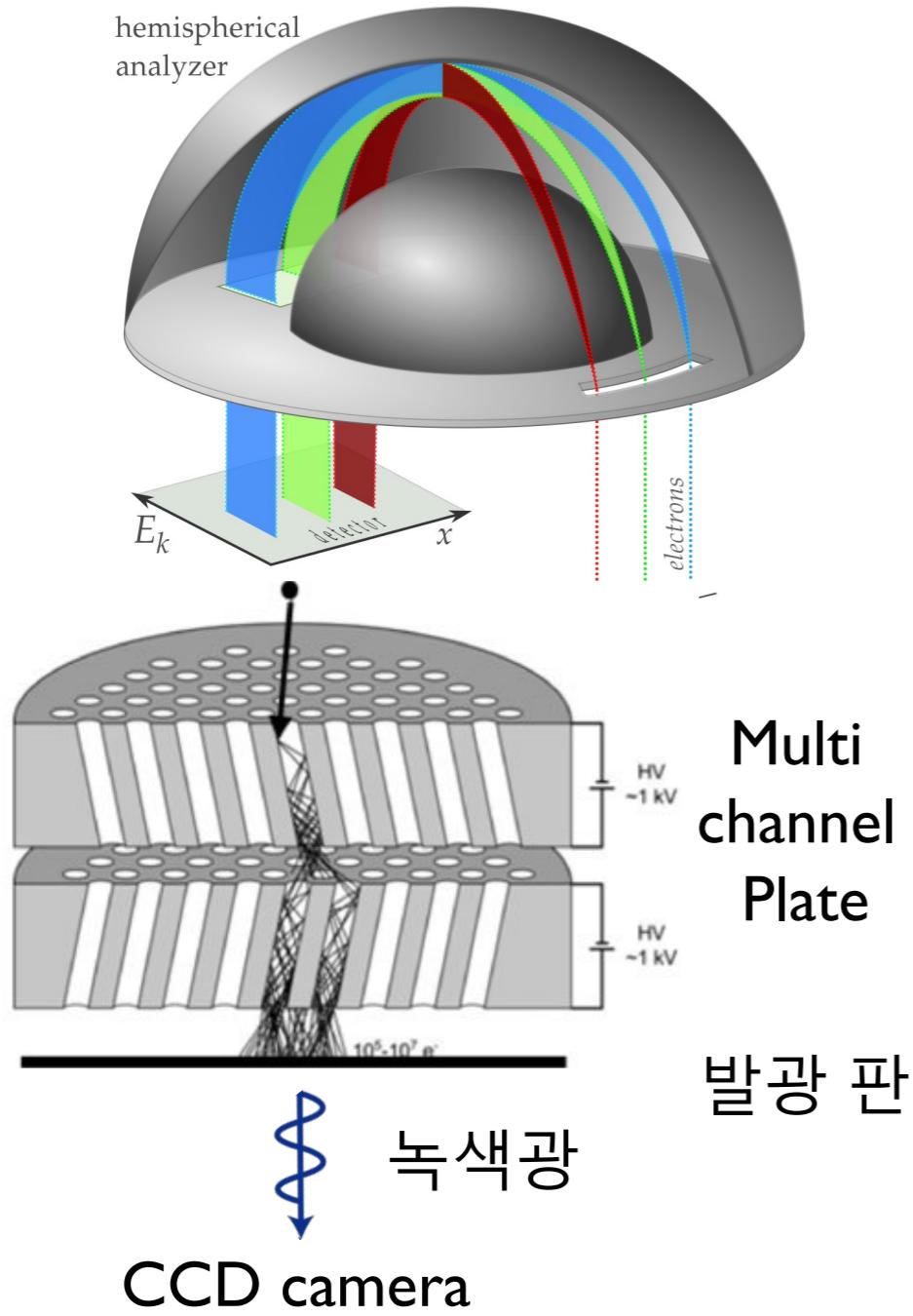
Time of flight electron analyzer



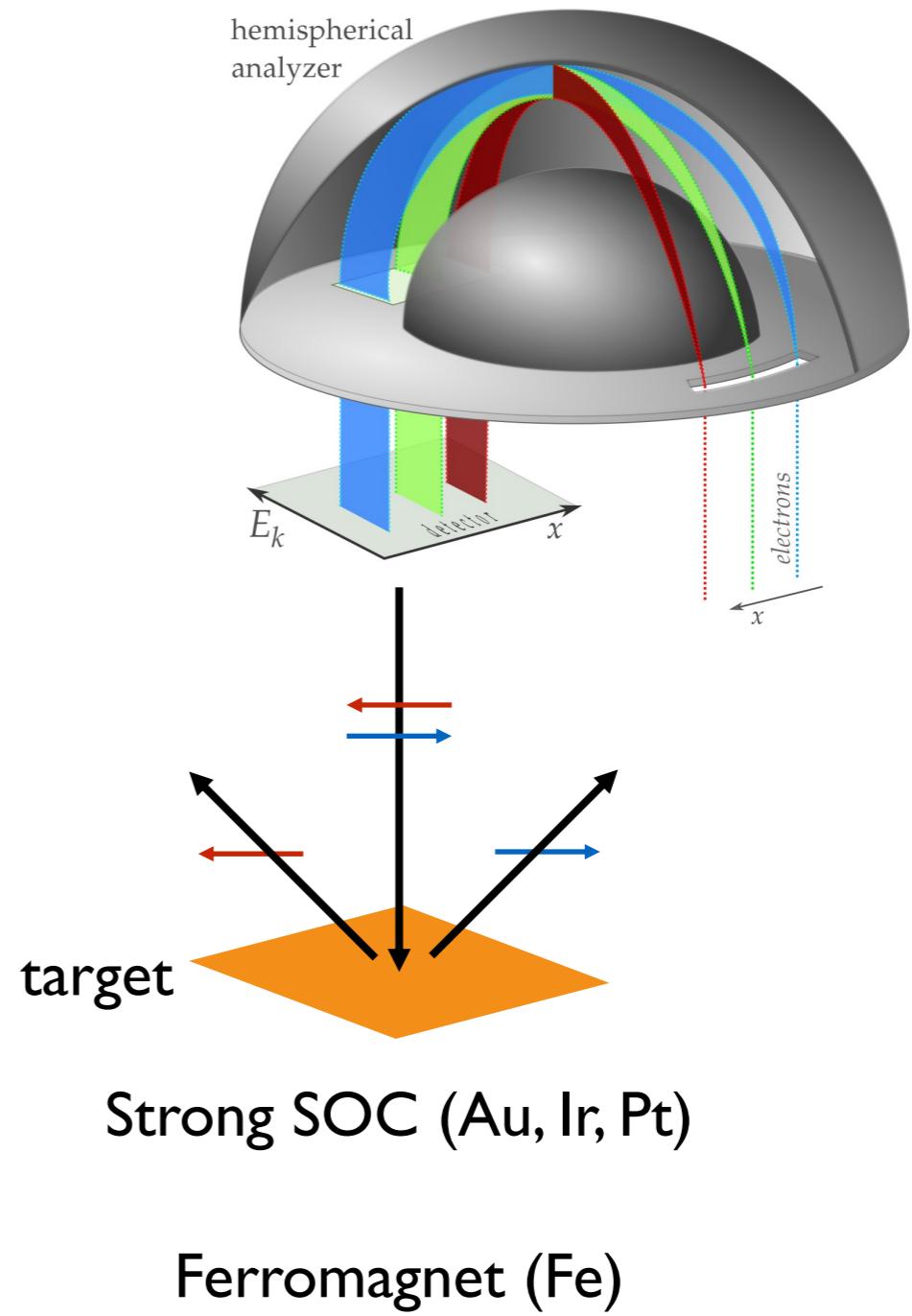
D. Kühn et al., *J. Electron Spectrosc. Relat. Phenom.* **224**, 45-50 (2018)

Electron Detection - spin resolving

기본 측정방법

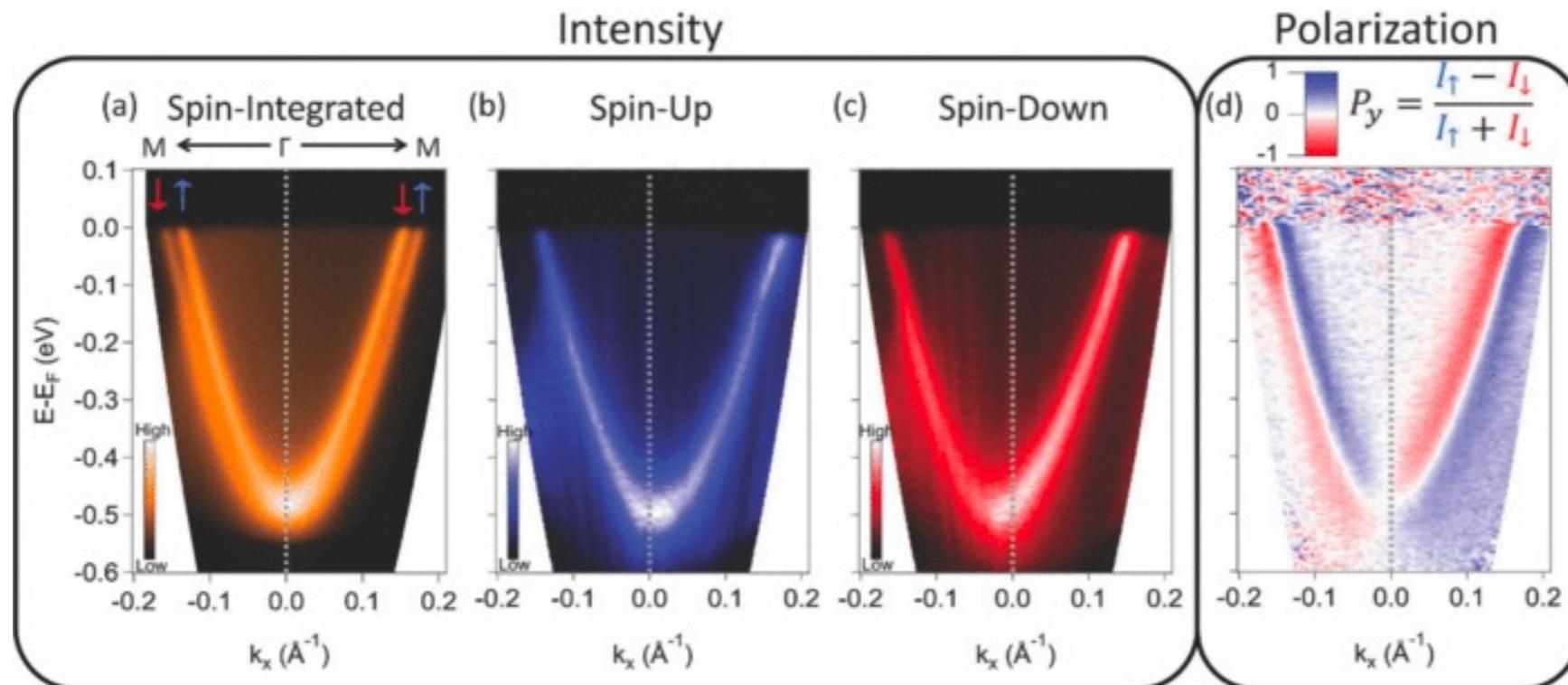


광전자와 spin 정보 측정



Spin-resolved ARPES

Rashba state on Au(111) surface



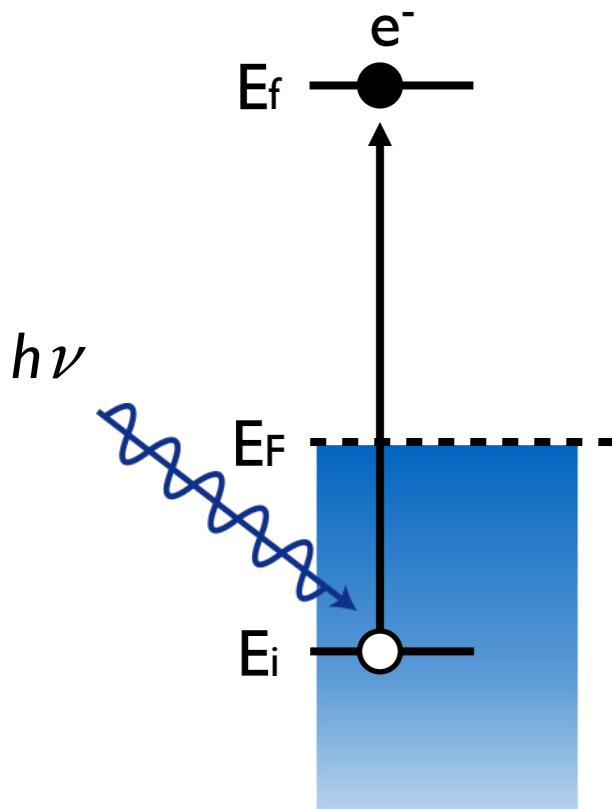
주의: 항상 같다는 보장이 없음

정리

- ✓ 각분해능 광전자 분광의 기초
 - ✓ 광전효과- 각분해능?
 - ✓ 관측법 및 관측결과를 전자구조로 매팅 하는 법
 - ✓ 기본 데이터 읽는 법
- ✓ 심화- ARPES로 얻을 수 있는 정보 / Intensity에 숨겨진 정보
 - ✓ light polarization dependence
 - ✓ Electron self energy info. in ARPES spectrum
- ✓ 심화- ARPES 기법 리뷰
 - ✓ 빛
 - ✓ 샘플
 - ✓ 전자 분광 및 검출

Thank you for your attention

More discussion on $A(\mathbf{k}, \omega)$



$$I(\mathbf{k}, E_{kin}) = \sum_{f,i} w_{f,i} \approx |M(k)|^2 A^-(k, \omega) f(\omega)$$

$$A^\pm(\mathbf{k}, \omega) = \sum_m |\langle \Psi_m^{N\pm 1} | c_\mathbf{k}^\pm | \Psi_i^N \rangle|^2 \delta(\omega - E_m^{N\pm 1} + E_i^N)$$

- ✓ N-I particle systems O/ photo-hole의 존재를 어떻게 느끼는가?
- ✓ Photo-hole O/ 형성되면 주변과 어떻게 상호작용하면서 decay 하지?

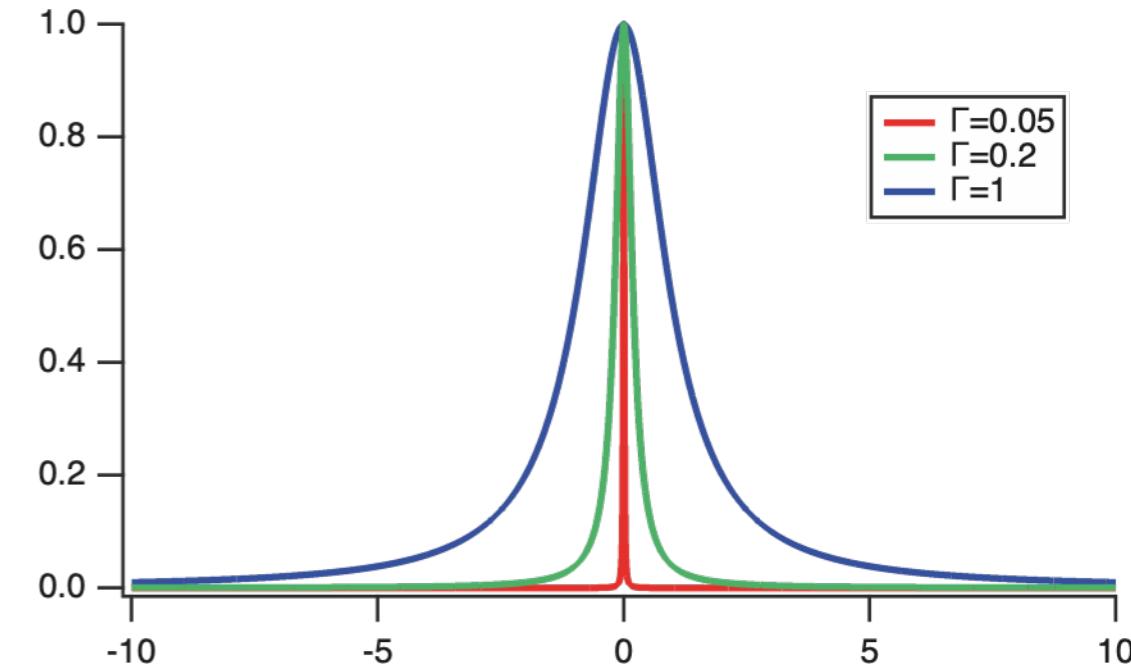
Information built in spectra

$$\omega_{fi} = \frac{2\pi}{\hbar} \left| \langle f | \vec{A} \cdot \vec{p} | i \rangle \right|^2 \delta(E_f - E_i - h\nu)$$

$$\Delta E \rightarrow 0 \quad \Delta t \rightarrow \infty$$

$$(\Delta E \Delta t \geq \hbar)$$

$$\delta(\omega - \omega') = \lim_{\Gamma \rightarrow 0} \frac{1}{\pi} \frac{\Gamma^2}{(\omega - \omega')^2 + \Gamma^2}$$



$$A(\omega - \omega') = \frac{1}{\pi} \frac{\Gamma}{(\omega - \omega')^2 + \Gamma^2} = \frac{1}{\pi} \text{Im} \underbrace{\frac{1}{\omega - \omega' + i\Gamma}}_{\text{Green's function}} = \frac{1}{\pi} \text{Im} G_0(\omega - \omega')$$

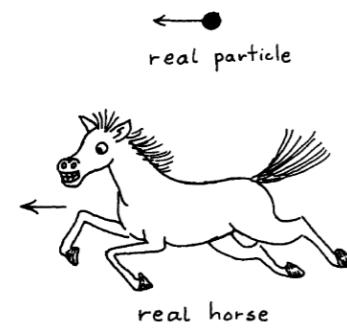
$$A(\mathbf{k}, \omega) = \frac{1}{\pi} \text{Im} \frac{1}{\omega - \epsilon_{\mathbf{k}} + i\Gamma} = -\frac{1}{\pi} \text{Im} G_0(\mathbf{k}, \omega)$$

Green's function

Interaction information built in the self-energy

Non-interacting particle

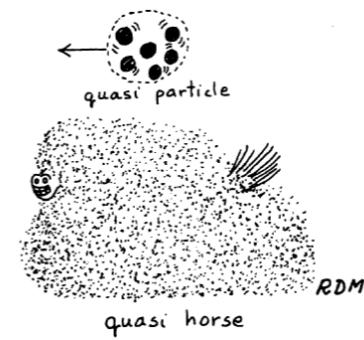
$$G_0(\mathbf{k}, \omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} + i\Gamma}$$



*life time
(real number)*

Interacting particle

$$G(\mathbf{k}, \omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} + \Sigma}$$

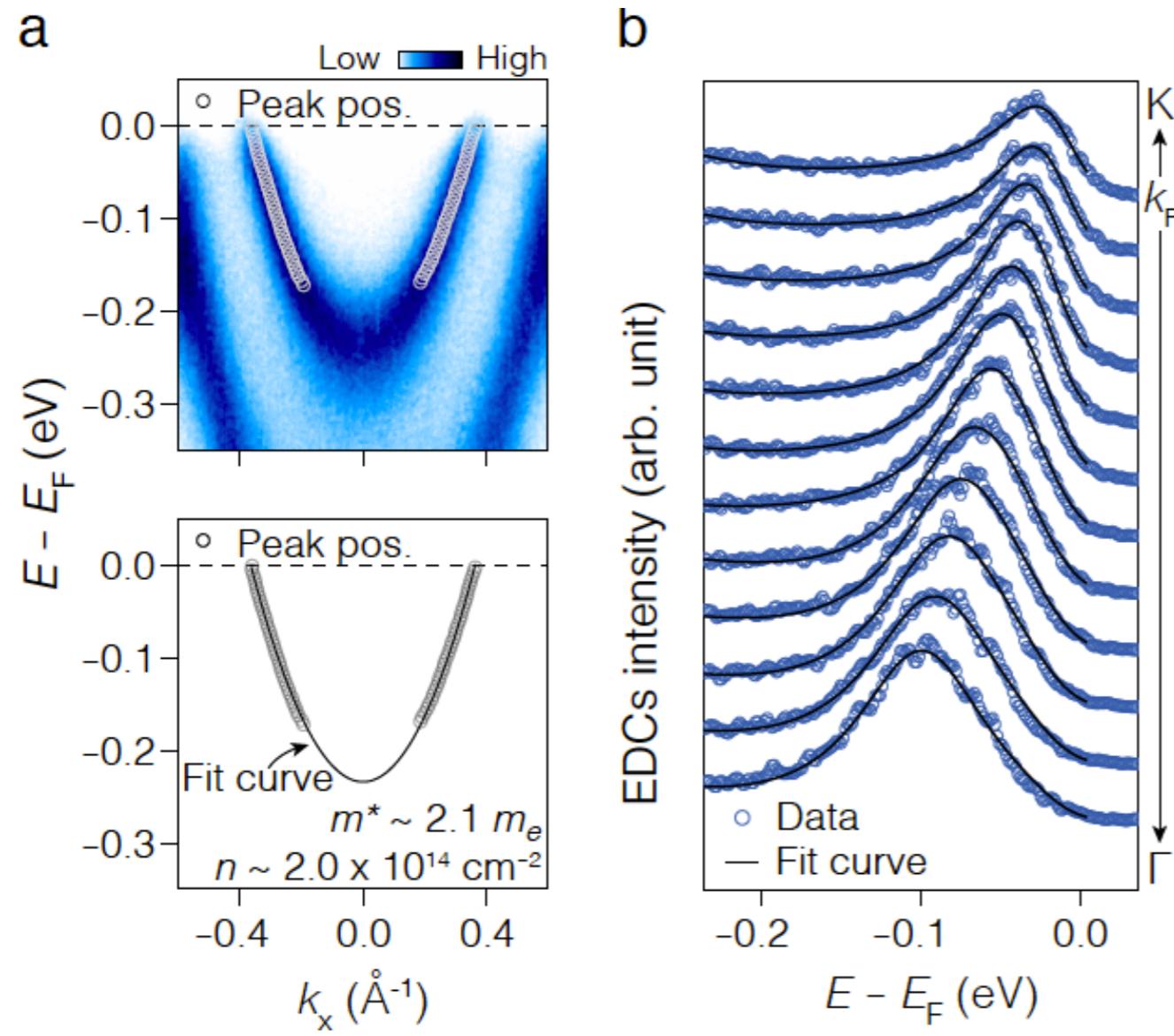


*self-energy
(complex function)*

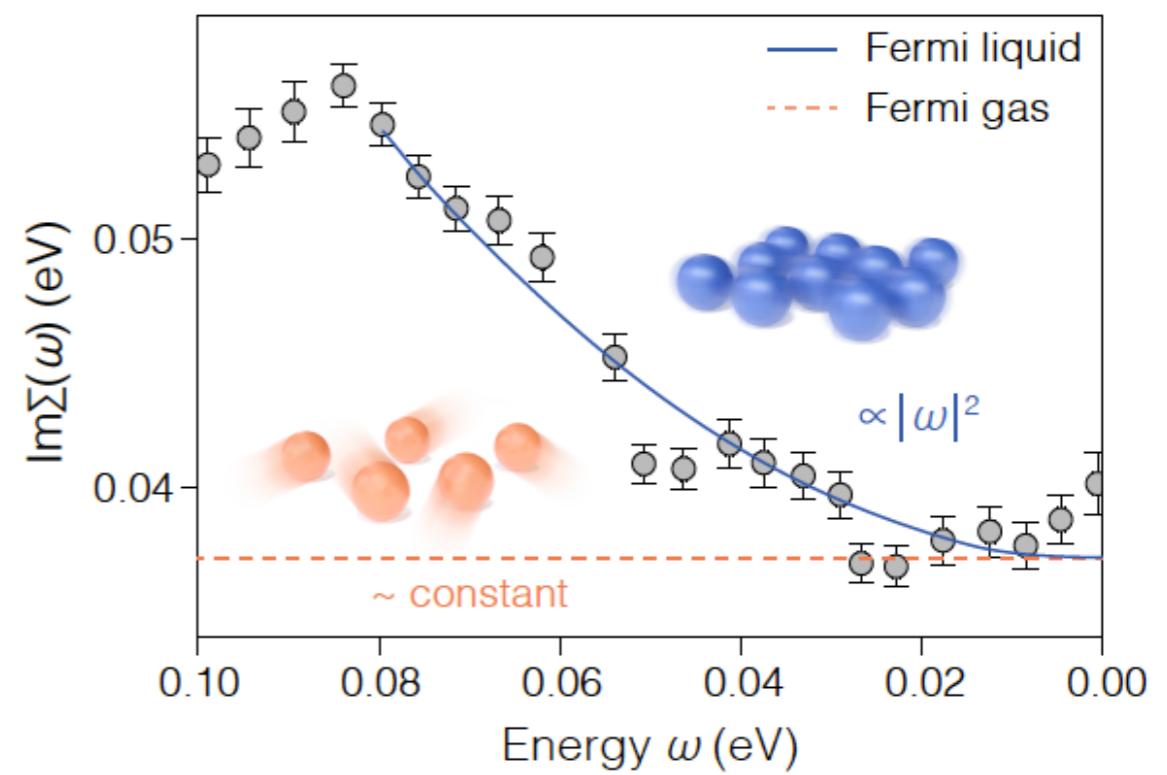
$$\Sigma(\mathbf{k}, \omega) = \Sigma'(\mathbf{k}, \omega) + i\Sigma''(\mathbf{k}, \omega) = \Sigma_{imp} + \Sigma_{e-ph} + \Sigma_{e-e}$$

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} G(\mathbf{k}, \omega) = -\frac{1}{\pi} \frac{\Sigma''(\mathbf{k}, \omega)}{[\omega - \epsilon_{\mathbf{k}} - \Sigma'(\mathbf{k}, \omega)]^2 + [\Sigma''(\mathbf{k}, \omega)]^2}$$

Example: e-e interaction

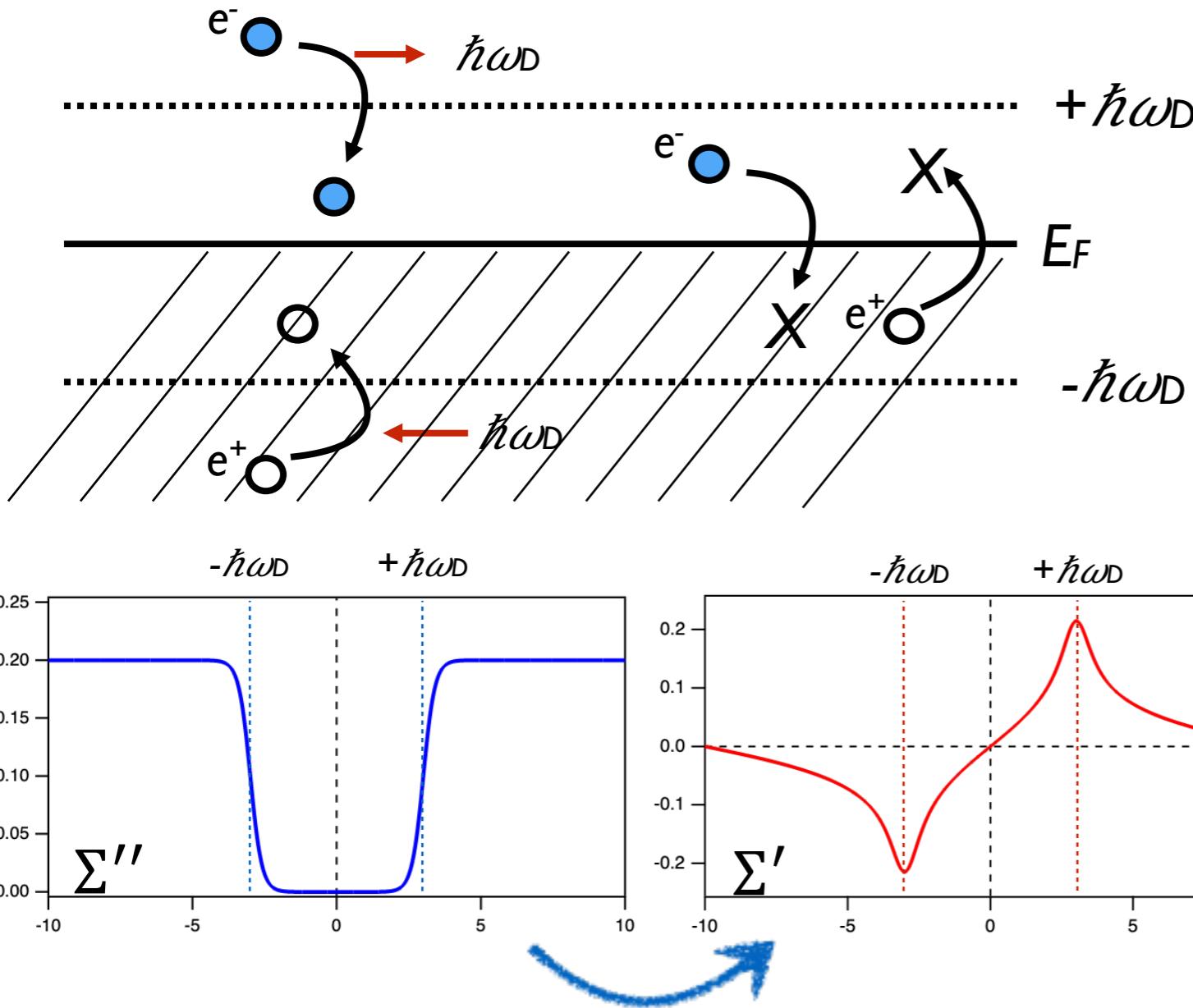


$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \frac{\Sigma''(\mathbf{k}, \omega)}{[\omega - \epsilon_{\mathbf{k}} - \Sigma'(\mathbf{k}, \omega)]^2 + [\Sigma''(\mathbf{k}, \omega)]^2}$$



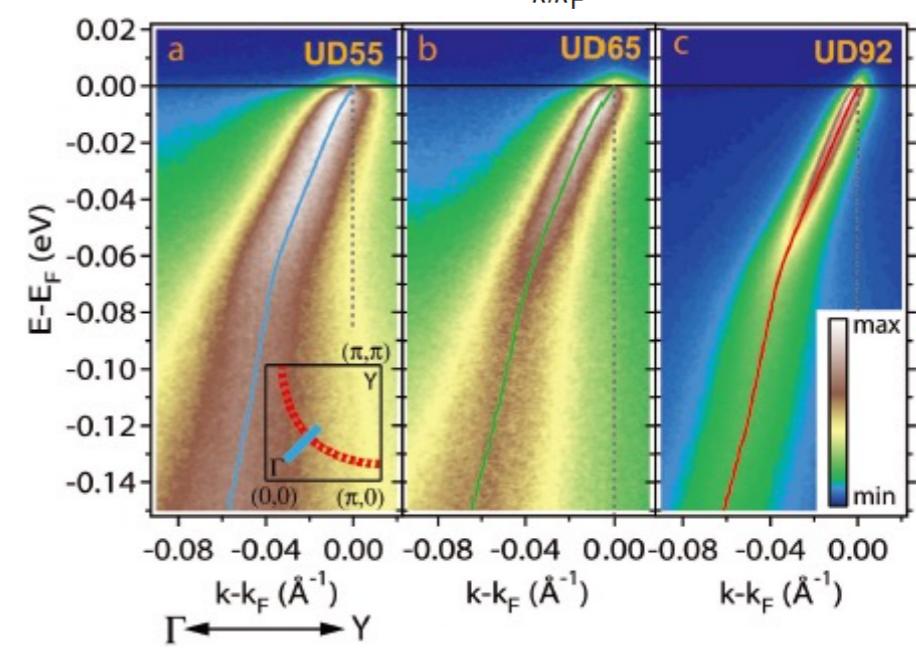
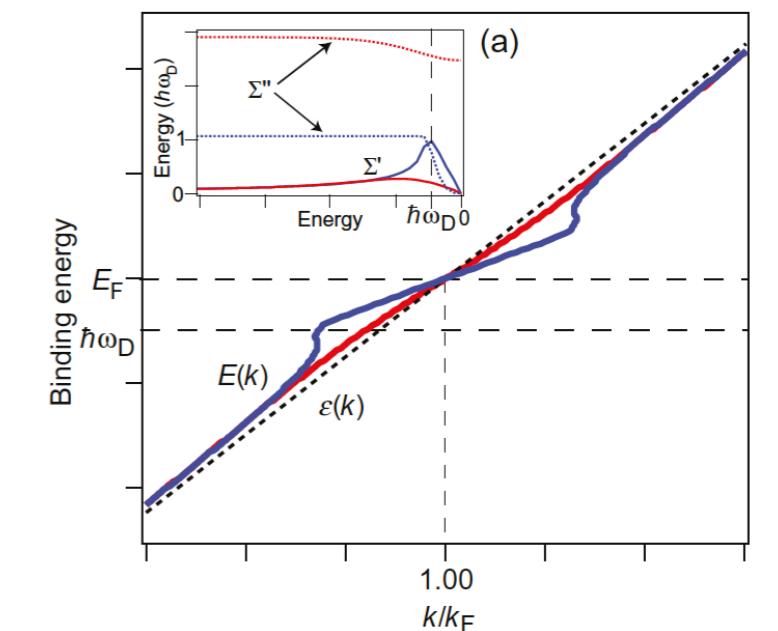
Example: e-phonon interaction

Let's consider an interaction with phonon



Kramers-Kronig relation, Hilbert transform

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \frac{\Sigma''(\mathbf{k}, \omega)}{[\omega - \epsilon_{\mathbf{k}} - \Sigma'(\mathbf{k}, \omega)]^2 + [\Sigma''(\mathbf{k}, \omega)]^2}$$



I. M. Vishik *et al.*, PRL 104, 207002 (2010)

More on $M(k)$: three-step vs. one-step model

$$M(k) = \langle f | A \cdot p | i \rangle = \langle f | e \cdot r | i \rangle$$

free electron *Atomic state*

