Ultra high-resolution Compton scattering

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Collaborators

- Compton scattering on graphite

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- Compton scattering on Li

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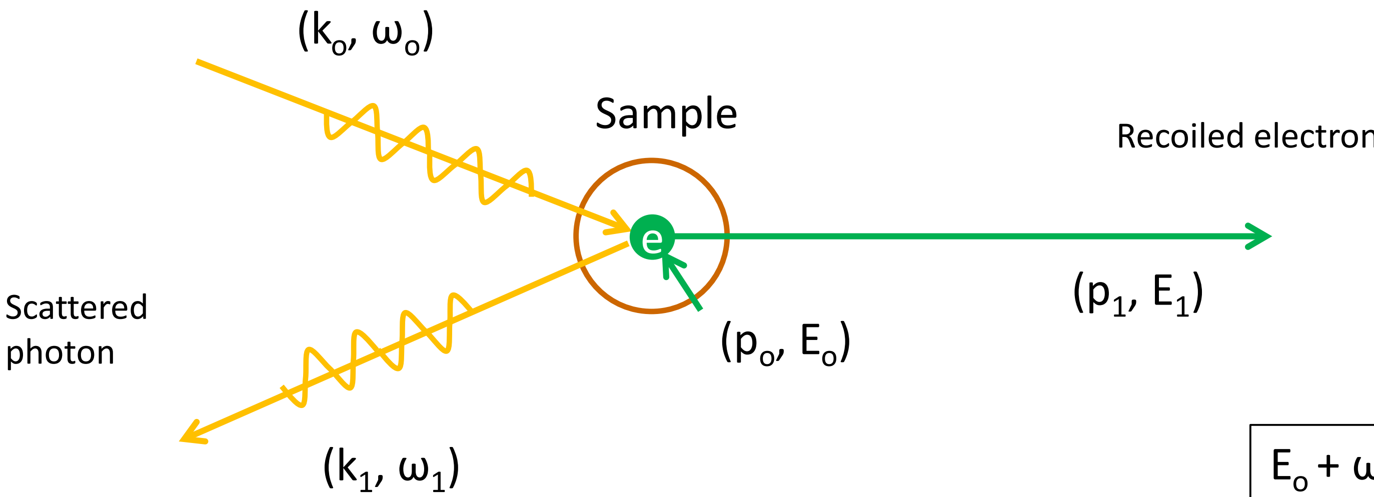
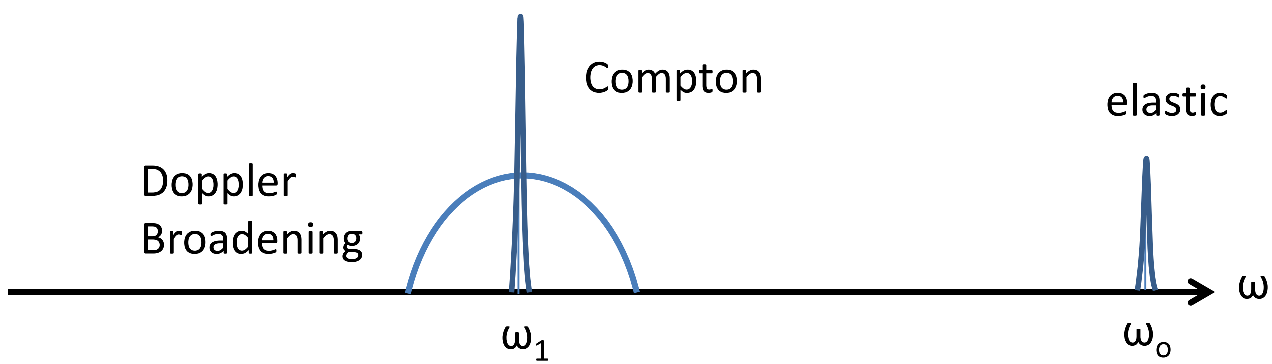
Markus Holzmann (ESRF)

Compton scattering



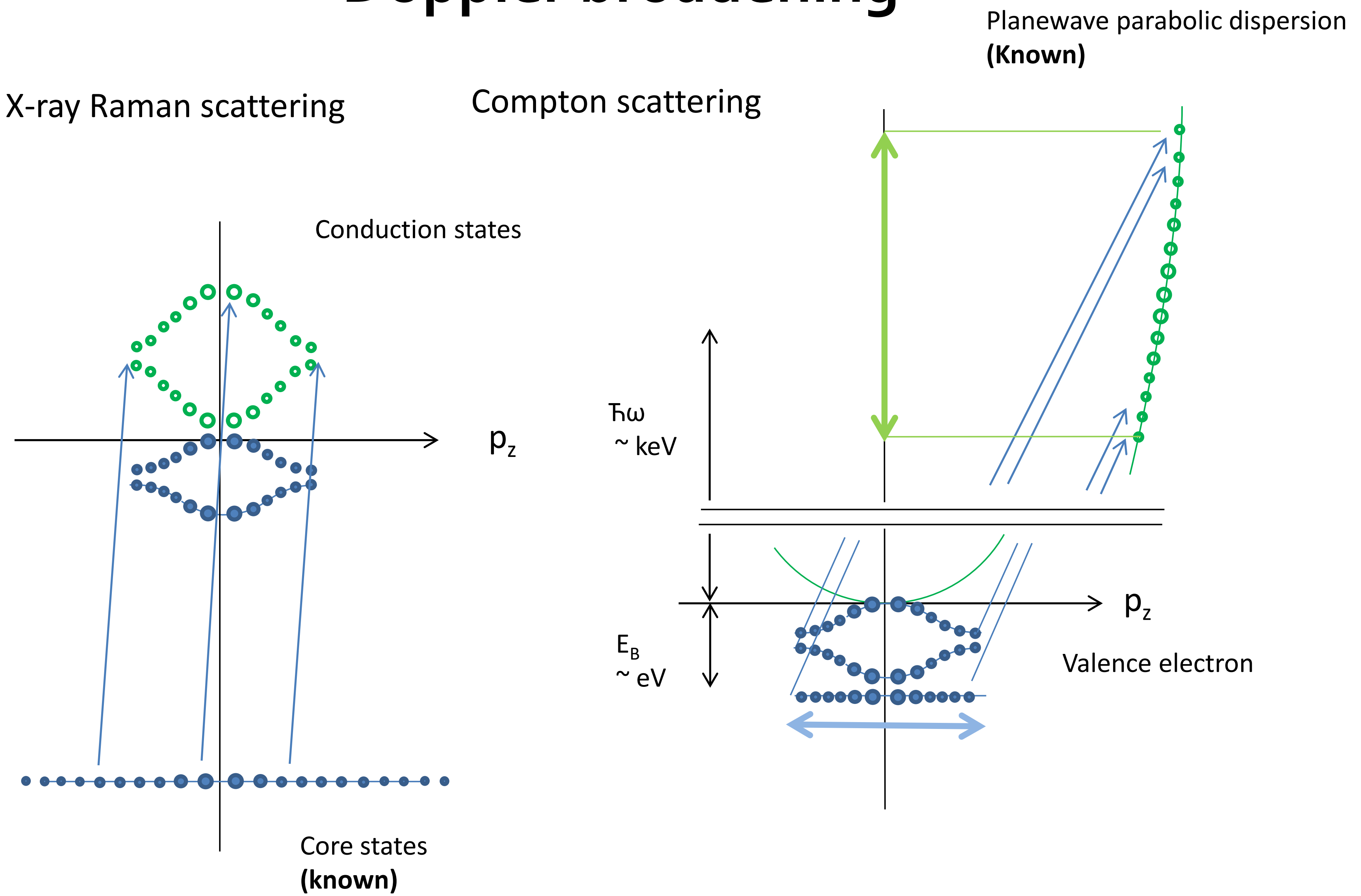
$$\boxed{\begin{aligned} &E_o + \omega_o = E_1 + \omega_1 \\ &\mathbf{p}_o + \mathbf{k}_o = \mathbf{p}_1 + \mathbf{k}_1 \end{aligned}}$$



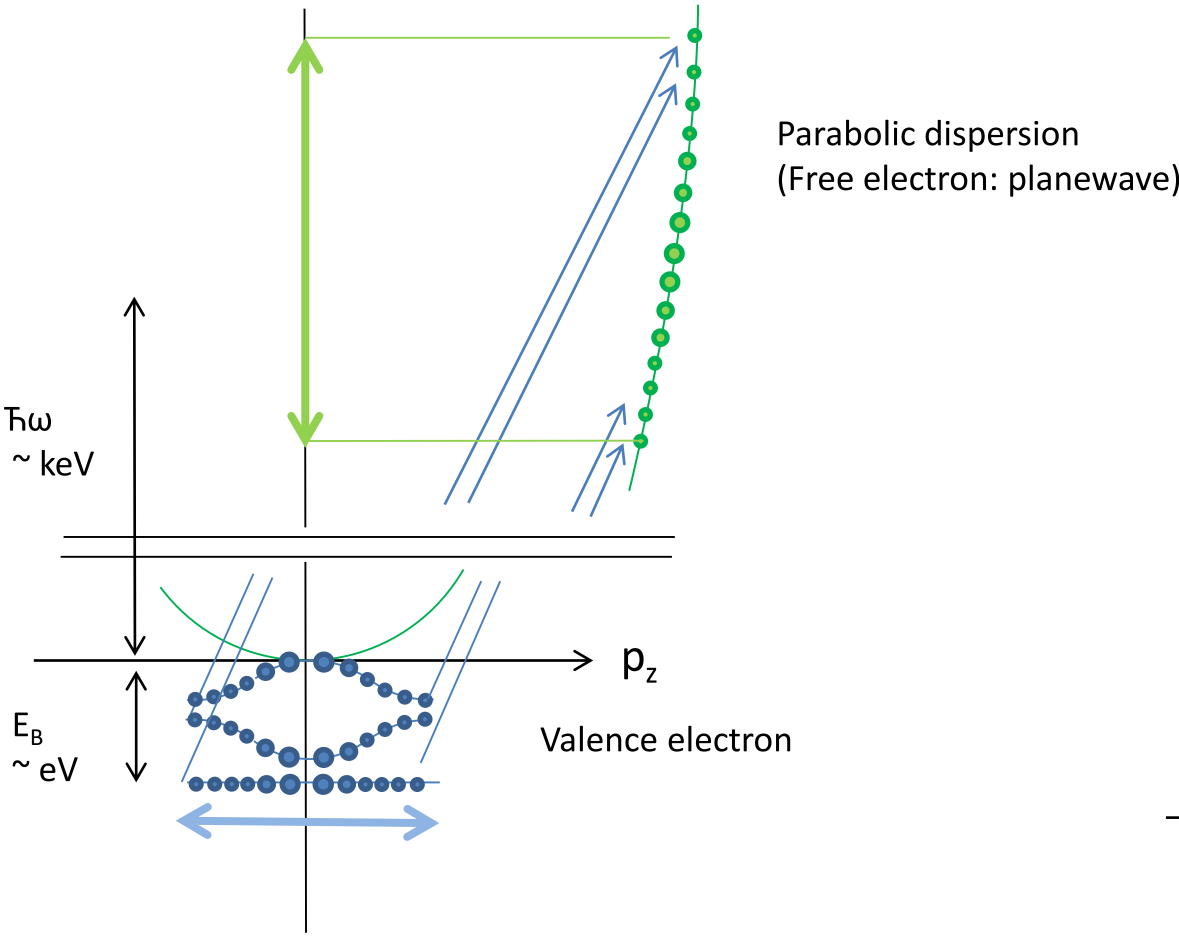
$$\omega_1 = \frac{\omega_o}{1+(\omega_o/mc^2)\,(1+\cos\theta)} + \frac{\mathbf{p}_o \cdot \mathbf{K}/m}{1+(\omega_o/mc^2)\,(1+\cos\theta)}$$

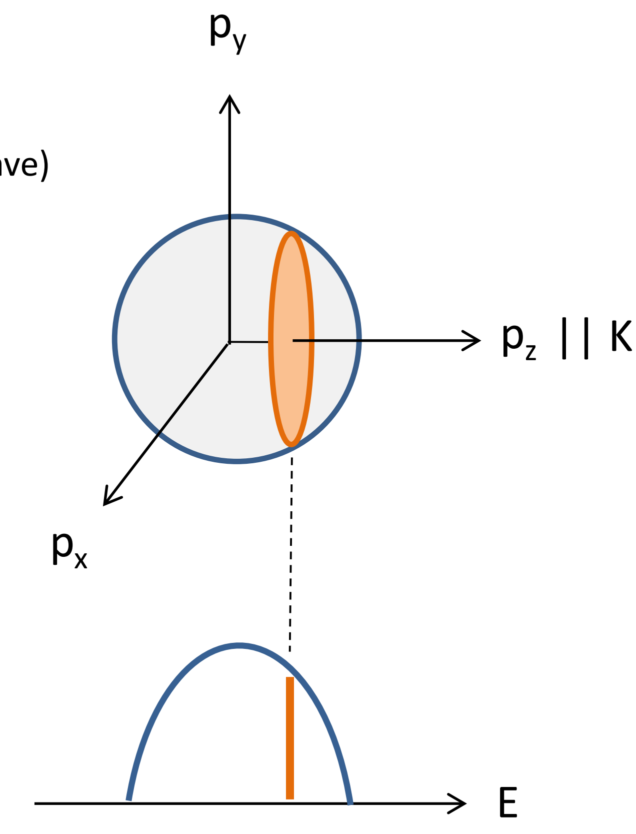
$p_o=0$ $\qquad$ $p_o \neq 0$

Doppler broadening



Compton Profile





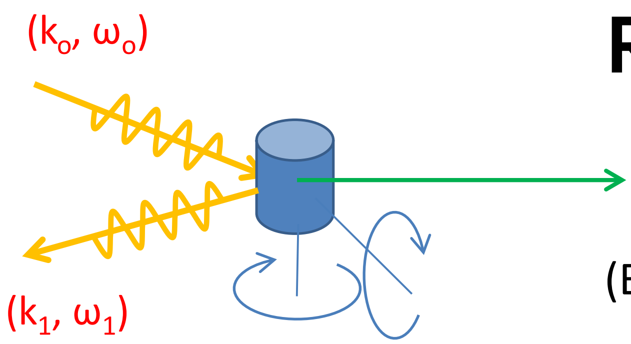
$J(p_z) \propto \iint n(\mathbf{p})dp_x dp_y$

Compton Profile

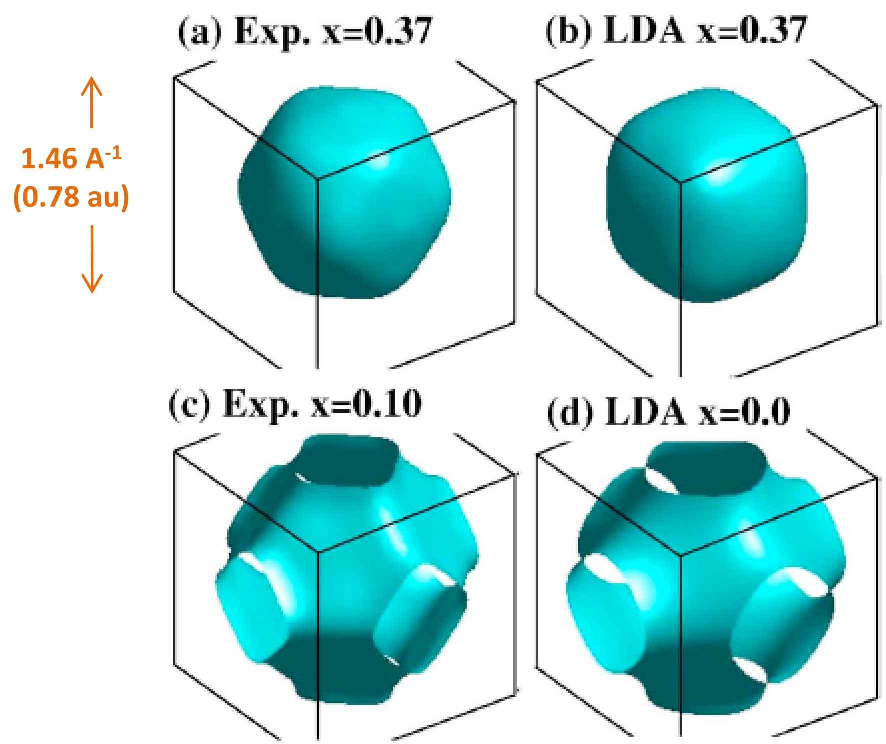
Key facts :

- ✓ $\hbar\omega >> E_B$ Impulse approximation : $E_B \rightarrow 0$
- ✓ One dimensional information along q , $J(dp_z) \rightarrow$ Reconstruction to get n(p)

Reconstruction

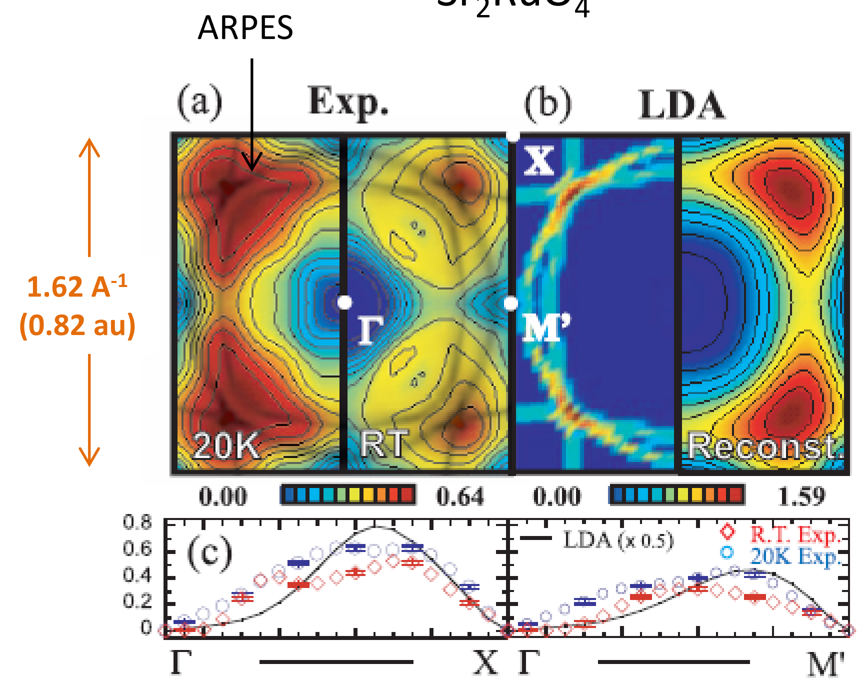


3D
(Ba,K)BiO_3



Hiraoka et al. PRB **75** 121101R (2007)

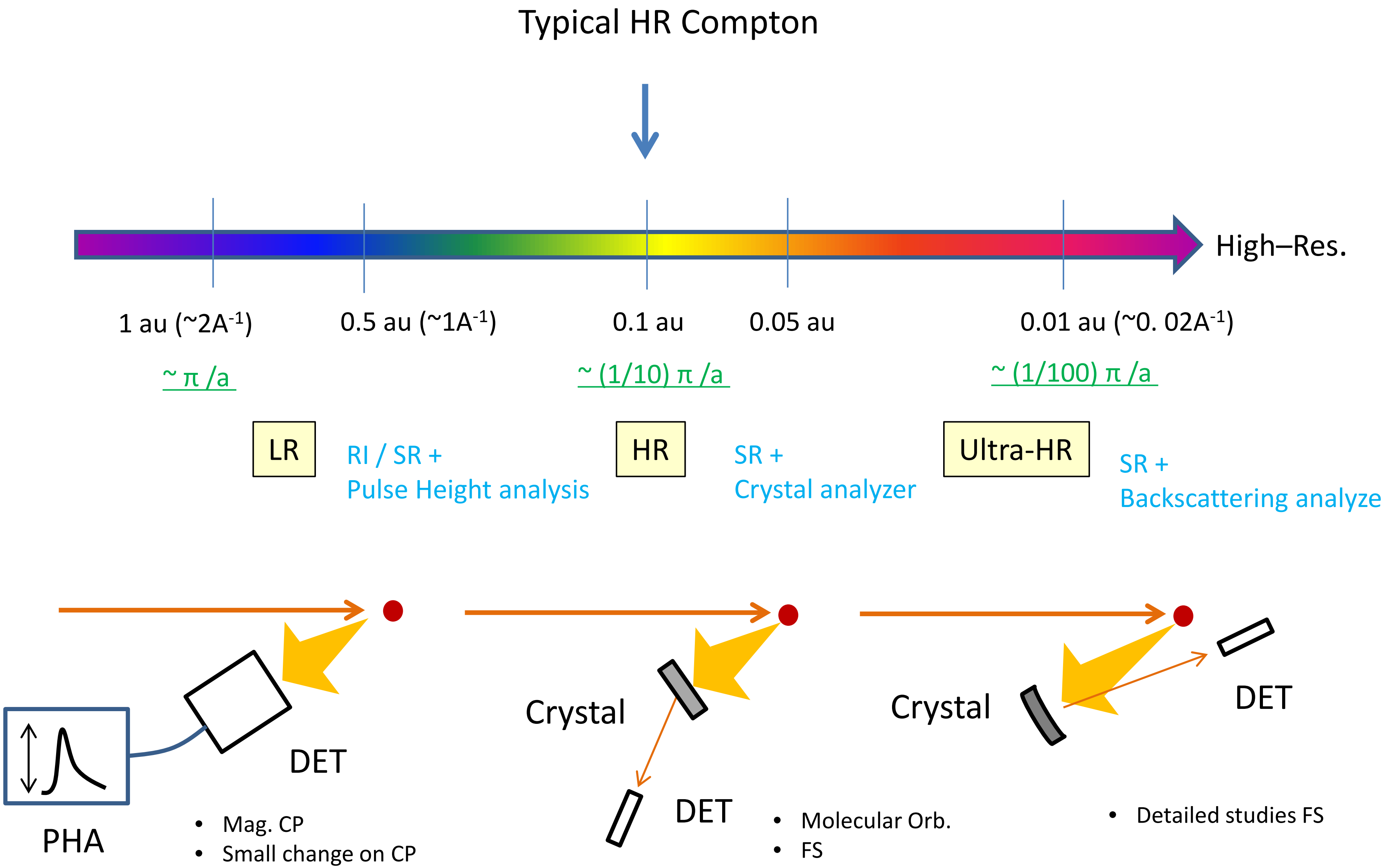
2D
Sr_2RuO_4



Hiraoka et al. PRB **74** 100501R (2006)

✓ *Typically available, ~0.1 au resolution is not high enough for detailed FS studies …*

Momentum resolution



Momentum resolution

Effective resolution =

Instrumental E (or p) resolution * final state effect

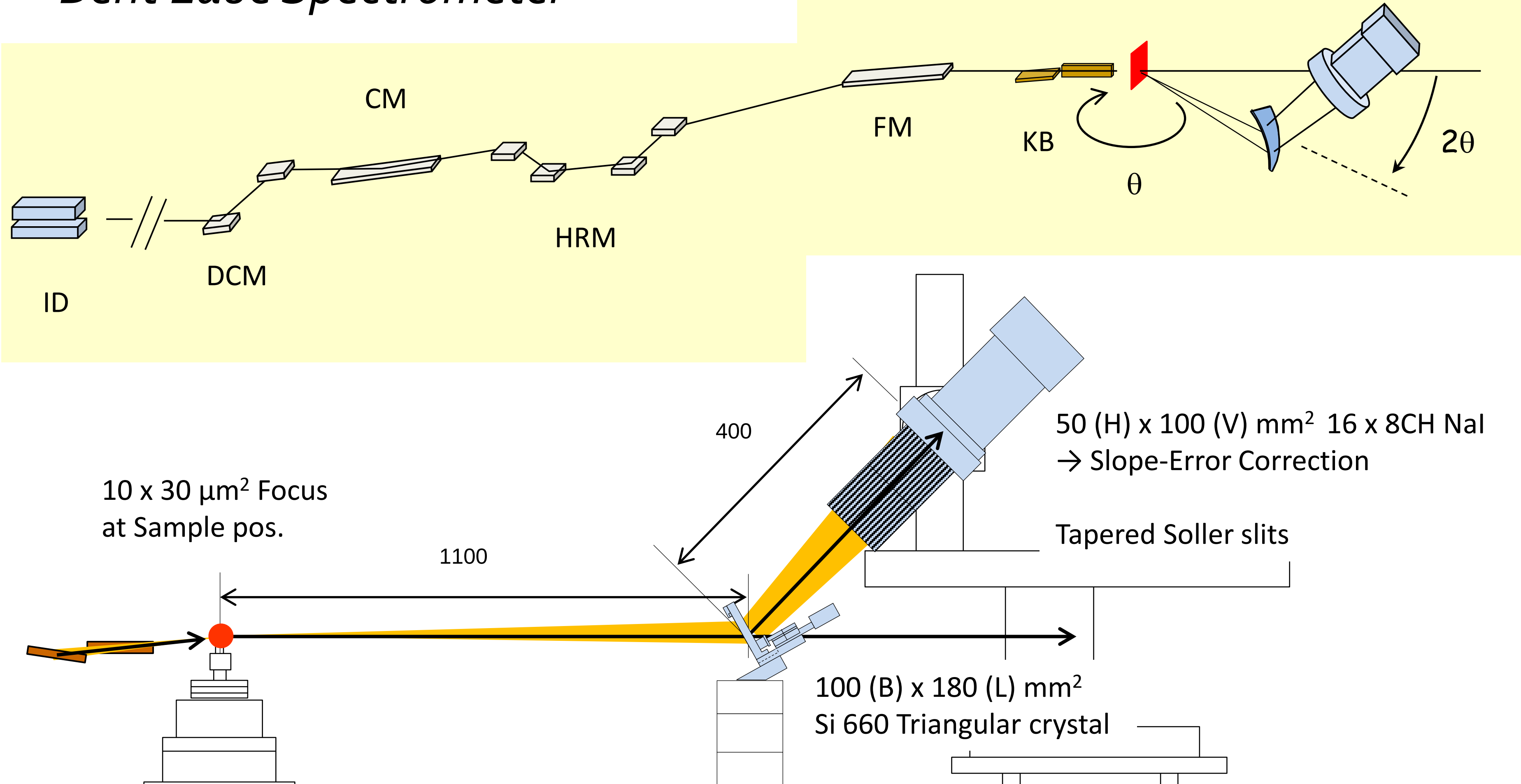
Low E (~ 10 keV)	~ 1 eV (E/dE~10,000 → 0.01 au)	**~10 eV (~ 0.1 au)**
High E (~ 100 keV)	**~100 eV (E/dE~1000→ 0.1 au)**	~1 eV (~0.001au)

Crossover happens at ~ 30 keV

Best balance for UHR Compton

High-E (20-30 keV) XRS spectometer

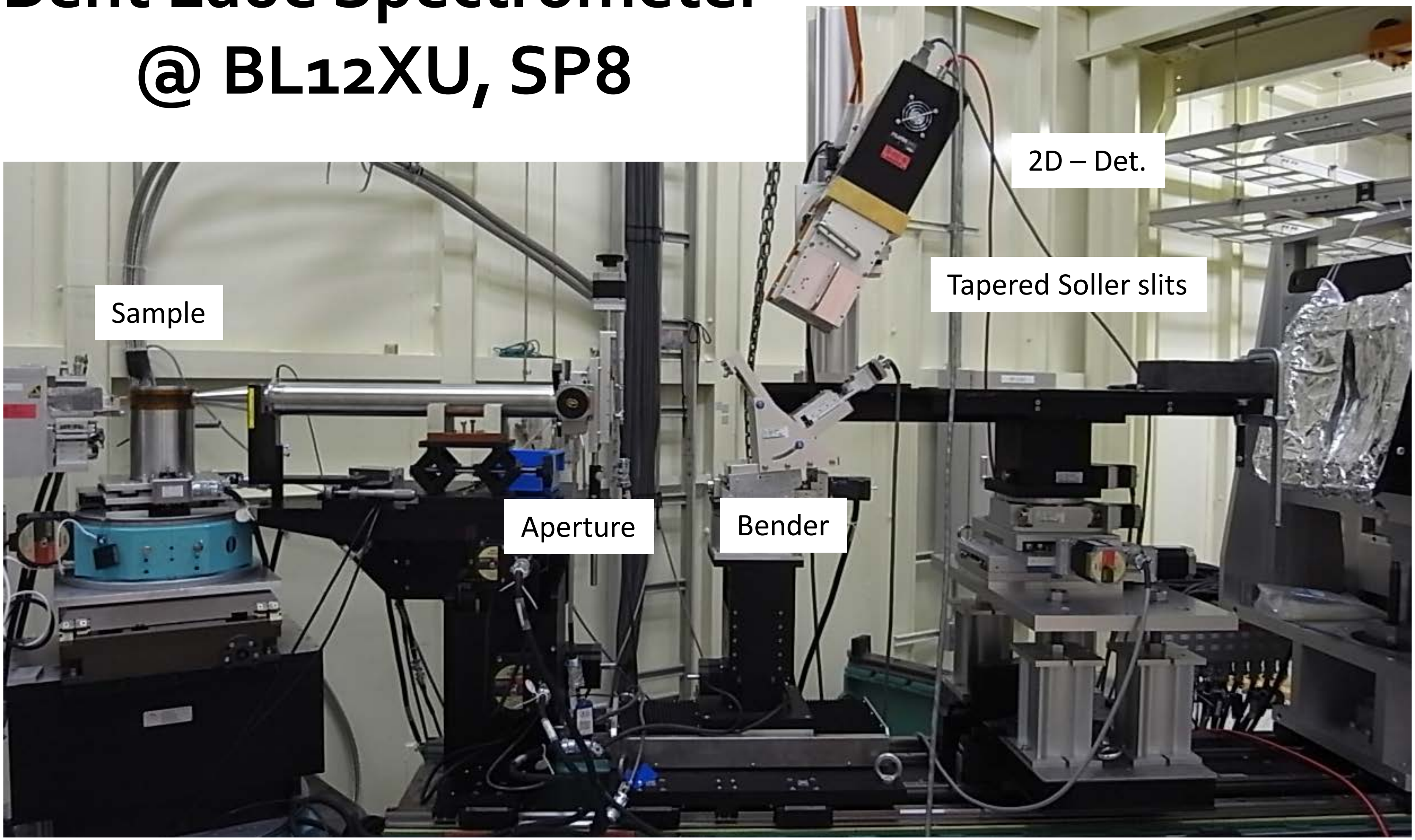
Bent Laue Spectrometer



Key factors : Small Bragg angle θ_B ; dE critically affected by dθ ($dE/E = d\theta/\tan\theta_B$)

- Small focus required (source size effect)
- Uniform curvature necessary ← Correction made by 2D detector

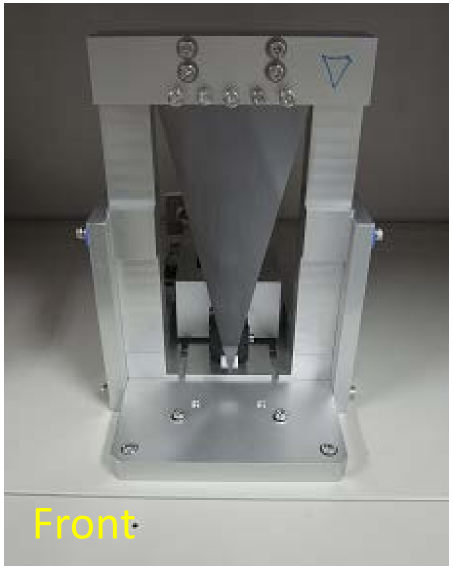
Bent Laue Spectrometer @ BL12XU, SP8



Bent Laue Analyzer

Triangular

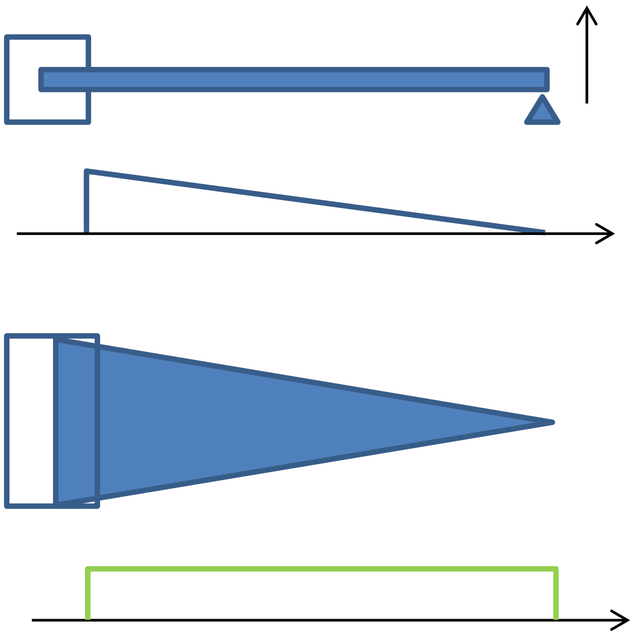
Currently used



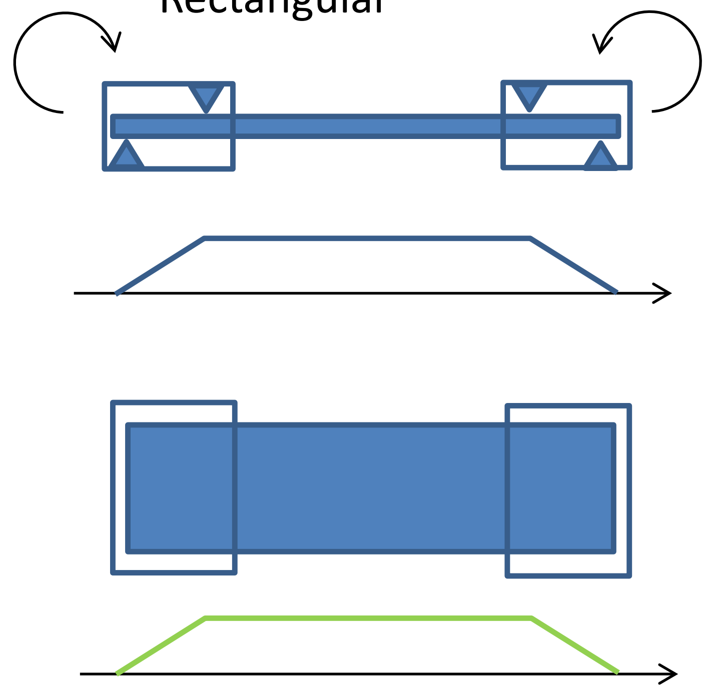
Rectangular

Triangular or Rectangular ? – *Both should work if properly bent*

Triangular (currently used)



Rectangular



Bending
Moment
Diagram

Bending
Stress
Diagram

- Single-end cramped
  → Stable
- Easy adjustment

- Only half-area available
- Bending and Bragg angle coupled

- Both ends free
  → Unstable, less reproducible
- Exactly equal force required at 4 points
  → More difficult to adjust

- Full area available
- Bending and Bragg angle decoupled

Specifications : Bent Laue spectrometer

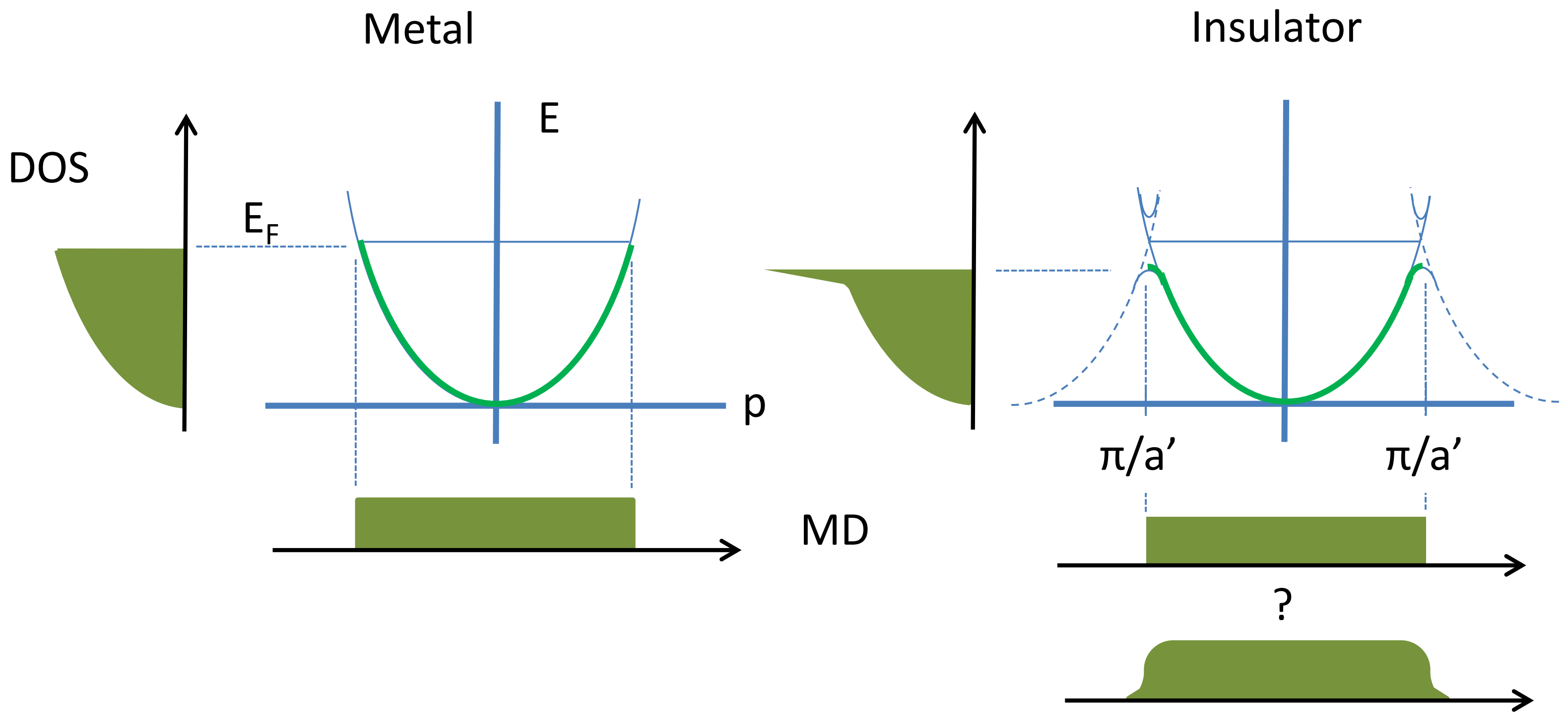
	Bent Laue
Energy	18 - 26 keV
dE	3 -5 eV (EXAFS mode, Si111 double crystal) 0.8 - 1.6 eV (XANES mode, Si220 channel cut)
Focus	10 (v) x 30 (h) μm^2
Flux	1 x 10^{13} phs./s @ 20 keV (EXAFS) < 2 x 10^{12} phs./s (XANES)
Q-range	0.2 $A^{-1}(1^{O})$ ~ 26.0 A^{-1} (150^{O})

UHR Compton at 26 keV

Instrumental resolution : Δ E = 5 eV → Δp = 0.016 au
Final state effect : Δ E ~ 5 eV → Δp ~ 0.016 au
Effect of Angular spread : $\Delta\theta = 0.23^{o}$ → Δp = 0.006 au
Overall p-resolution: Δp =0.024 au ←Not final goal (0.01 au) but Not bad !

E may be still too low to get high intensities on high-Z samples but okay for low-Z samples

II. Band gap and momentum distribution in Graphene/Graphite

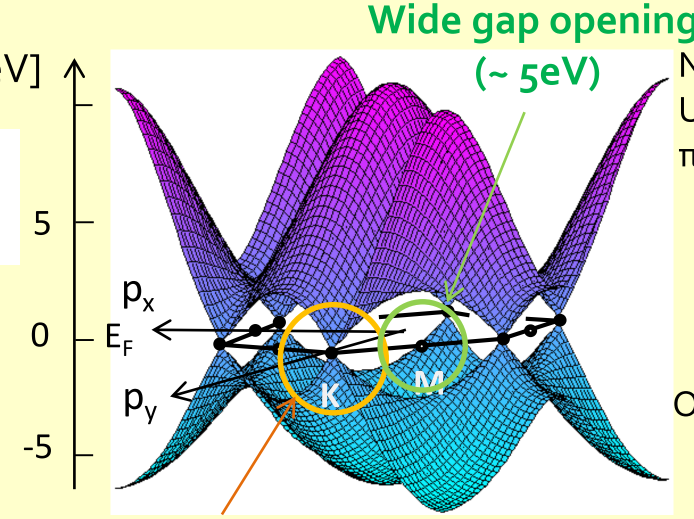


- ✓ DOS certainly changes when M-I transition or SC transition happens
- ✓ How about momentum distributions ?
  Change or No change ? How we can see it ? Really observable ?

Graphene : Ideal sample to study MD broadening

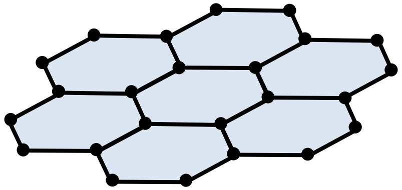
- Consideration on nearly free electron (NFL) model -

2D Band Dispers.

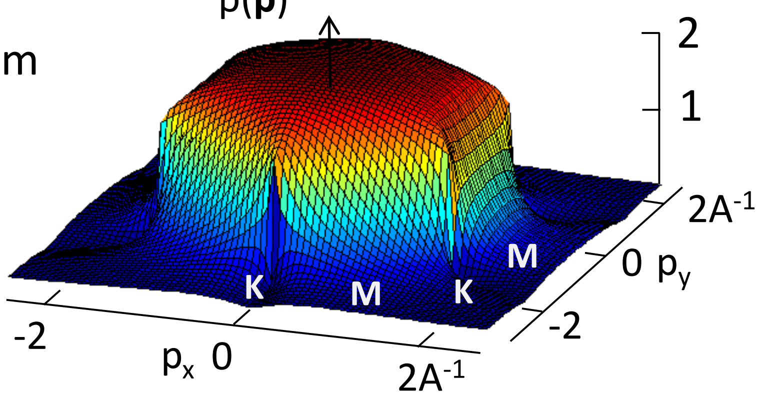


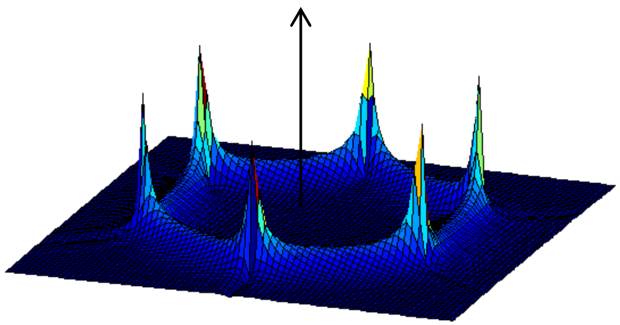
Dirac point : Linearly crossing bands (massless elec.)

Graphene :
Hexagonal layer



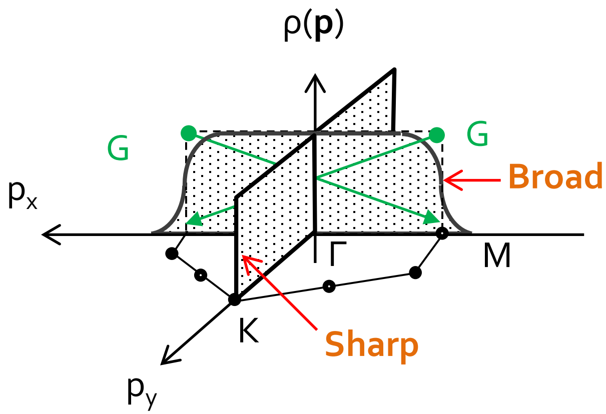
Momentum
Density





Prediction of a diverging behavior at K

Broadening vs Band gap

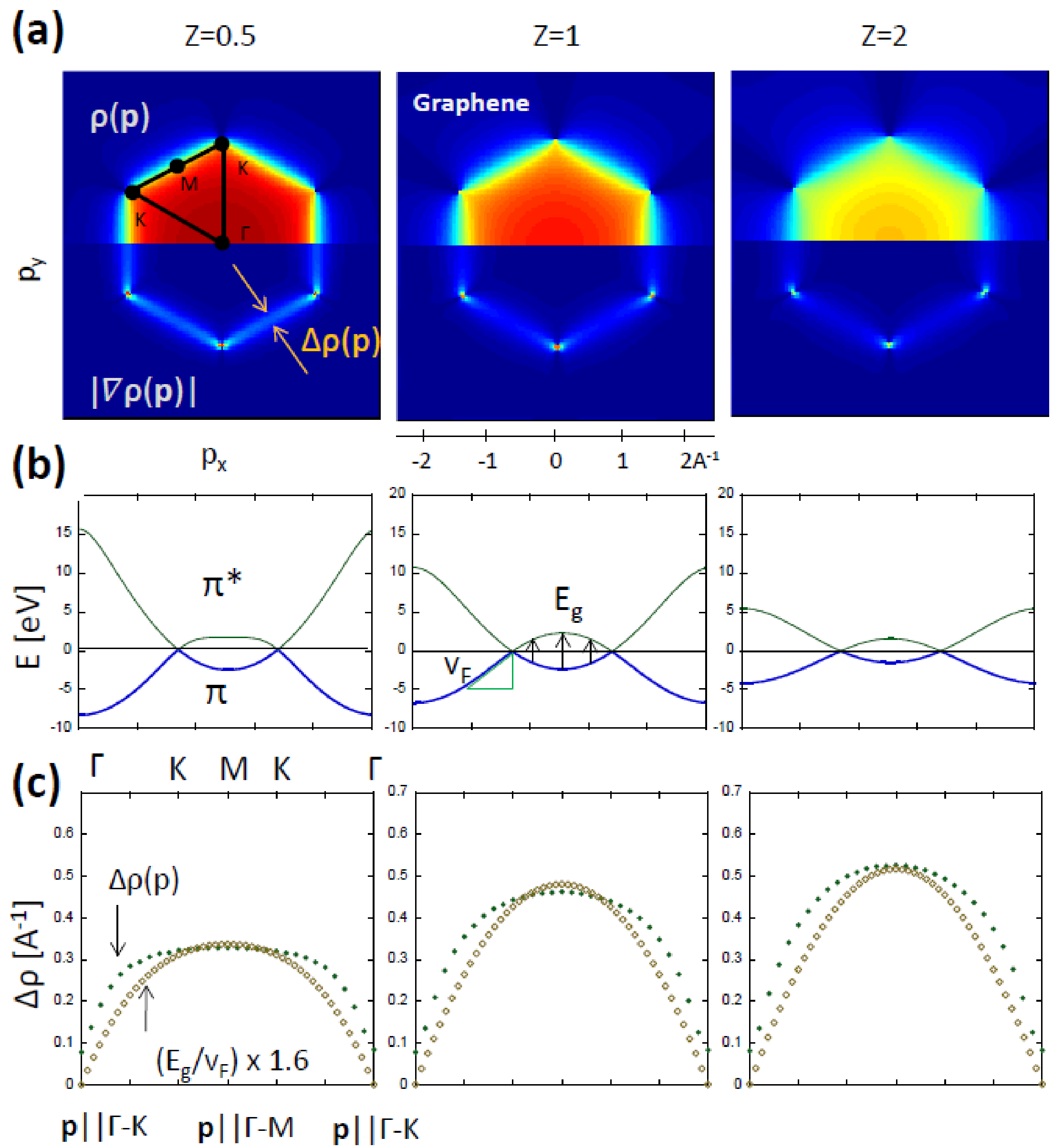


Wide Gap (at M) — Strong mixing ψ_k and $\psi_{k\pm G}$ thr. **G**

No Gap (at K) — No mixing ψ_k and $\psi_{k\pm G}$ thr. **G**

$\Delta\rho(p) \sim \eta(E_g/v_F)$, where η = 1.6

Note: FWHM of $g(x)=\exp\{-(x/\beta)^2\}$ is
$\Delta x = 2(\ln 2)^{1/2}\,\beta \sim 1.6\,\beta$

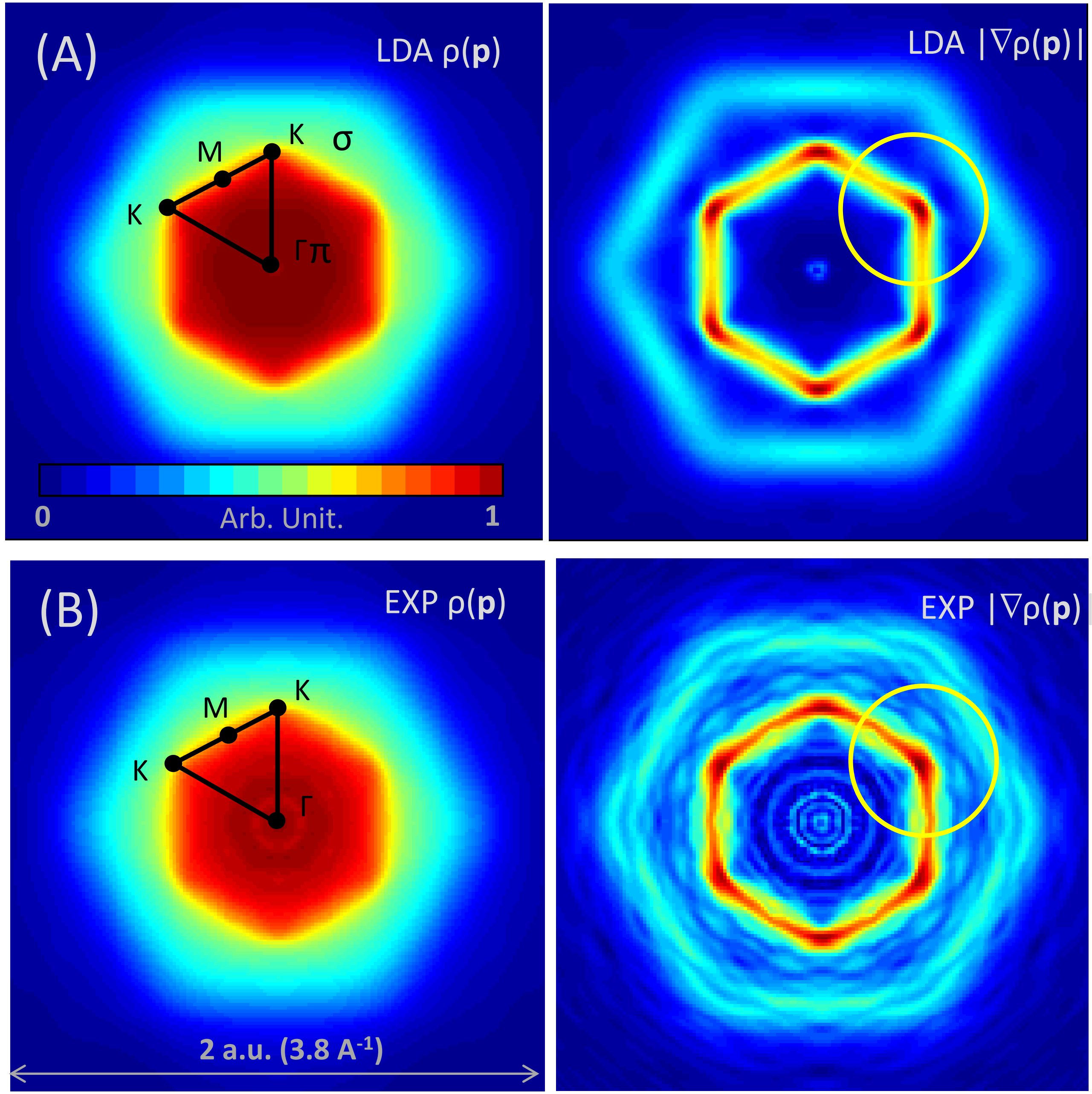


Graphite

Difference :
No linear crossing
But still gap-less

MD Reconstructed from 5 CPs

Clear exp. evidence of MD broadening as a function of Eg



N. Hiraoka and T. Nomura SREP **7** (2017) 565

Summary

Compton scattering experiments were performed at 0.024 au resolution.

I. Momentum density renormalization in Li

Good agreement with QMC : Z_F = 0.51 for Liq. and 0.60 for Sol.

II. Band gap and Momentum broadening on graphene/graphite

$\Delta p = \eta \cdot E_g / v_F$,where η=1.6

UHR Compton of 0.01-au resolution at ~ 50 keV