Science with Intermediate Energy X-Rays

Argonne NATIONAL LABORATORY

Workshop August 2004
~50 participants

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Outline

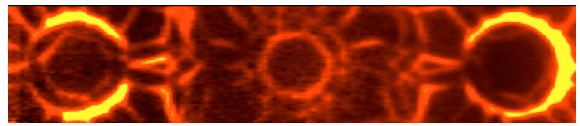
From Murray:

- What is the highest impact revolutionary science that is on the horizon, but not possible with APS capabilities today?
- How can this science be accomplished through a major APS upgrade? Please include a brief discussion of technical needs.

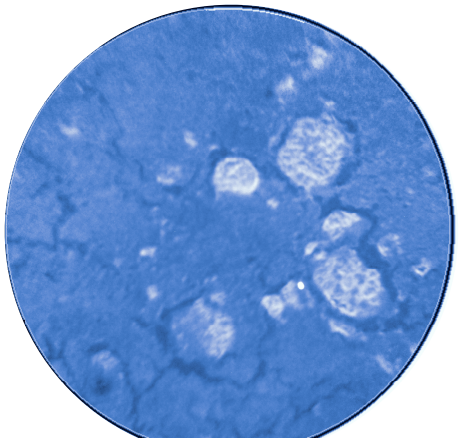
Why are these techniques so useful?

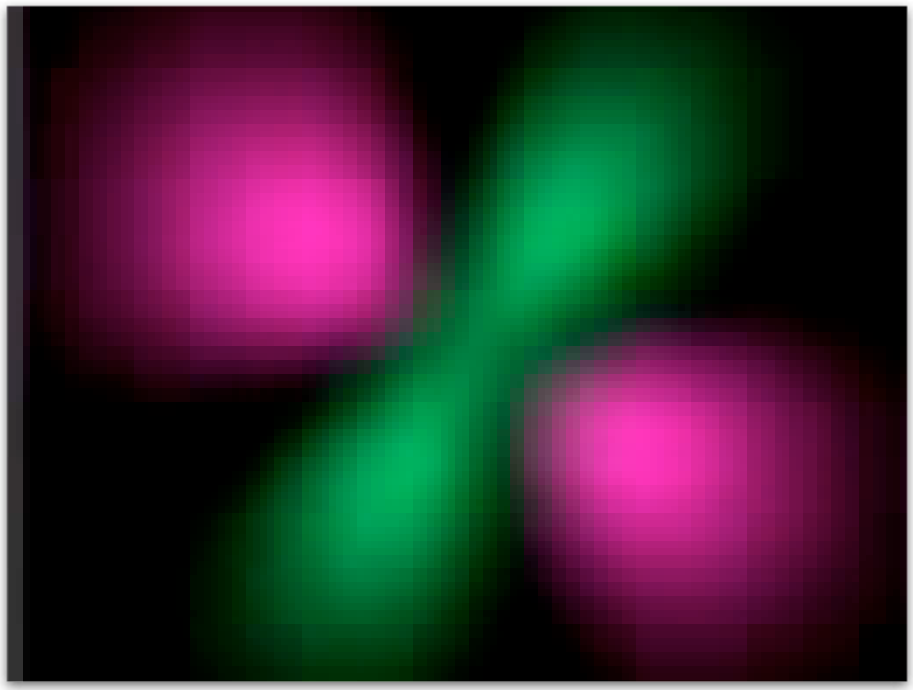
Because all the

Physical



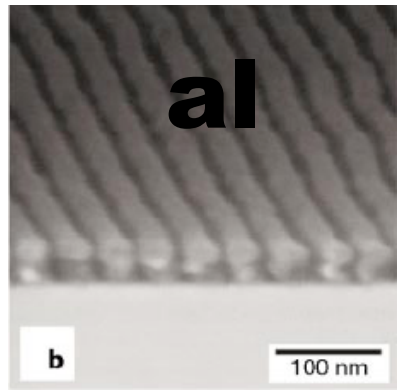
Chemical





Mechanic

al

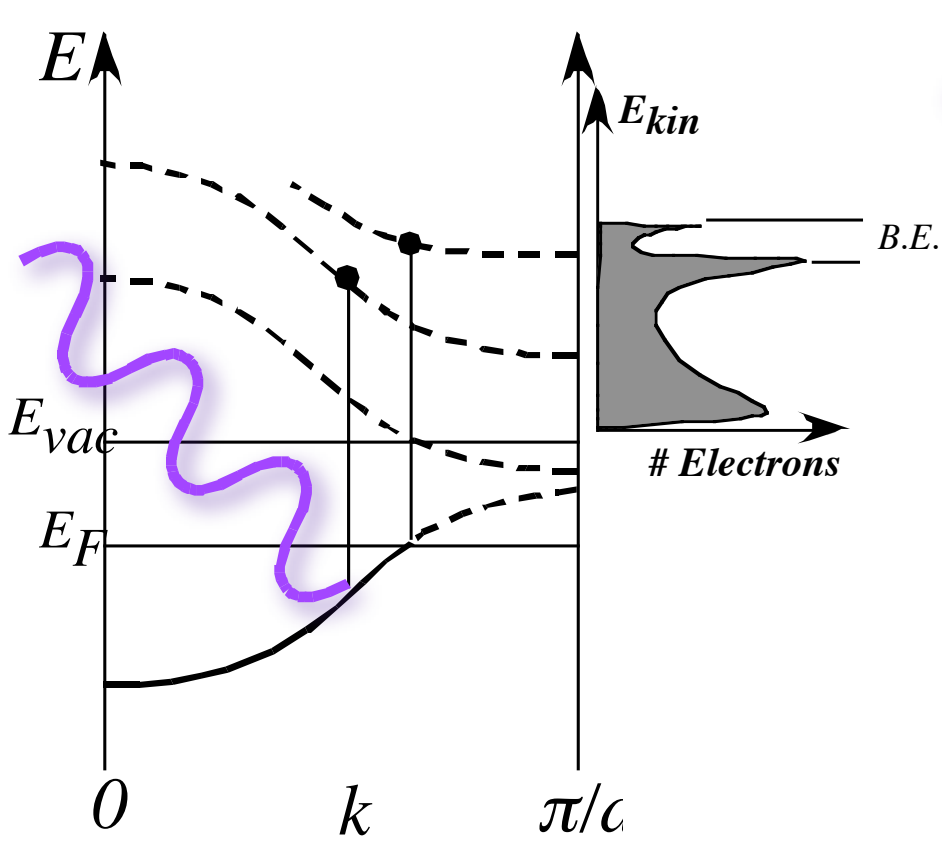


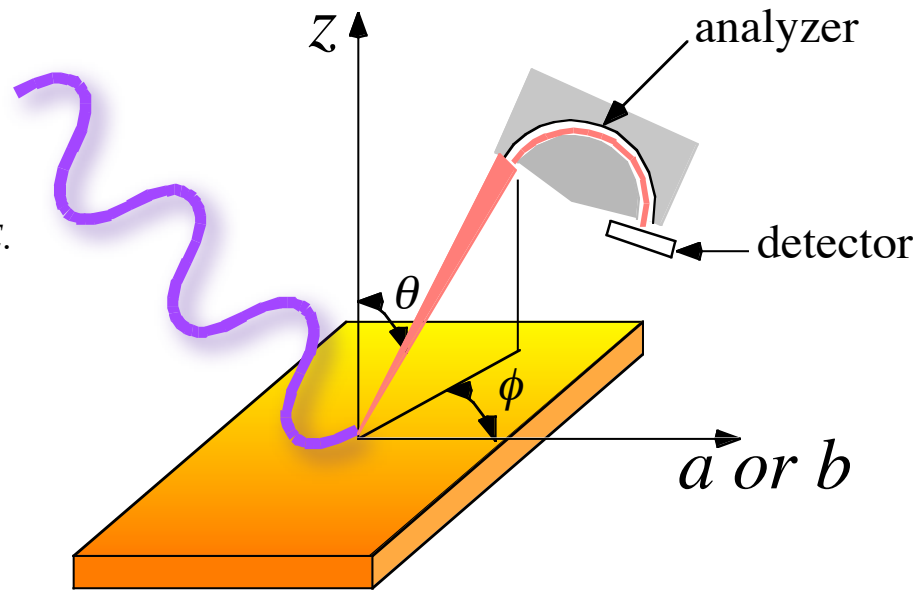
properties of materials
are determined by valence electrons

These are measured by

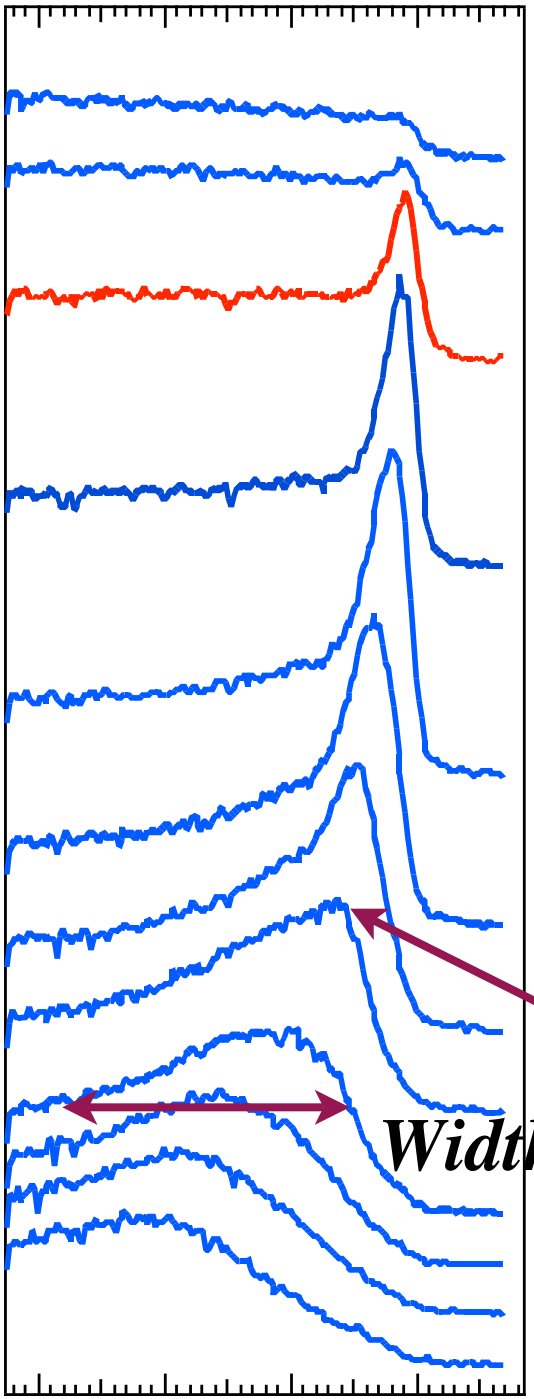
ARPES and RSXS

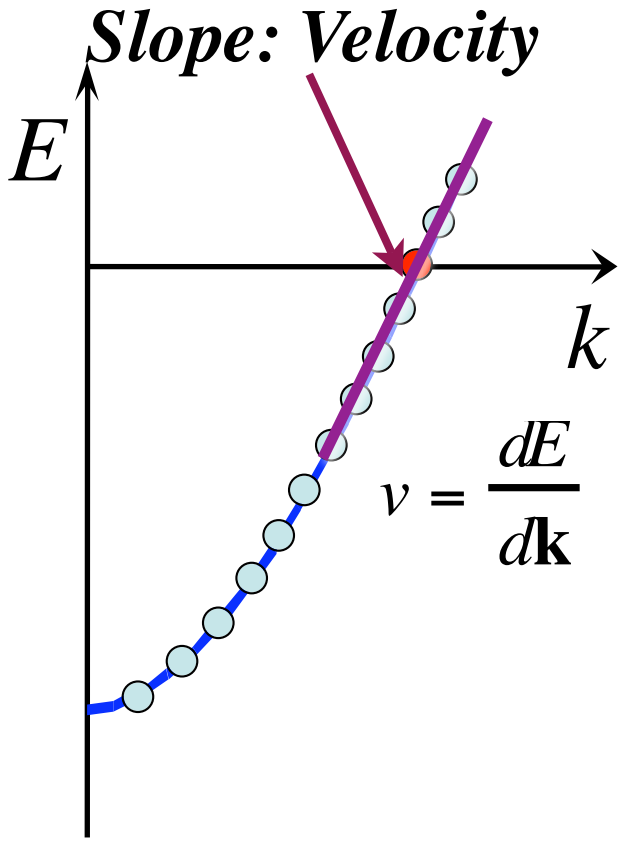
Angle resolved photoemission





$$\vec{k}^{f}_{//} = \vec{k}^{i}_{//} = \sqrt{\frac{2mE}{\hbar^2}} sin\theta$$



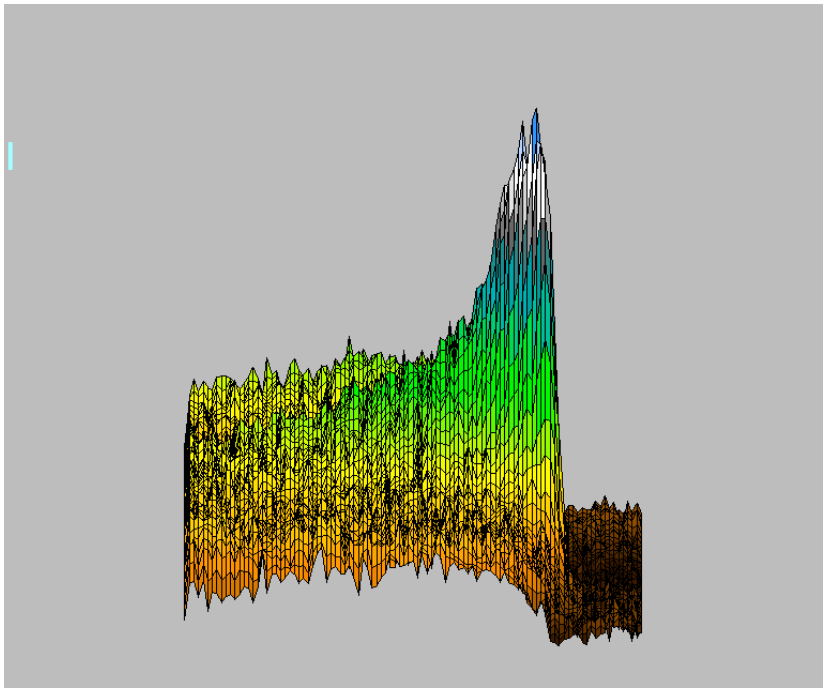


Position: Energy

Width: 1/Lifetime

Lineshape provides most complete information on many-body interactions

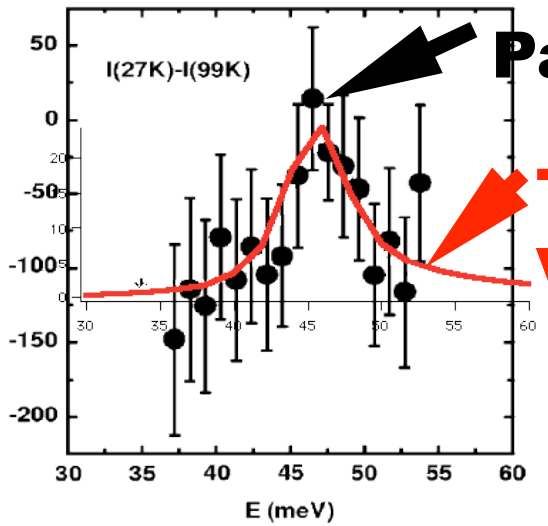
$$I(k,\omega) = \frac{1}{\pi}\Im mG(k,\omega)$$



Examples Inelastic Neutron Scattering

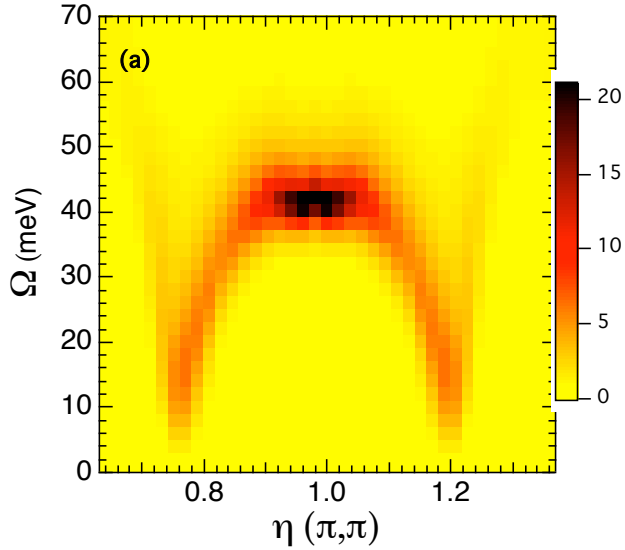
$$\chi_0(q,\Omega) = \frac{1}{\pi^2}\sum_k \int_{-\infty}^{\infty} d\nu\ d\epsilon\,[ImG(k,\nu)\ ImG(k+q,\epsilon) + ImF(k,\nu)\ ImF(k+q,\epsilon)\ \frac{n_F(\nu)-n_F(\epsilon)}{\Omega+\nu-\epsilon+i\delta}$$

$$\chi(q,\Omega) = \frac{\chi_0(q,\Omega)}{1-J(q)\chi_0(q,\Omega)}$$

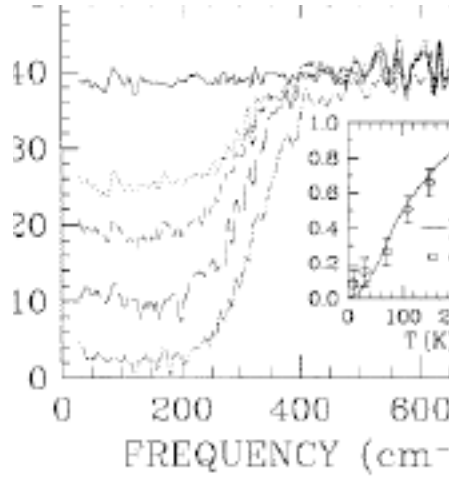


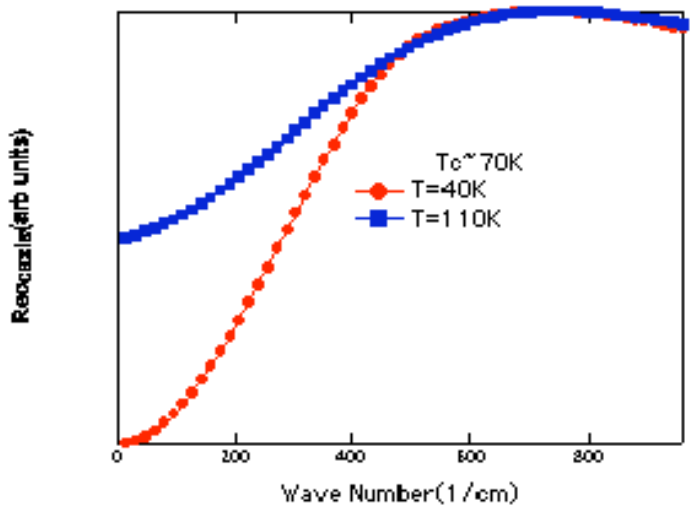
Pailhes PRL 93

This work



Optical conductivity

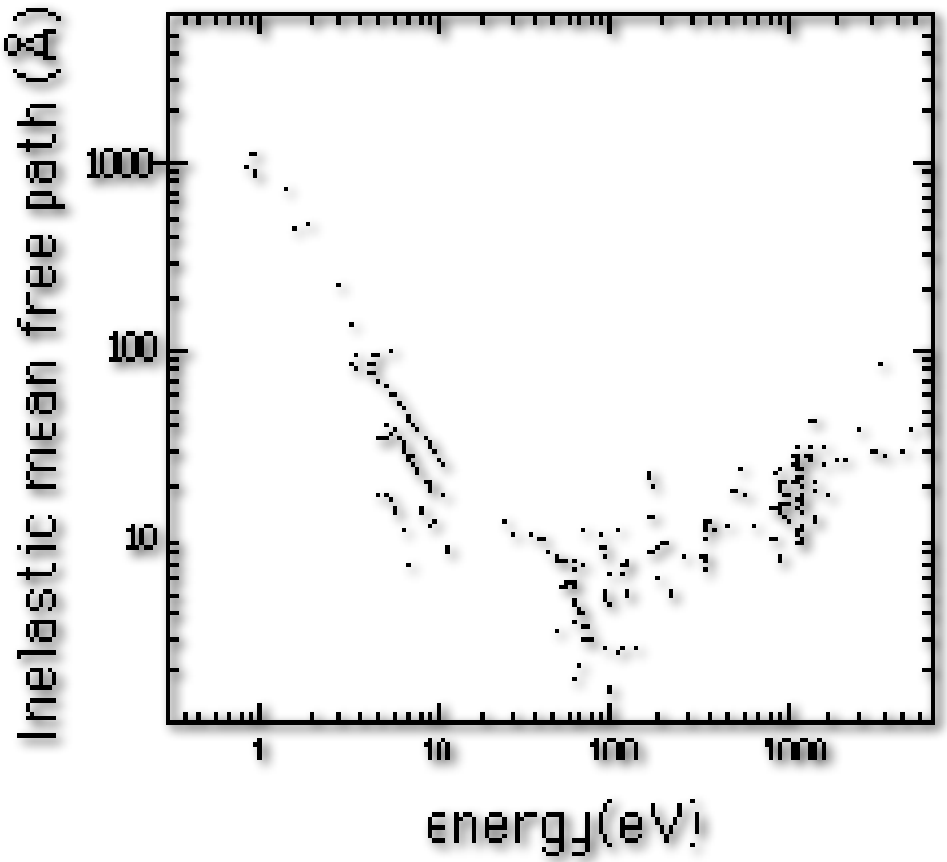


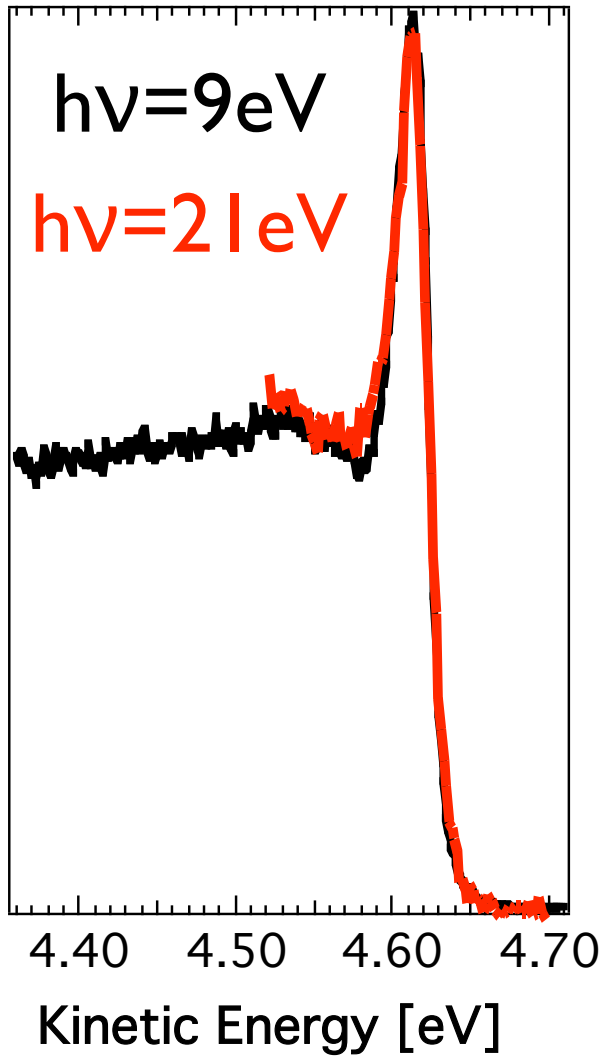


ARPES normally uses hv ~5 to 150 eV

Why do we want higher energy?

ARPES is surface sensitive



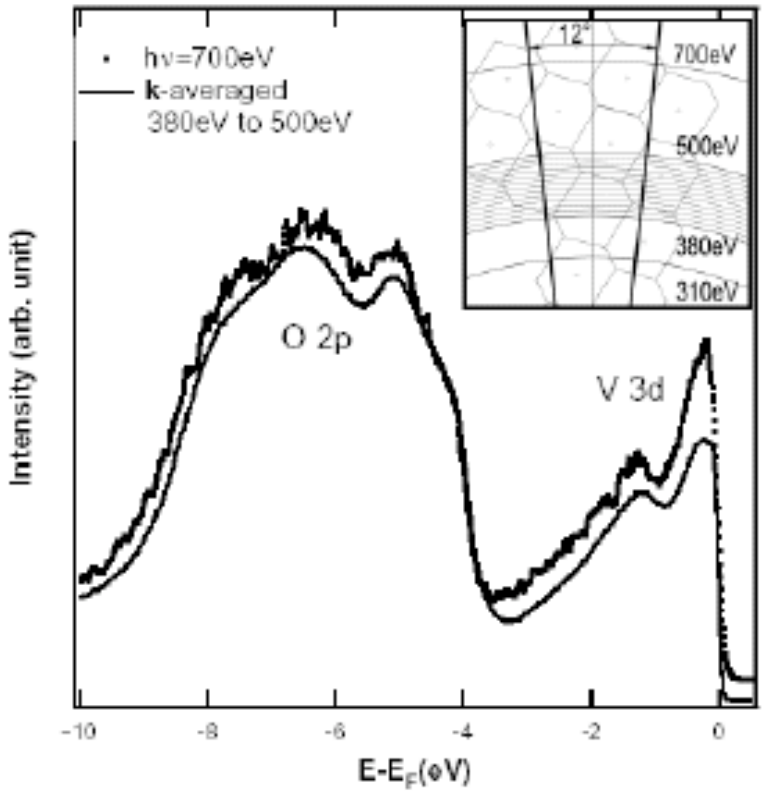


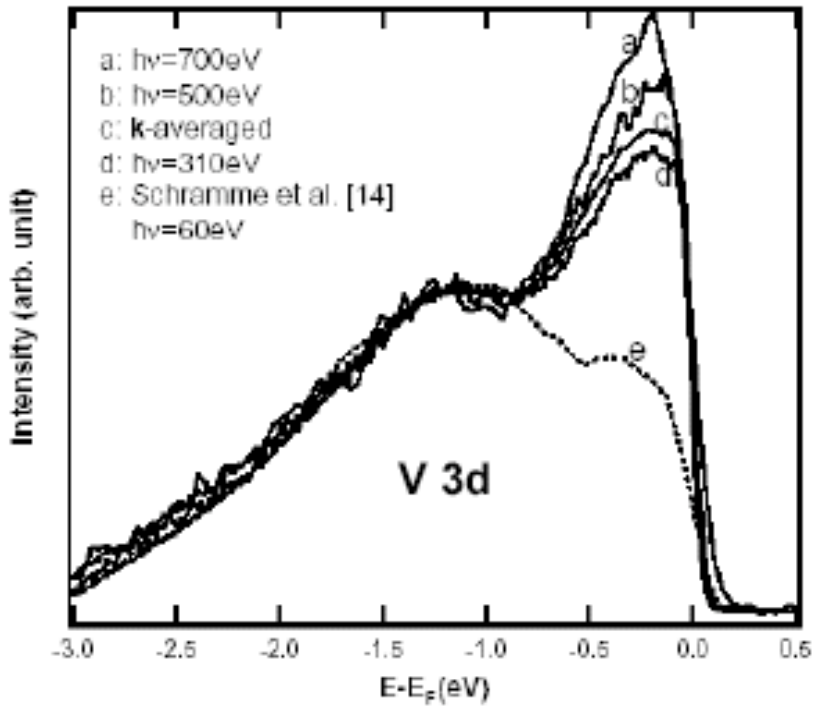
MUST go to higher energy!

Does high hν work? YES

Newly observed E_F peak for V_2O_3

New results achieved with high photon energy and small (approx 100 μm diameter) photon spot.



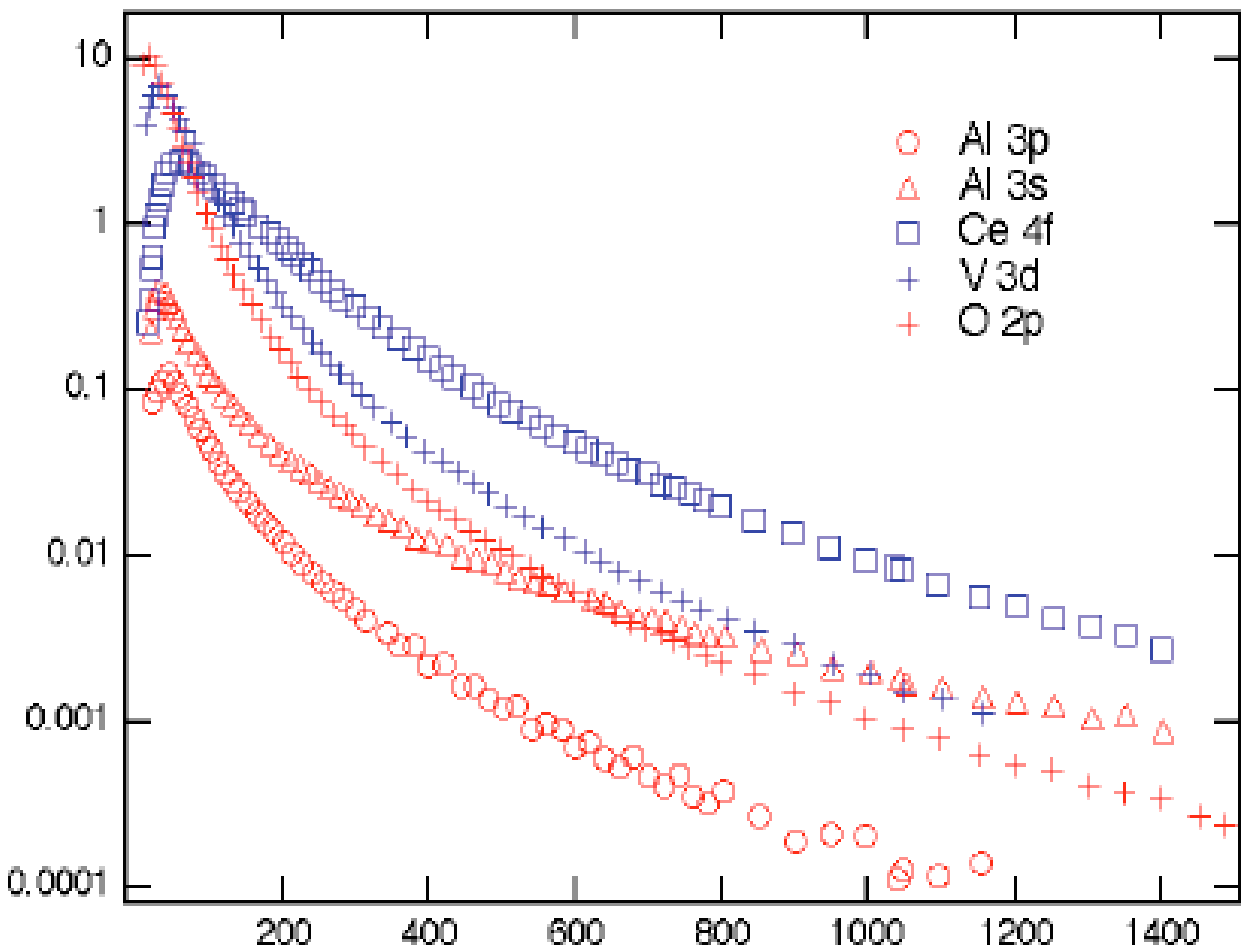


SPring8 collaboration with
S. Suga et al.
Early small spot work
at ALS with J. D. Denlinger

Monotonic increase of peak with increasing hν ⇒
Probe depth increase outweighs any k_z dependence

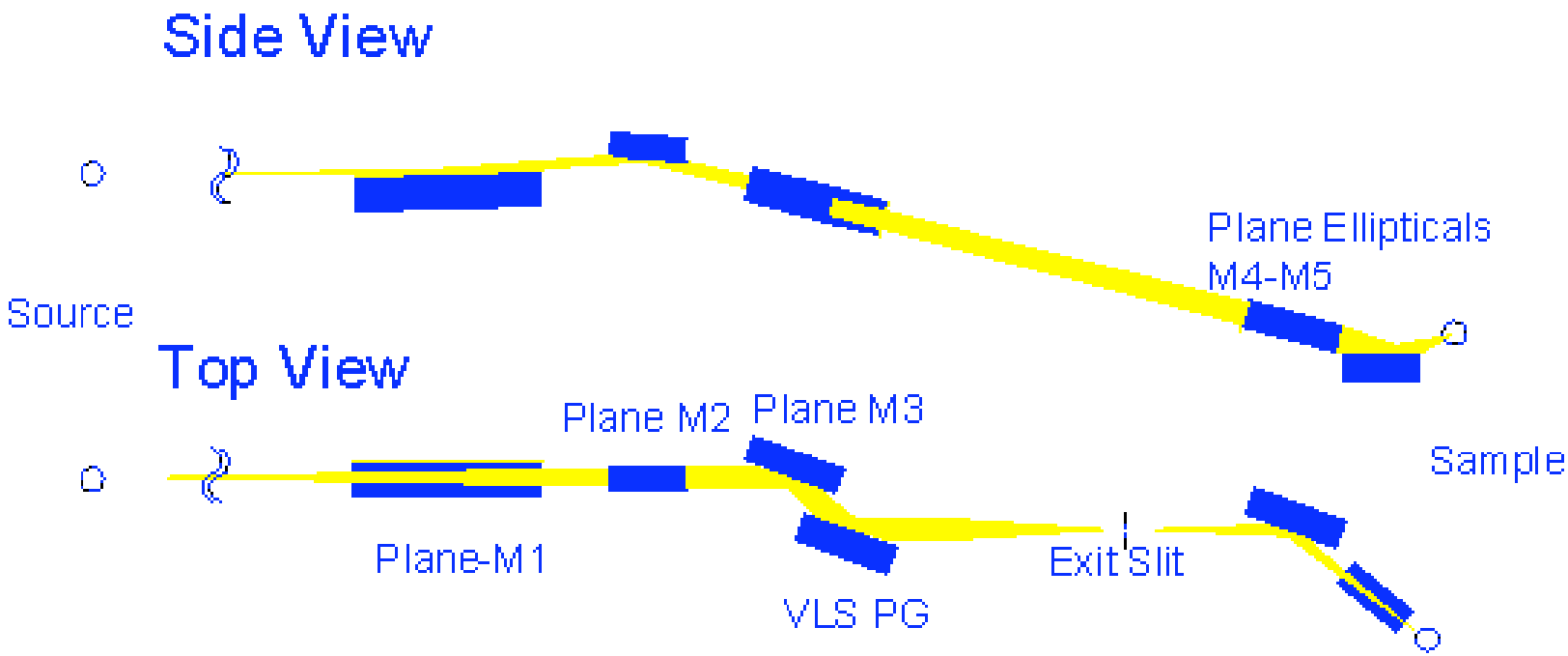
What does this have to do with the APS upgrade? Plenty...

I) High hν photoemission cross-sections small



What does this have to do with the APS upgrade? Plenty...

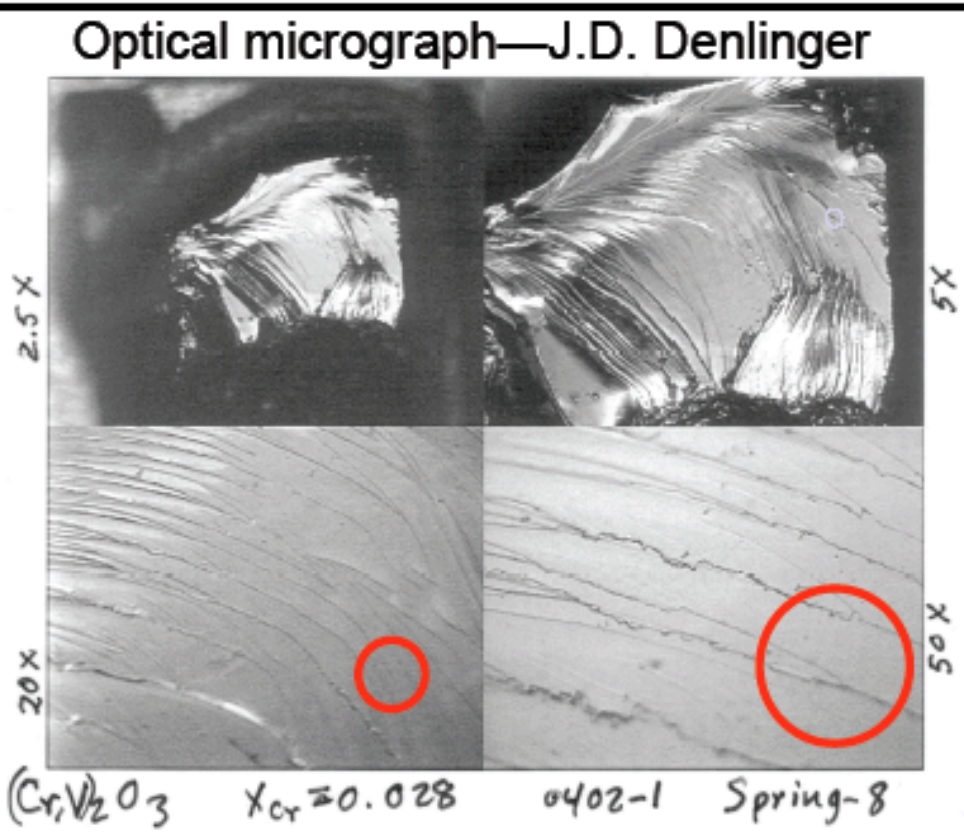
2) Mono uses gratings



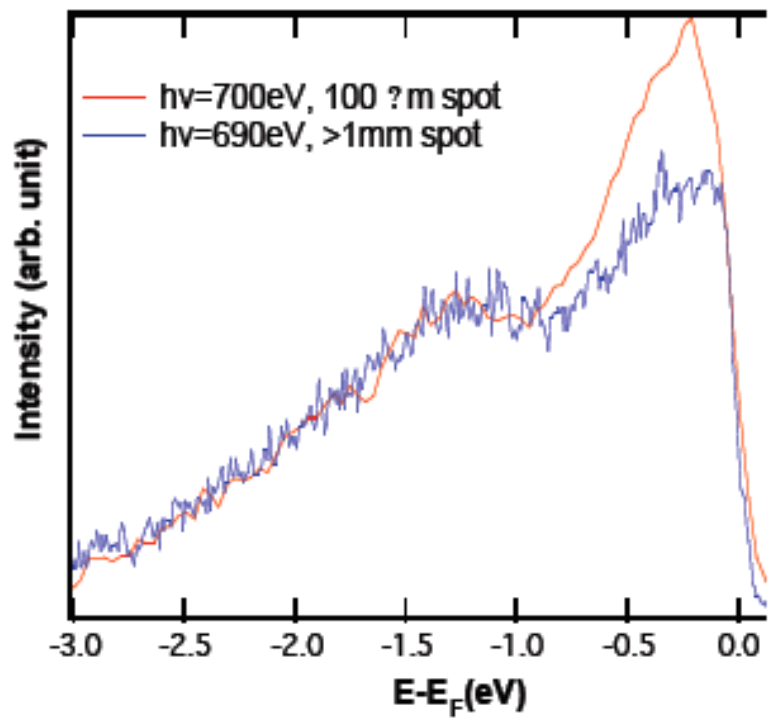
Need highest possible brilliance to achieve desired performance

What does this have to do with the APS upgrade? Plenty...

3) Small spot essential for large E_F peak !



○ = 100 μm spot size



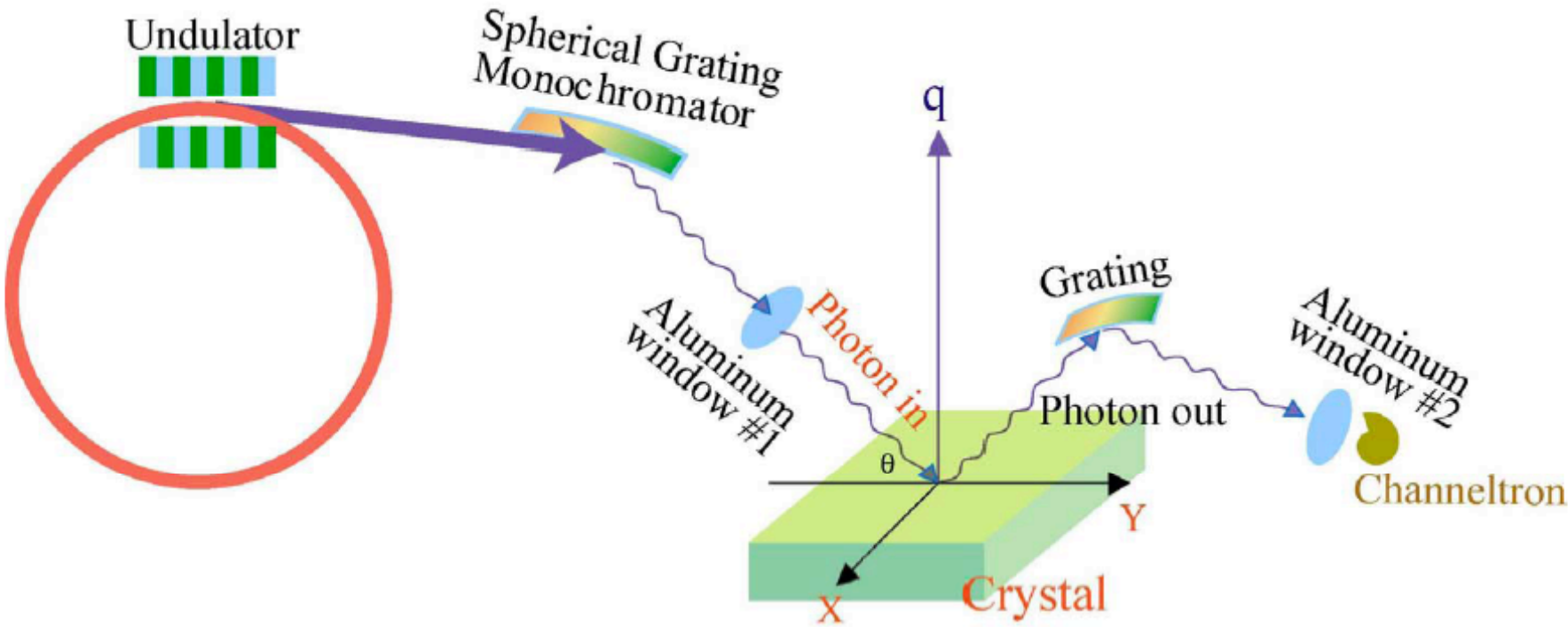
With small spot can select probing point to <u>avoid steps and edges as much as possible</u>

E_F peak much reduced with larger spot

Difference for 300 eV to 500 eV

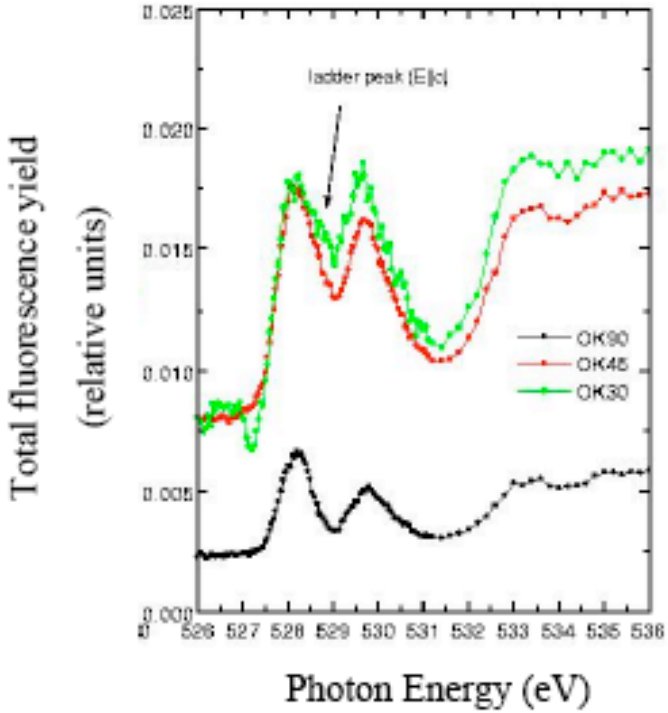
range even larger

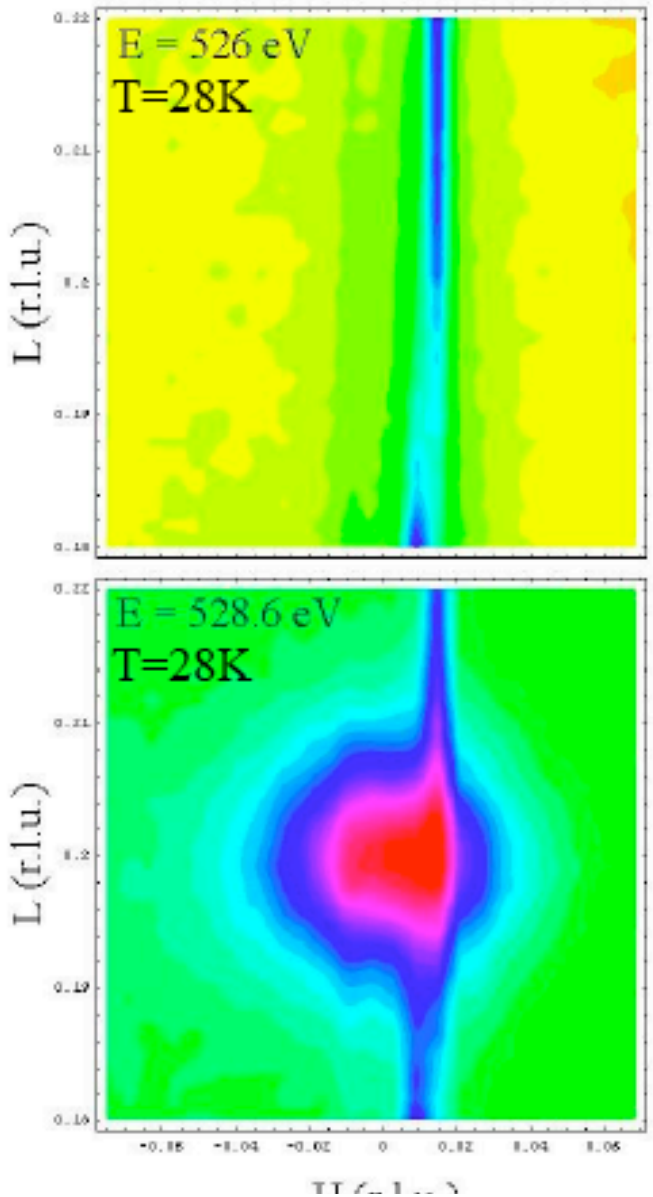
Resonant Soft X-ray Scattering



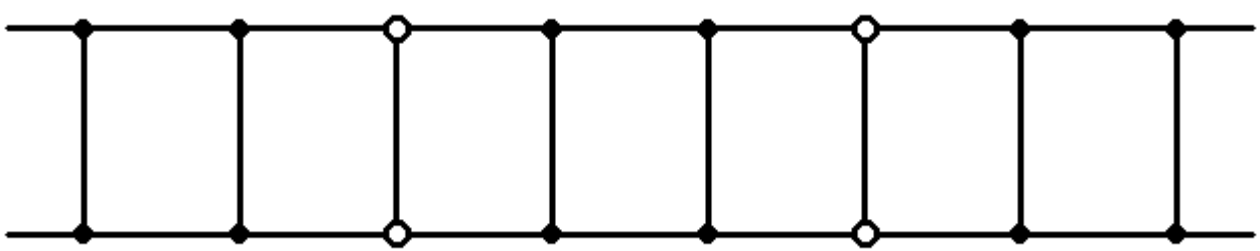
- Many collective phenomena at longer wavelengths
  - Spin ordering
  - Magnons
  - Polarons, bi-polarons, etc
- Weak phenomena need resonant scattering
- LOW-lying energy levels participate in these phenomena

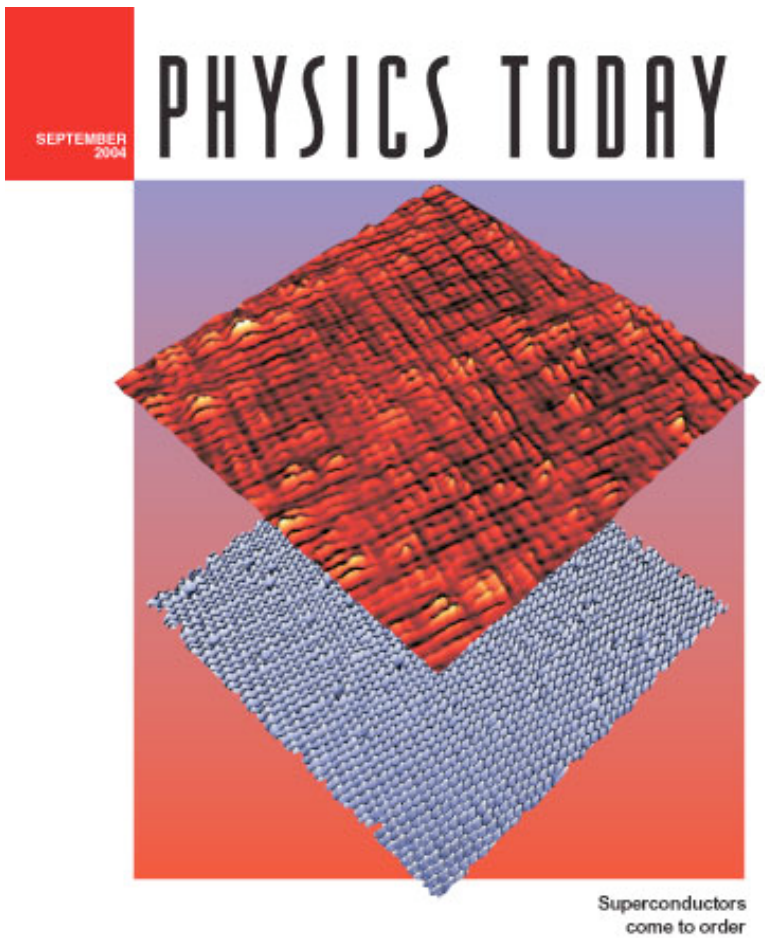
Valence modulation in $Sr_{14}Cu_{24}O_{41}$



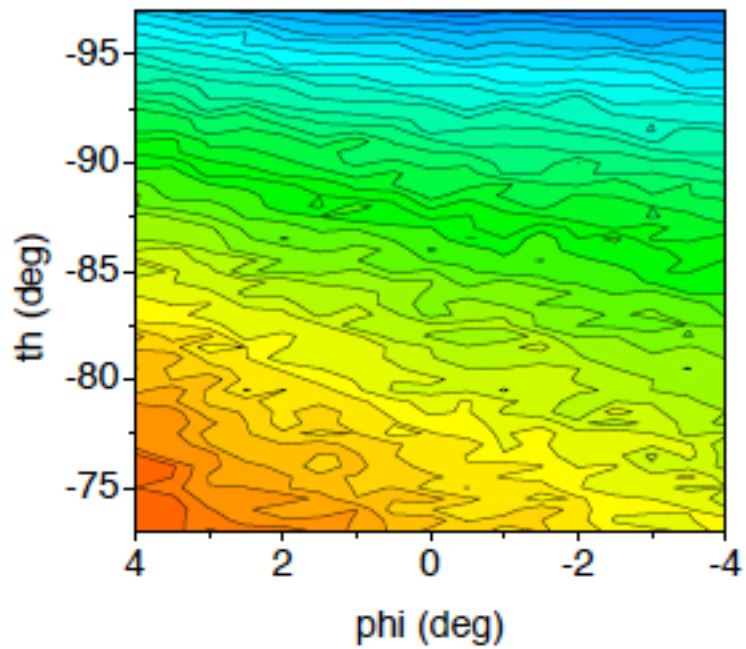


- $L = 0.200 \pm 0.009$ r. l. u. $\Rightarrow$ l $= 5.00 \pm 0.24\ c_L$.
- *Does not index to 27.3 Å unit cell.*
- $x_c = 255$ Å, $x_a = 274$ Å
- No measurable off-resonant signal $\Rightarrow$ purely electronic phenomenon



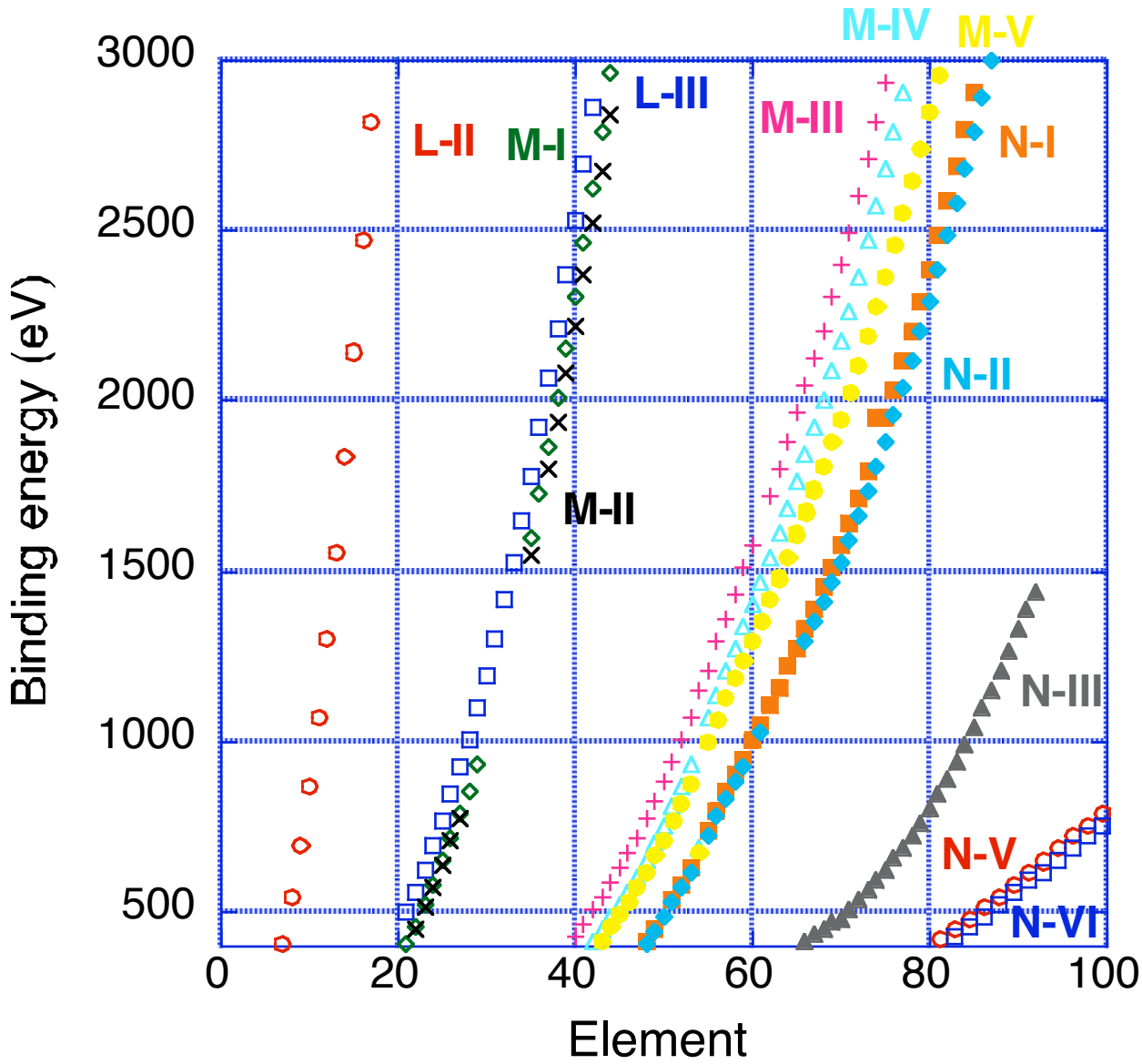


$$Na_xCa_{2-x}CuO_2Cl_2$$

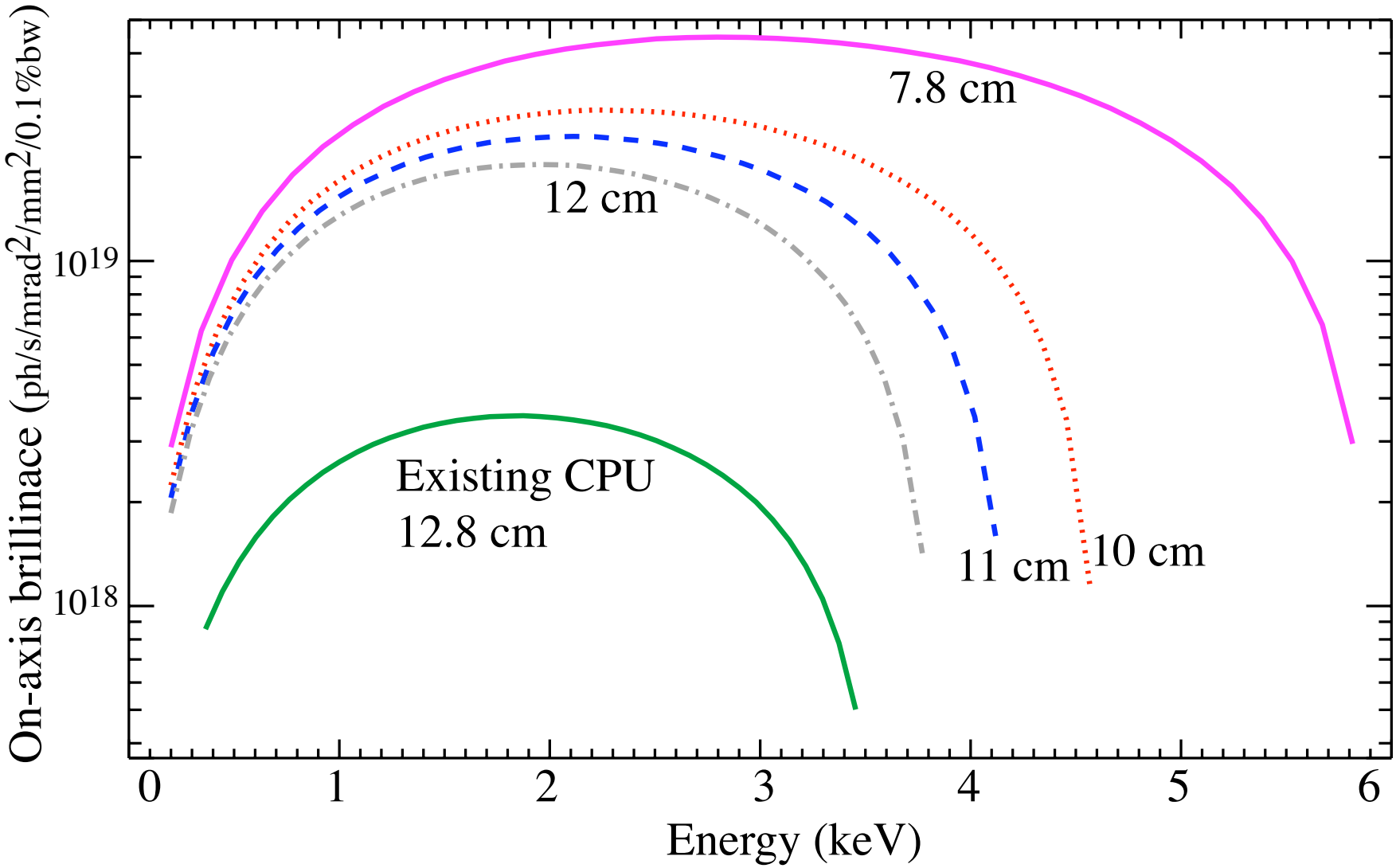


A 2D scan at 933 eV, centered at (0.25, 0, 1.5) and ranges from H ~ 0.15 to H ~ 0.35. The sloping background is due to the variation of sample absorption with phi and theta.

Need Soft X-Rays to look at all possible resonant excitations



A 2.5 m APPLE II device



Expected performance with current APS

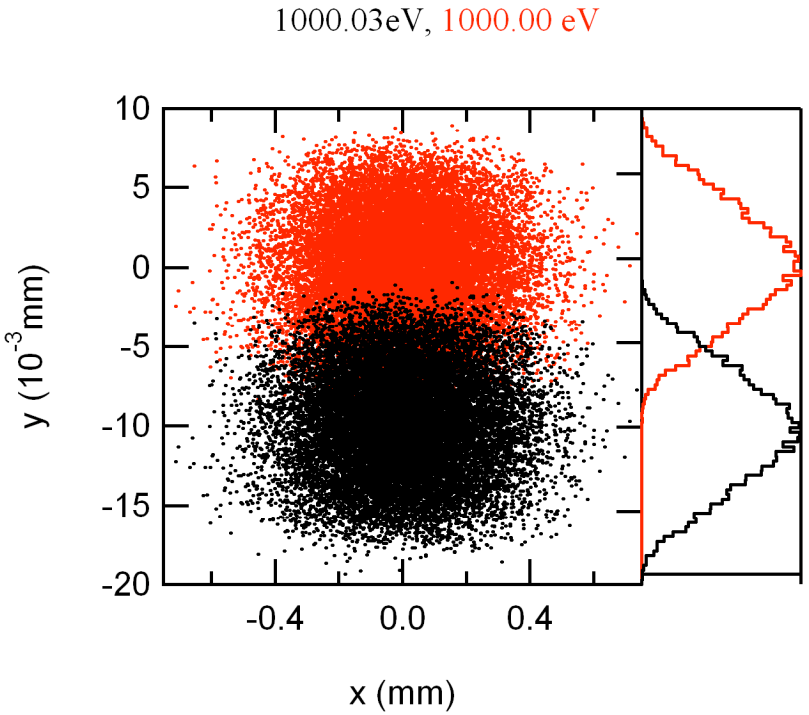


Fig. 4.8: Ray traces at the exit slit for 1000 and 1000.03 eV with the HRG including slope errors.

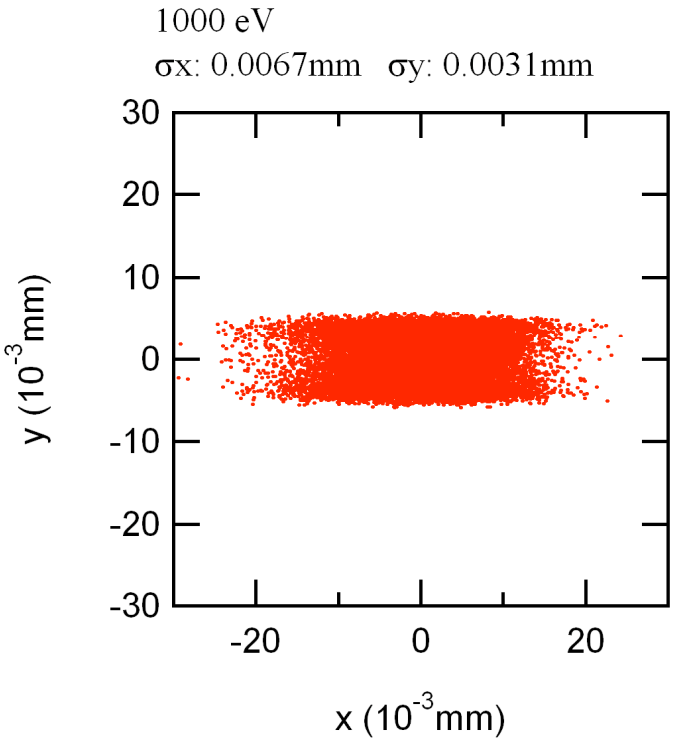


Fig. 4.9: Ray traces at the sample position including slope errors.

An 8-10 m device should make this the cutting-edge IEX source in the world!