Soft X-Ray Scattering from Hard and Soft Matter

The scientific case for a new undulator beamline with dedicated instrumentation for resonant scattering from a broad range of materials.

Heterogeneity is ubiquitous

How are chemical/functional heterogeneities distributed over nm – μm distances in materials? What differences exist between bulk and spatially confined materials?

Can the spatial distribution of heterogeneities be controlled during self-assembly?

What energetics, interactions, proximity effects exist in nanoscale composites or assemblies? How can they be modified to influence functionality?

What forms of energy conversion can be found in heterogeneous nanoscale materials?

What chemical/functional properties?

- electronic structure (bands, bonds, anisotropies, …)
- optical absorption/emission (PVs, LEDs, etc.)
- magnetism
- ferroelectricity (polarization)
- piezzoelectricity (strain)
- self-assembly, dynamics
- others ?

Workshop motivation

Measurements that are sensitive to the distribution of these chemical/functional properties over nm – μm dimensions are needed, and will accelerate the development of nanoscale materials.

Soft x-ray resonant scattering is one such tool that is underdeveloped generally and especially at the ALS.

The ALS and Molecular Foundry coexist at LBNL.

Workshop goals: Define impact, uniqueness

Develop compelling scientific case for a world-class beamline facility for resonant scattering studies of nanometer-scale structure in a broad range of materials:

- magnetic, correlated electron, multifunctional systems,…
- polymers, liquid crystals, bio-materials,…

Establish general technical specifications for beamline.

Discuss optimal end-stations for these studies.

Why q-resolved scattering with soft x-rays?

- Dipole transitions to Fermi edge or anti-bonding molecular orbital states yields *strong resonant enhancements* to chemical and functional properties.
  $\Rightarrow$ Unique, new scattering contrast mechanisms.

- Scattered intensity/absorption length $\propto \lambda^3$
  $\Rightarrow$ Scattering from *very* small volume of material

- Spatial resolution ~ $\lambda/2$: 1 nm up to several μm.
  Angles 10 x larger for given q ($q = 4\pi\sin\theta/\lambda$)

- *Broadly applicable* (materials, geometries)
  - lateral, depth resolution
  - *in situ*, dynamic studies
  - …

Contrast mechanisms at soft x-ray core levels

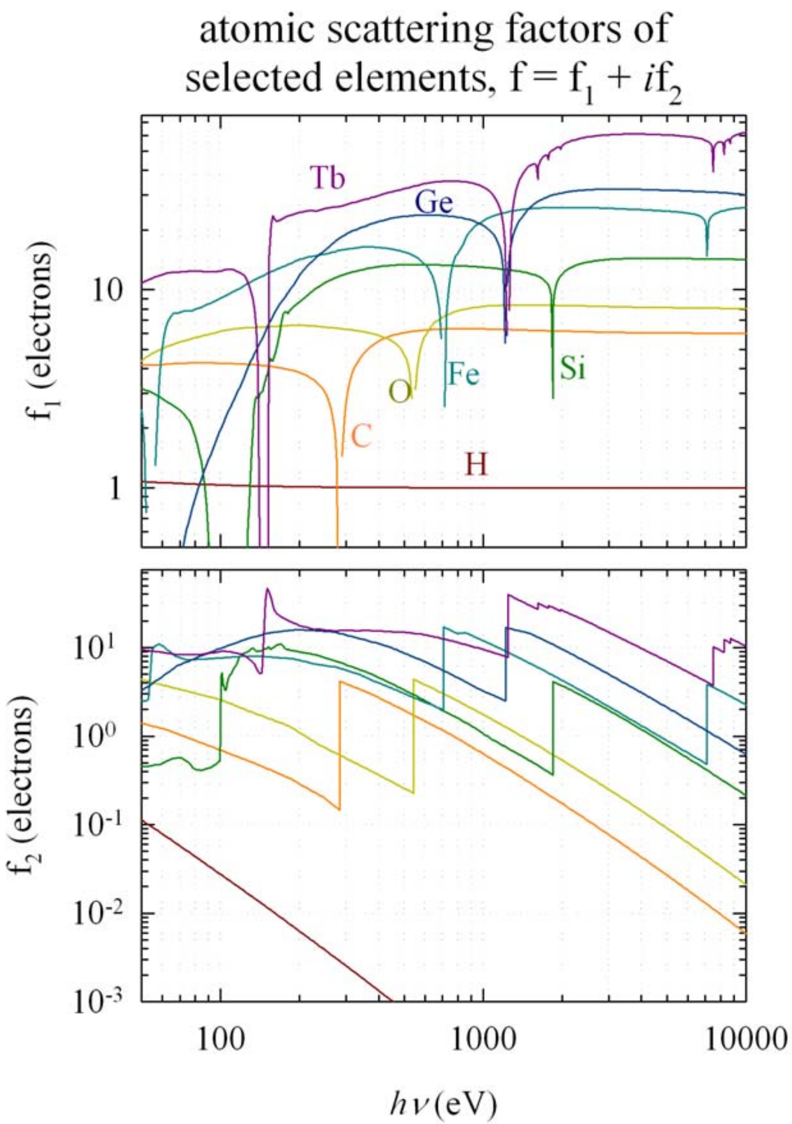
Contrast mechanisms

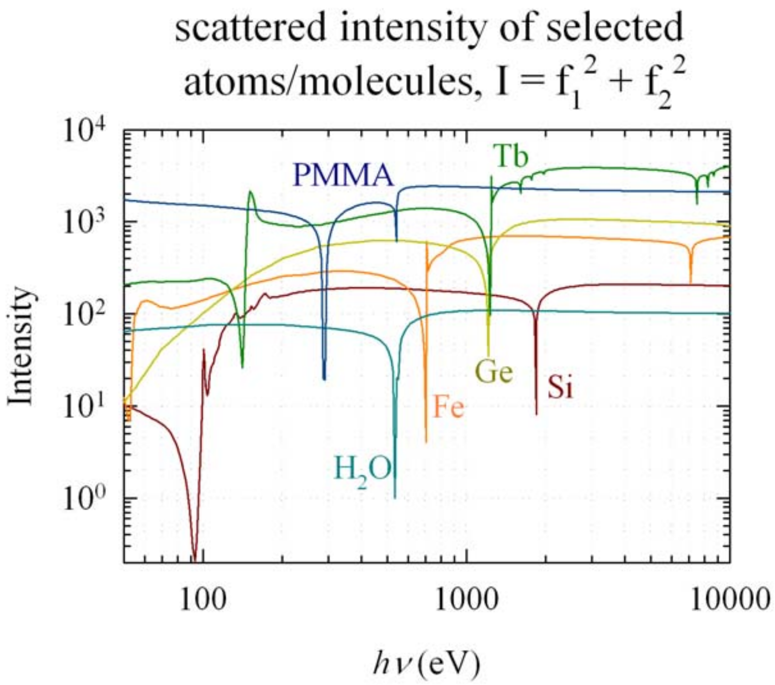
- charge, orbital sensitivity
- magnetic sensitivity (MCD, MLD)
- bond-specific sensitivity
- structural anisotropy (LD, CD)
- others ?

Chemical/functional properties

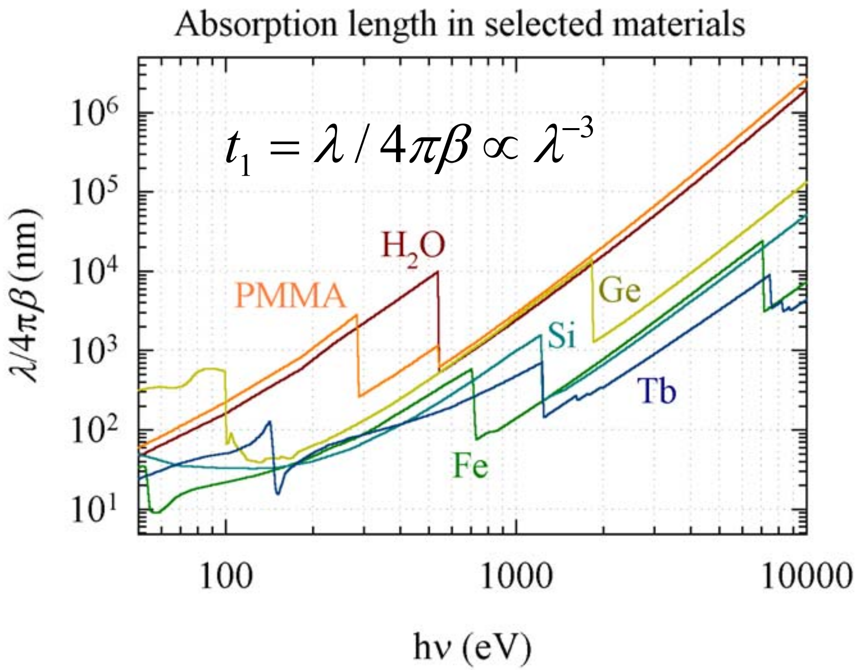
- electronic structure
- optical properties
- magnetism
- ferroelectricity
- piezzoelectricity
- assembly, dynamics
- others ?

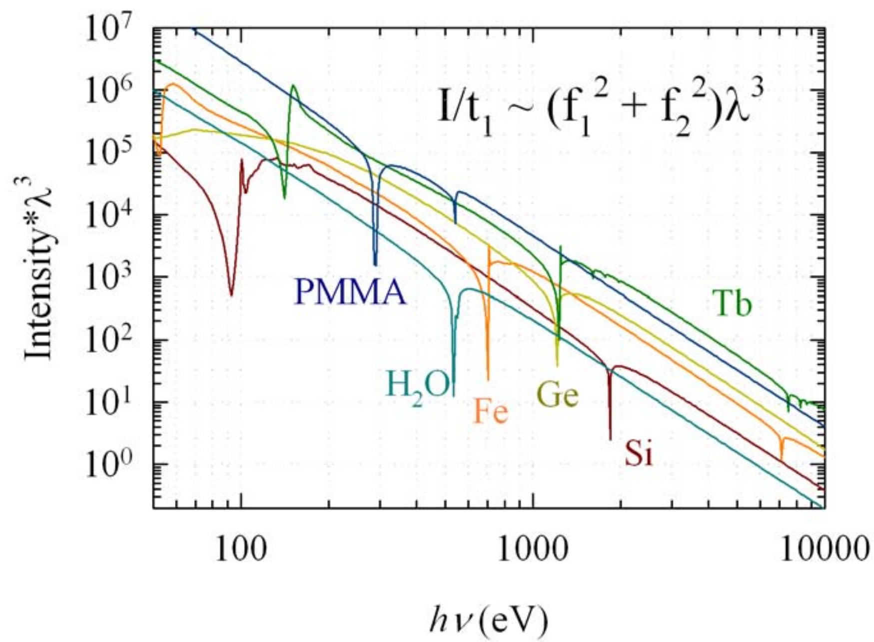
Energy trends in scattering factors, intensities





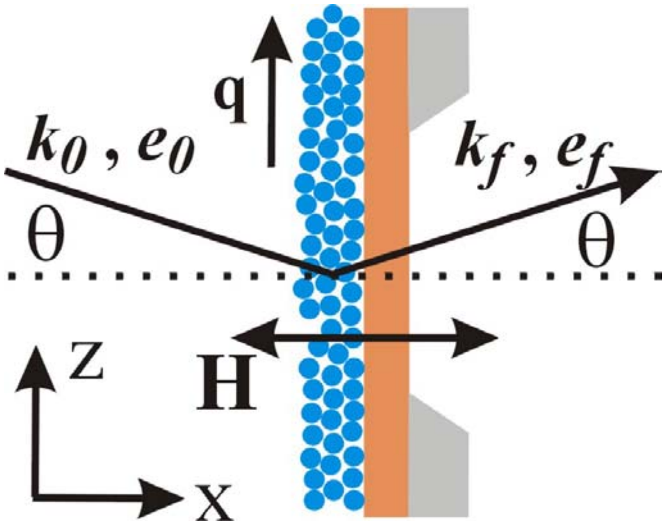
Scattered intensity/absorption length favors long λ to study nanoscale (*i.e.*, thin) materials.





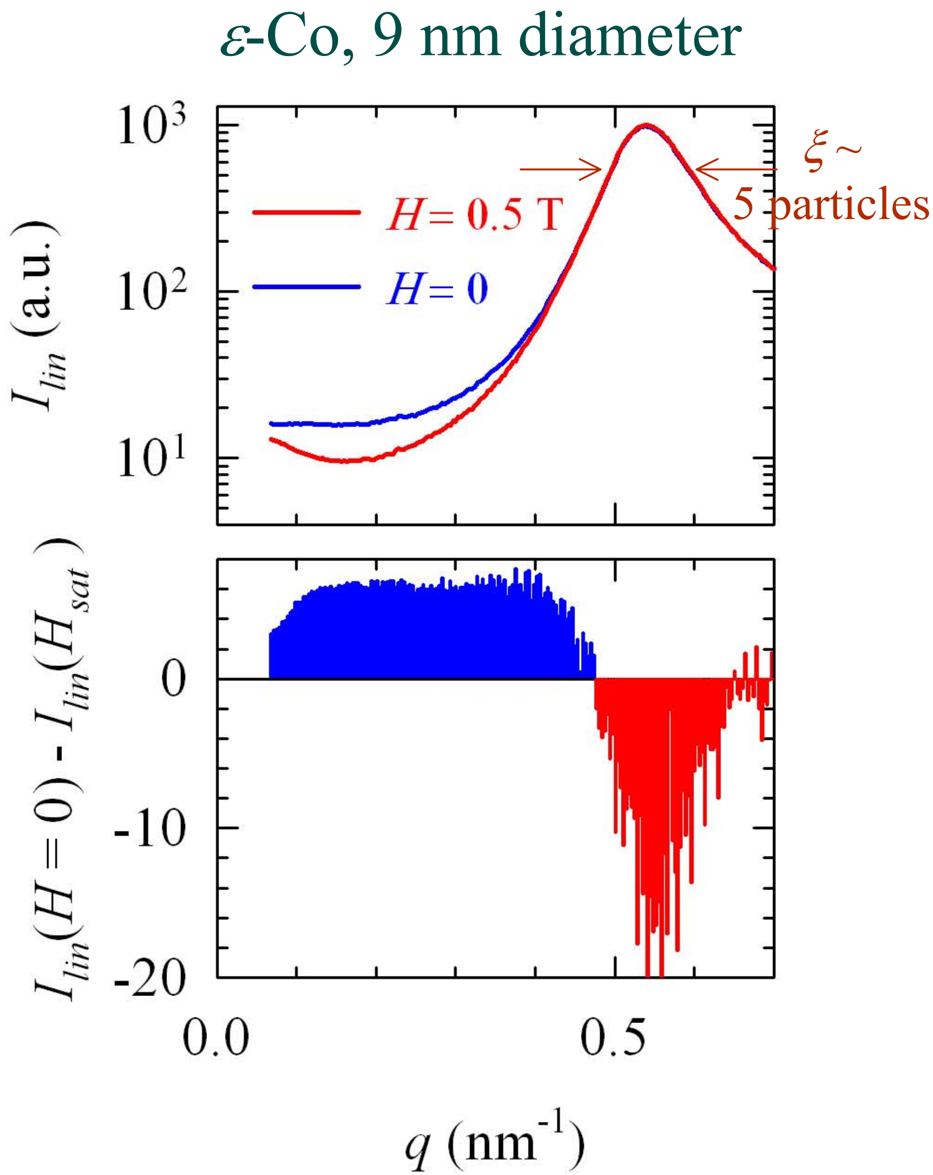
$$\beta(\omega) = \frac{r_0}{2\pi}\lambda^2 \sum_i N_i f_{2\,i}(\omega)$$

Example: Dipolar interactions in dense Co nanoparticle assemblies – are they significant?



$$I_{lin}(q,H) = I_{charge-charge}(q) + I_{mag-mag}(q,H)$$

$\Delta I_{lin}(q,H)$ gives remanent paramagnetic scattering.



Stronger than random paramagnetic scattering in ε-phase sample indicates significant dipolar interactions

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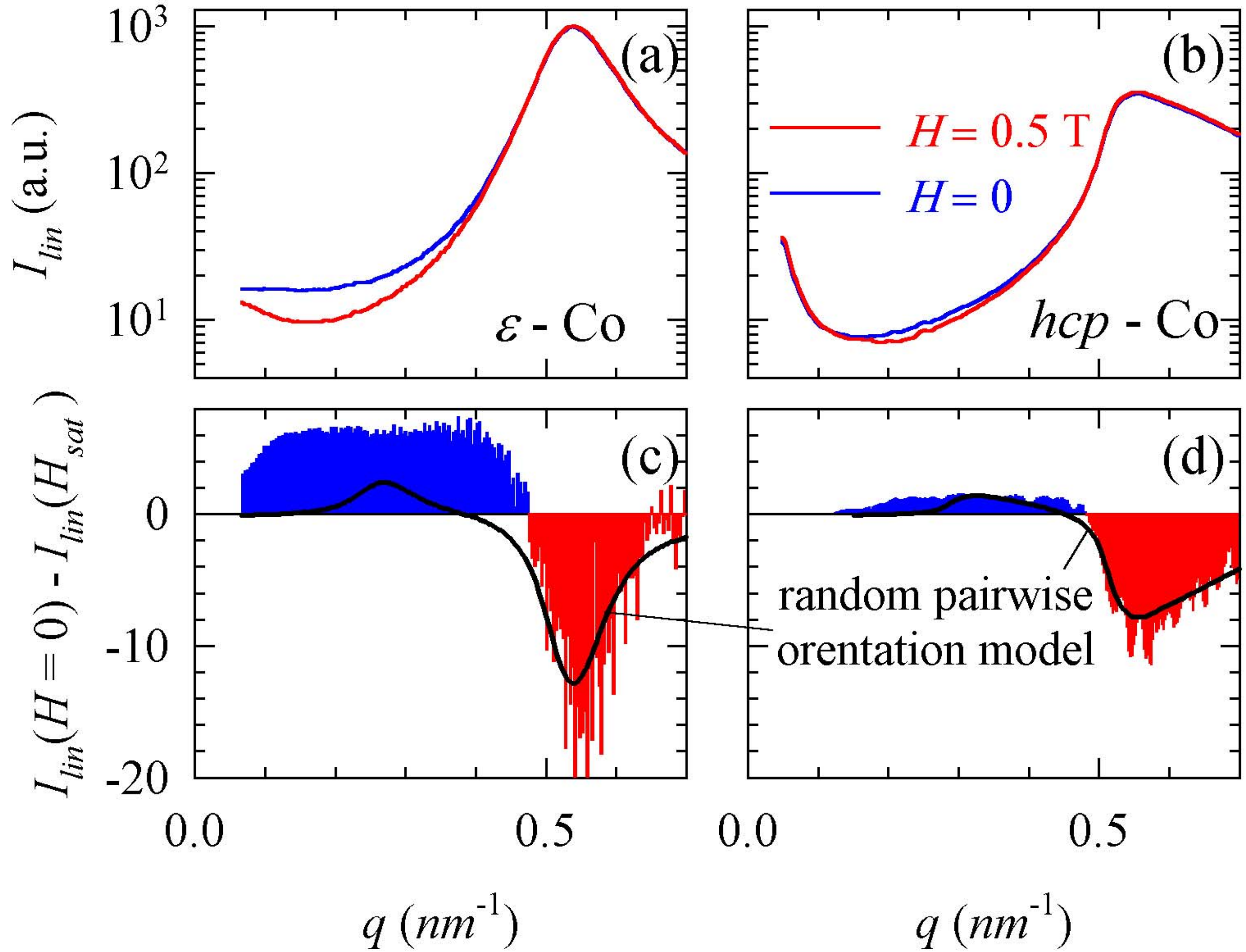


General beamline plan: chicane long undulator into two short EPUs, one for scattering

Resolving power 3000 to 7500 (and higher at reduced flux)

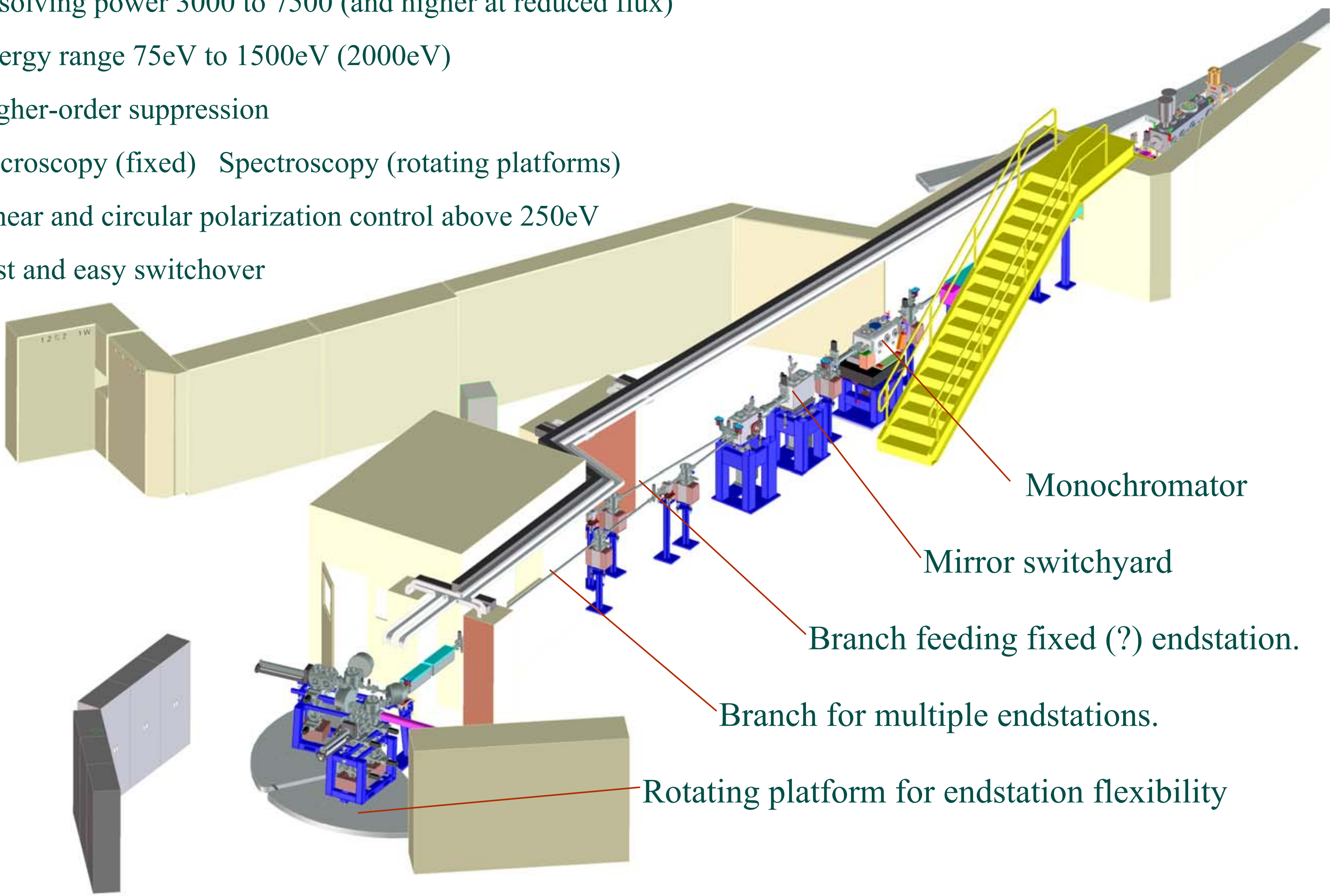
Energy range 75eV to 1500eV (2000eV)

Higher-order suppression

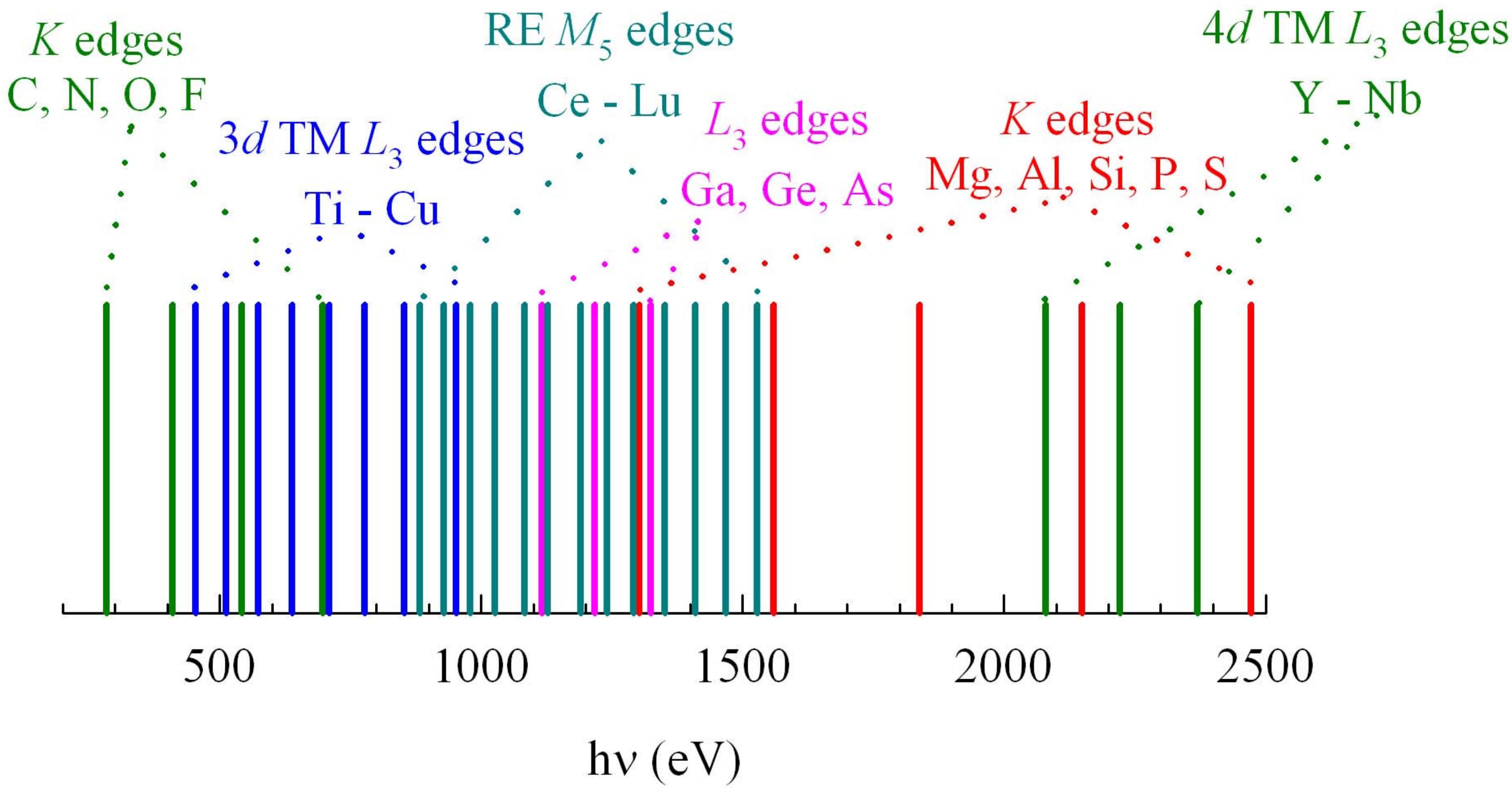
Microscopy (fixed) Spectroscopy (rotating platforms)

Linear and circular polarization control above 250eV

Fast and easy switchover



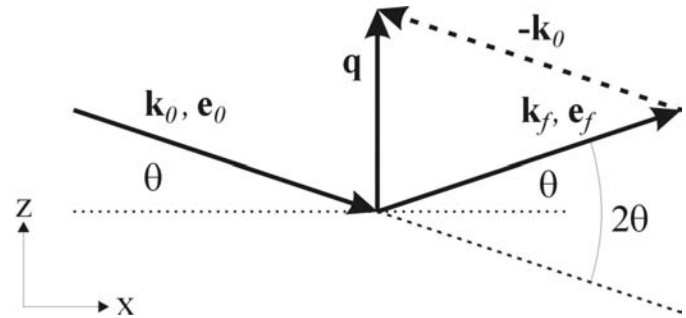
What energy range is required?

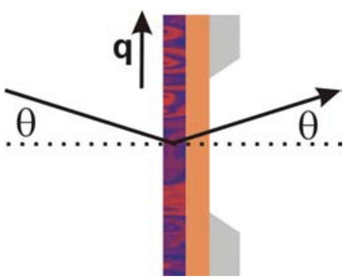


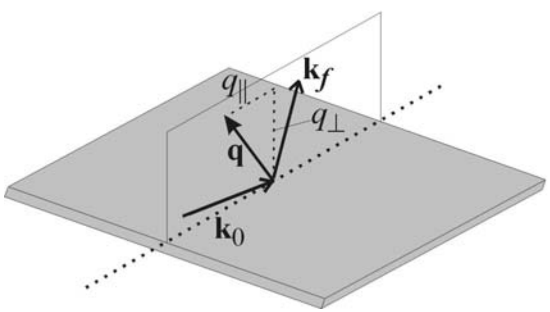
Beamline specifications?

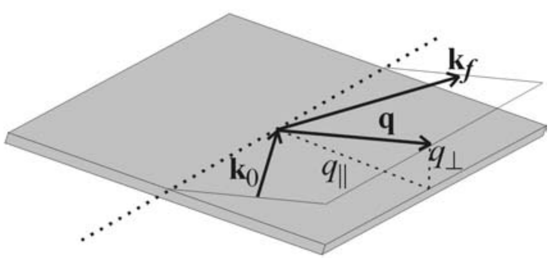
- Energy range?   (150 eV – 2???
- Energy resolution (temporal coherence)?
- Energy scanning?
- Energy stability?
- Maximize flux?
- Maximize transverse coherence?
- Spot size?
- Sensitivity to beam motion?

Scattering geometries: what is needed?



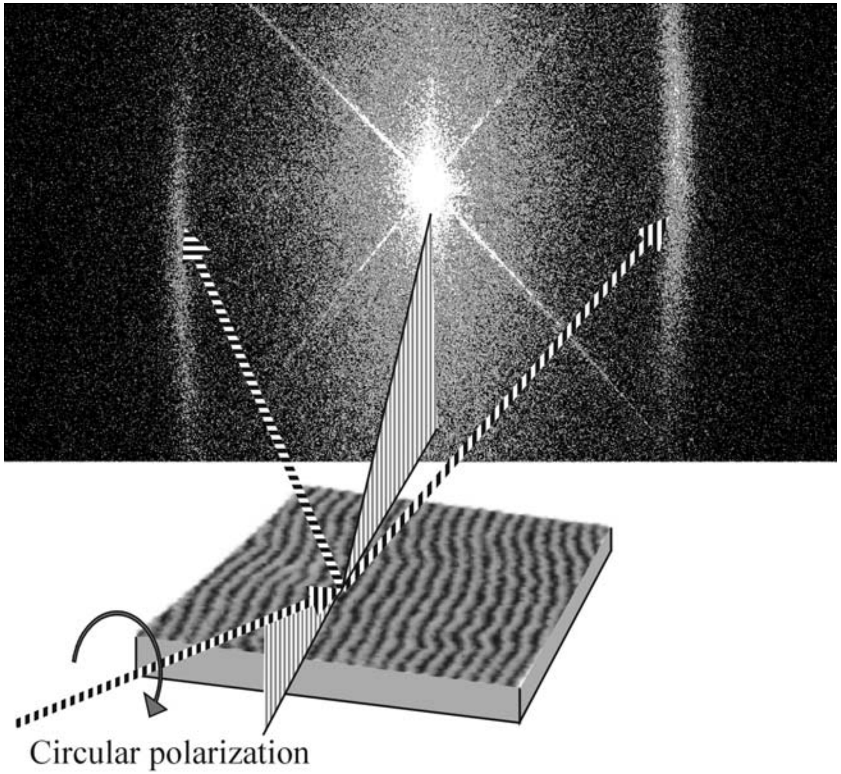






- Transmission
- Specular reflection
- Off-specular reflection
- Grazing incidence
- Single crystal diffraction

Detector schemes: what is best?



K. Chesnel

- CCD, 2-D array
- Linear array
- Apertured detector
- Large angular range
- Other ?

Sample environments: Hard matter/magnetism

Applied fields (H, E)?

Temperature range?

Vacuum requirements?

Sample transfer?

In situ sample prep., processing?

Sample environment: Soft matter

Vacuum requirements?

Temperature?

Applied fields?

In situ processing?

Provision for liquid, wet, frozen samples?

Endstations needed to satisfy hard and soft matter communities?

One for each?

More than one for each?

Future flexibility important?

What development is needed?