XRD endstation:
condensed matter systems

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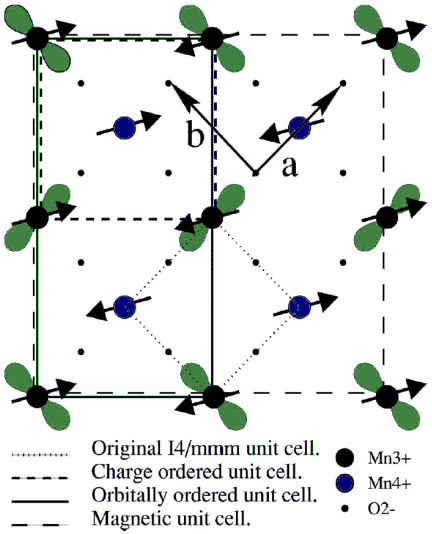
Outline

- Motivation
- Baseline XRD setup
- R&D setup
- Two-color operation and split&delay line
- Sample preparation

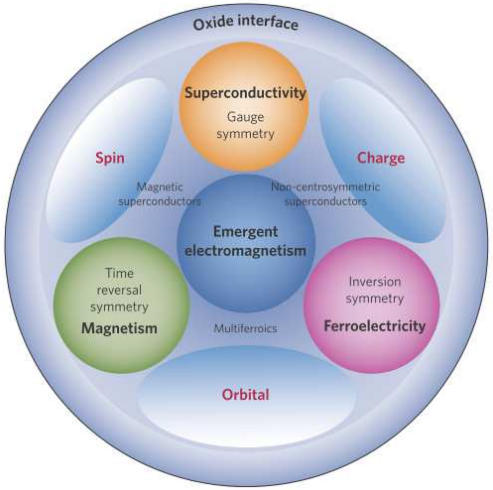
Motivation

Physics of comples materials is determined by different degrees of freedom (i.a. nuclear, charge, spin, orbital) and their interplay

Charge, orbital and spin order in $La_{0.5}Sr_{1.5}MnO_4$

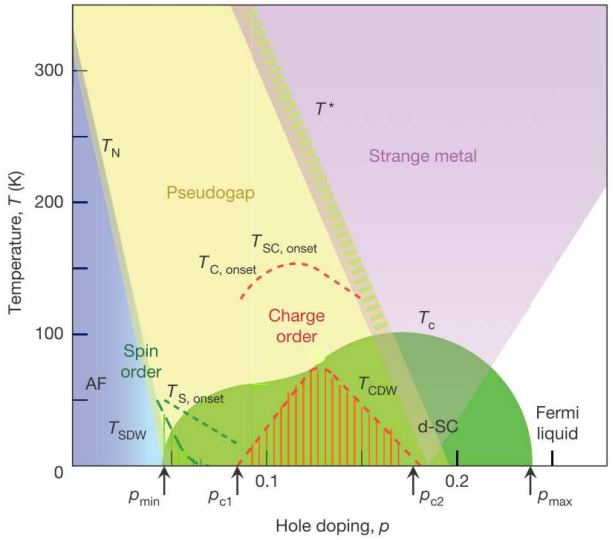


C. W. M. Castleton and M. Altarelli, Phys. Rev. B 62, 1033 (2000).



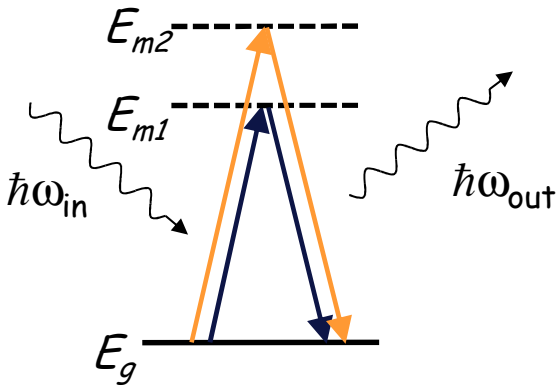
H.Y. Hwang et al., Nature Materials 11, 103 (2012).

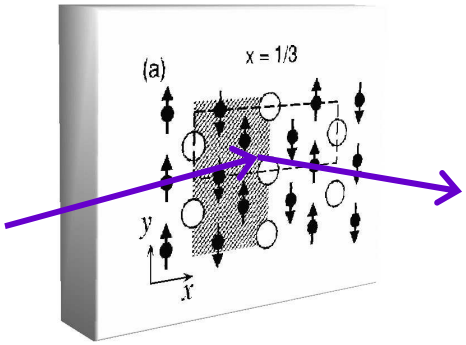
Phase diagramm of copper-oxide superconductors

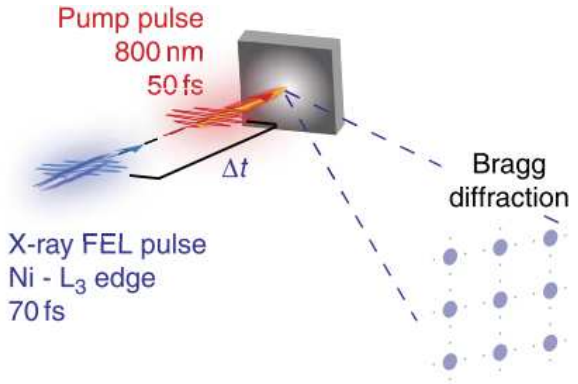


B. Keimer et al., Nature 518, 179 (2015).

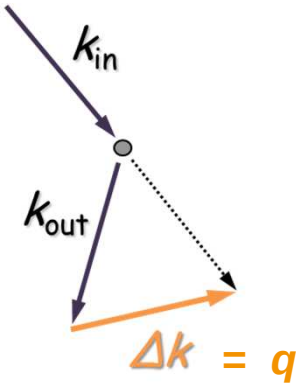
Resonant x-ray diffraction

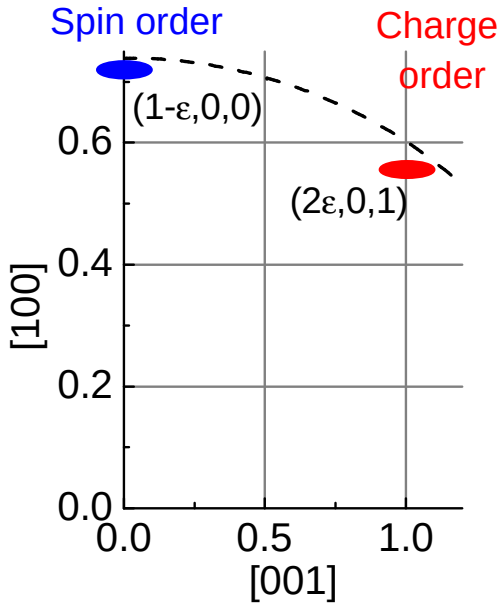


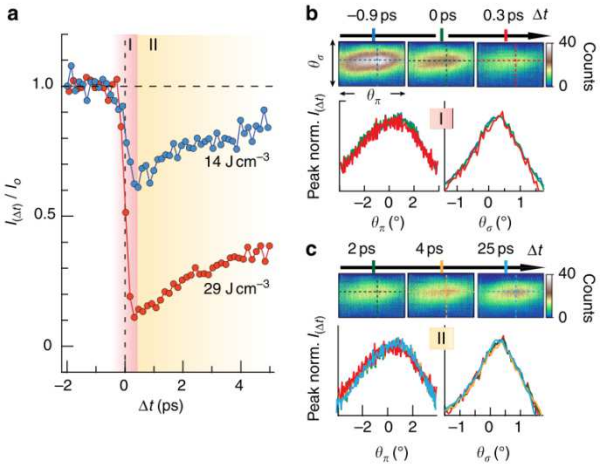




Laue condition:



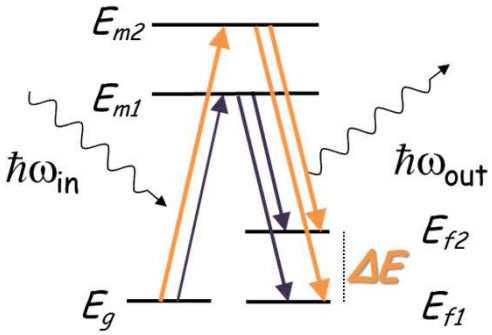


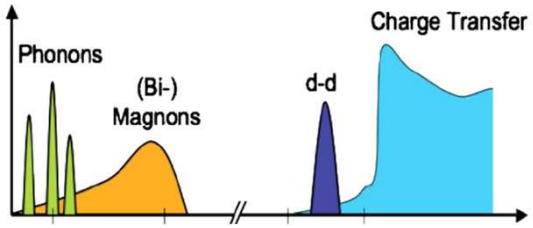


W.S. Lee et al., Nature Communications 3, 838 (2012).

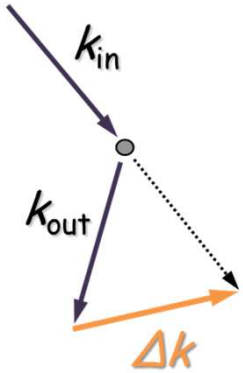
Schüssler-Langeheine & Schlappa et al.

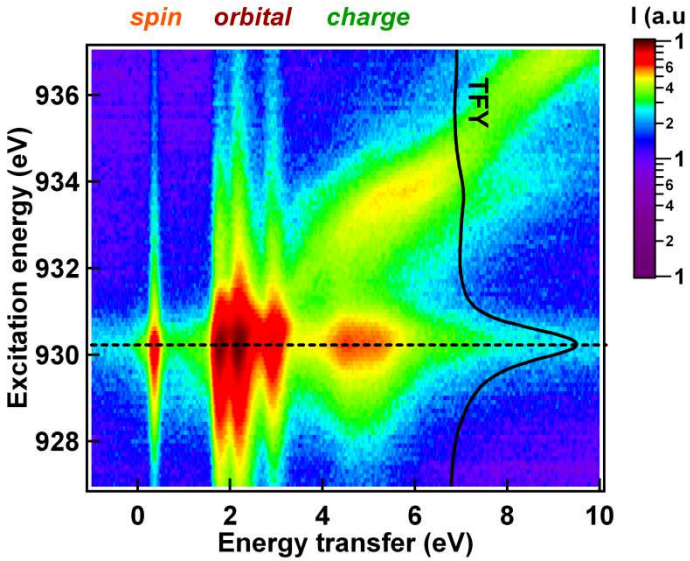
Resonant inelastic x-ray scatttering (RIXS)

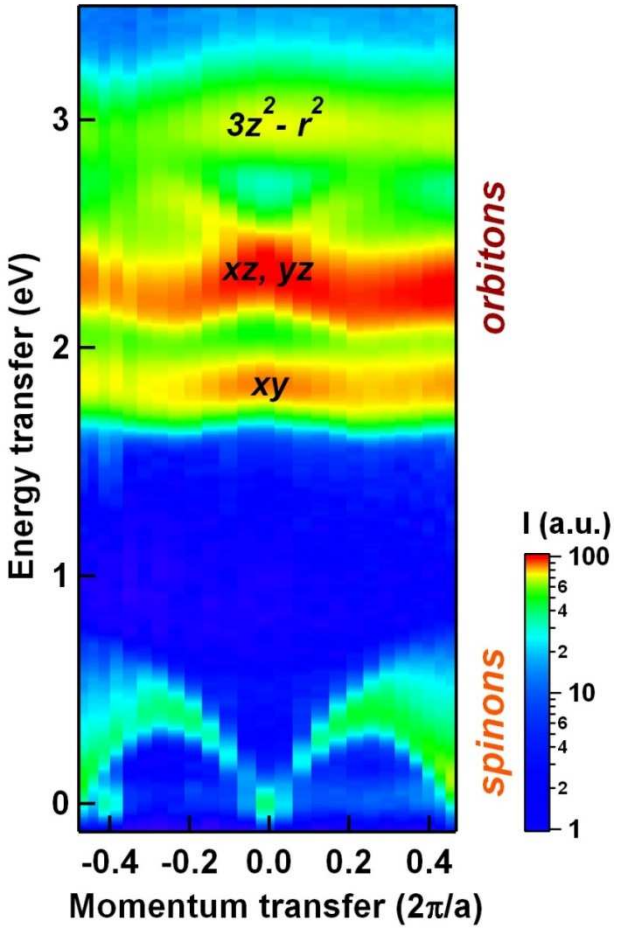




L.J.P. Ament *et al.*, Rev. Mod. Phys. 83, 705 (2011).







J. Schlappa *et al.*, Nature 485, 82 (2012).

See also talk: Stefan Neppl

Baseline SCS setup: X-ray Resonant Diffraction (XRD)

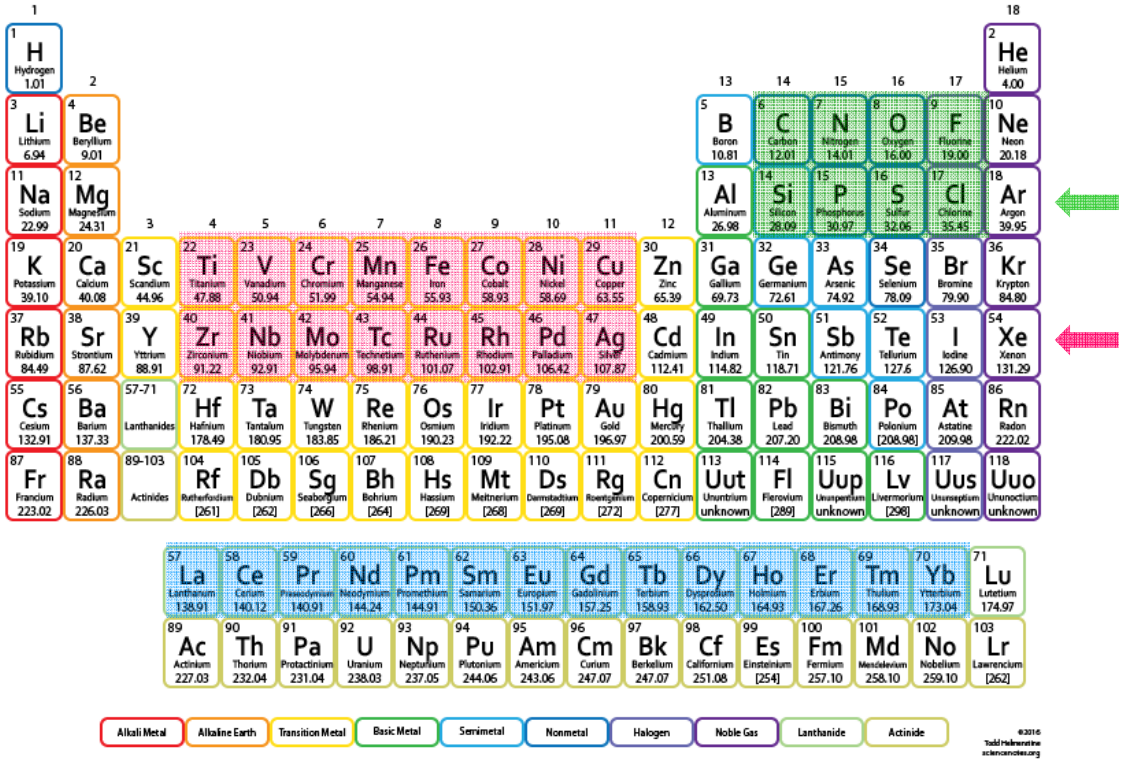
- Solid samples
- Techniques: Spectroscopy and Diffraction
  - Resonant x-ray diffraction
  - Reflectivity
  - X-ray absorption
  - Resonant inelastic x-ray scattering (hRIXS)
  - Pump-probe experiments / Nonlinear studies/ Single-shot experiments
- Soft and tender x-ray range: 0.25 keV – 3 keV
- Pump laser: UV / Optical / IR / THz

Resonances in the energy range: **250 – 3,000 eV**

***K*-edges**

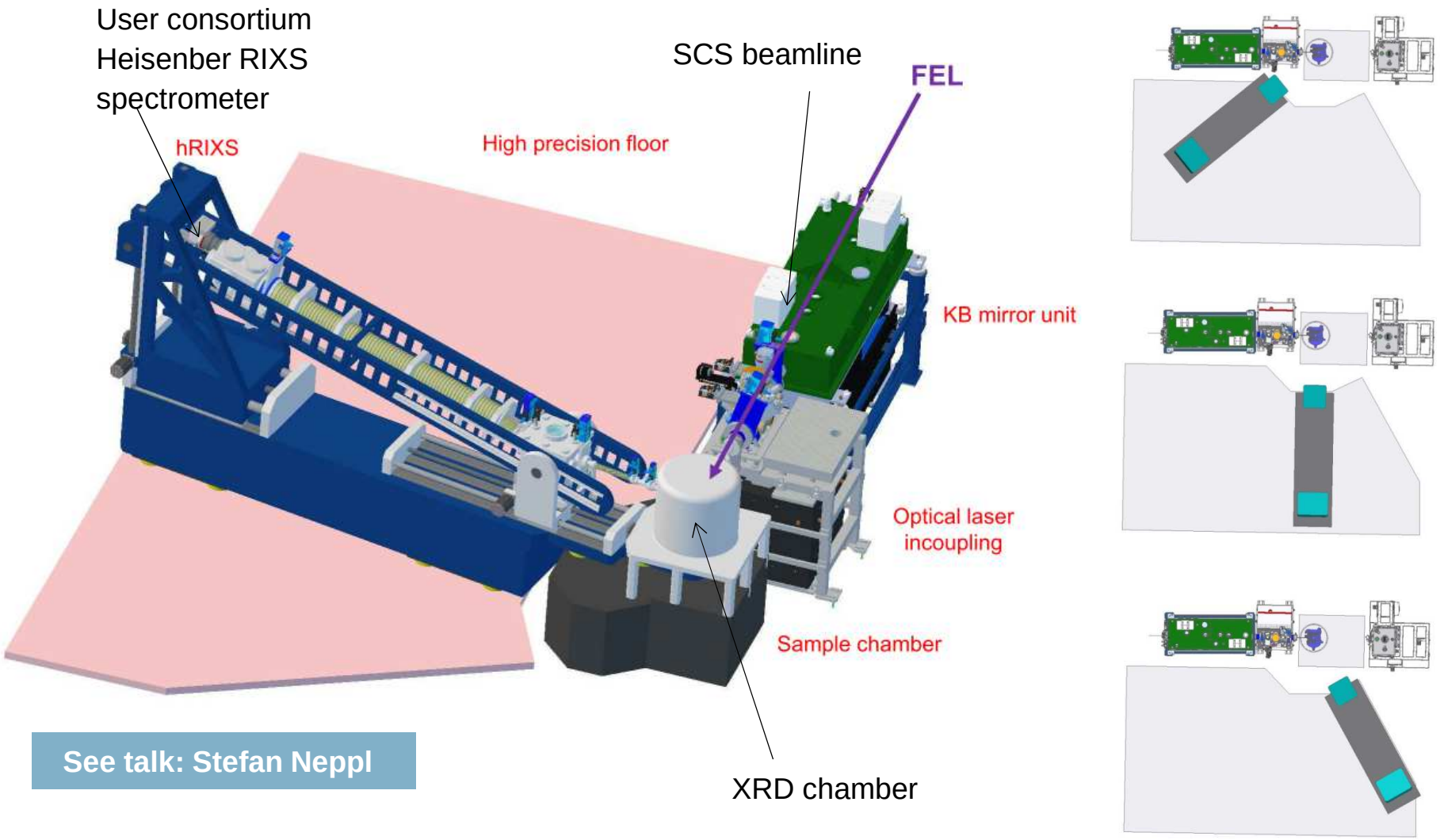
***L*$_{2,3}$-edges**

***M*$_{4,5}$-edges**



Particularly: accessibility of **structural reflections** down to **~ 2 Å**

Experimental setup:

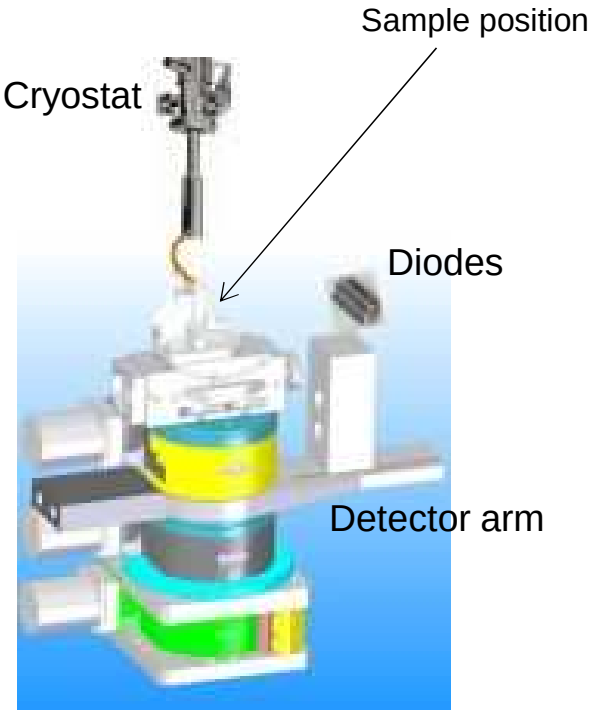


See talk: Stefan Neppl

XRD sample environment:

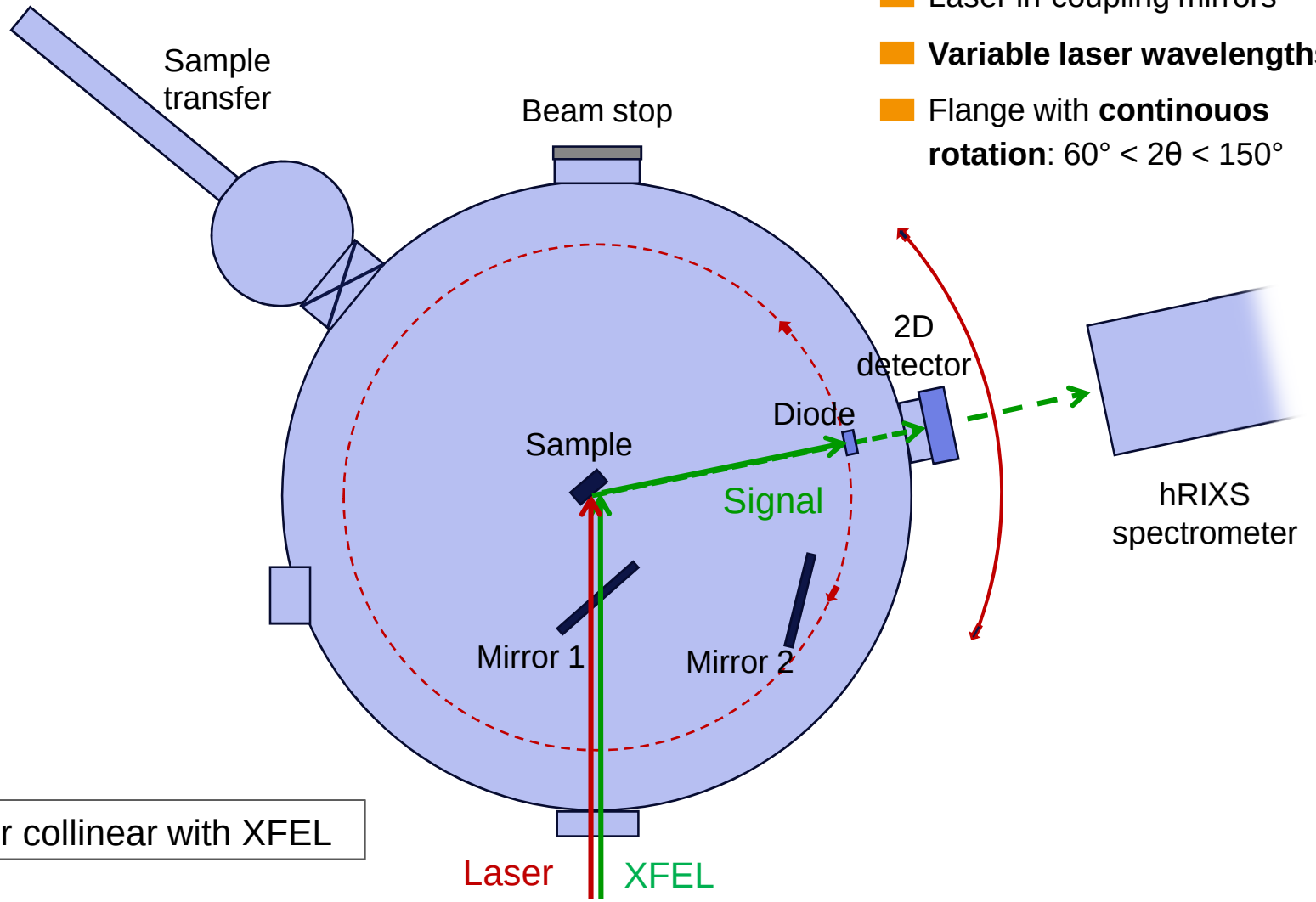
- **UHV**, solid samples
- Temperature range: **20–300 K**
- Sample motion: **6 degrees**
- Detector motion: 1 degree (2θ)
- Planned for Q1, 2018

Motion	Range	Resolution
X	± 10 mm	0.05 µm
Y	± 10 mm	0.05 µm
Z	± 10 mm	0.05 µm
Azimuth	± 180 deg	0.05 deg
Flip	± 30 deg	0.05 deg
Theta	± 180 deg	0.01 deg
TwoTheta	± 180 deg	0.01 deg



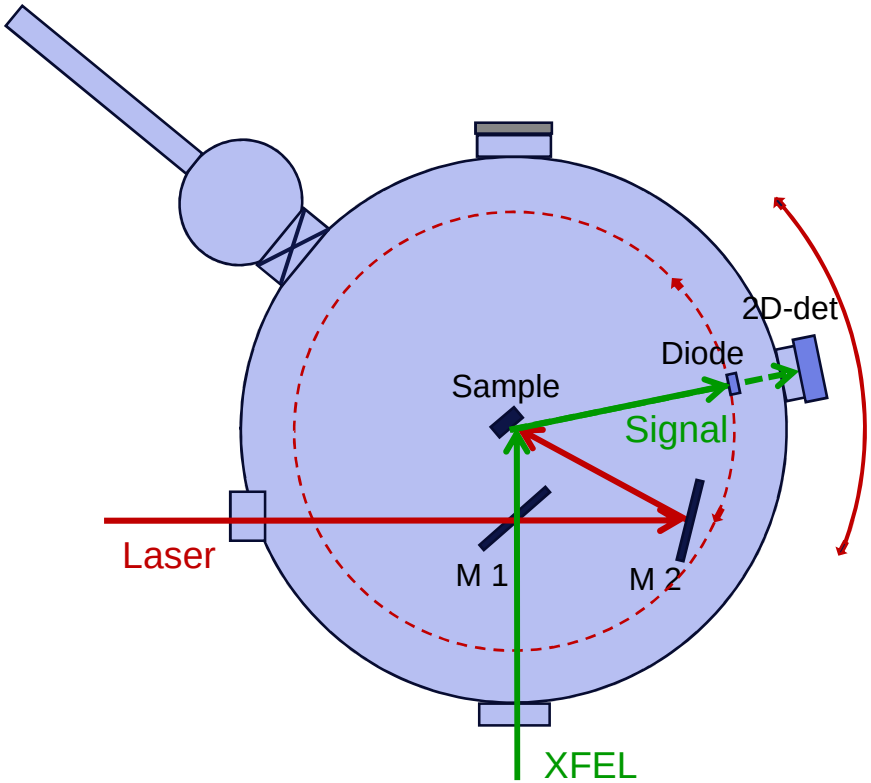
XRD experimental geometry:

- Sample transfer system
- Laser in-coupling mirrors
- **Variable laser wavelengths**
- Flange with **continouos rotation**: 60° < 2θ < 150°

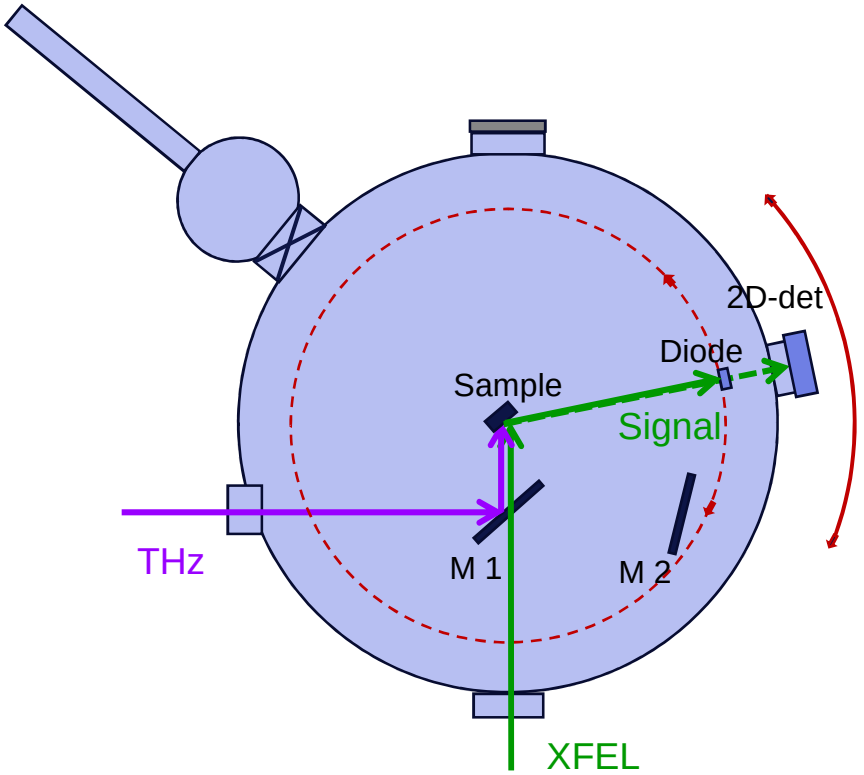


Laser collinear with XFEL

XRD experimental geometry:



Laser non-collinear with XFEL



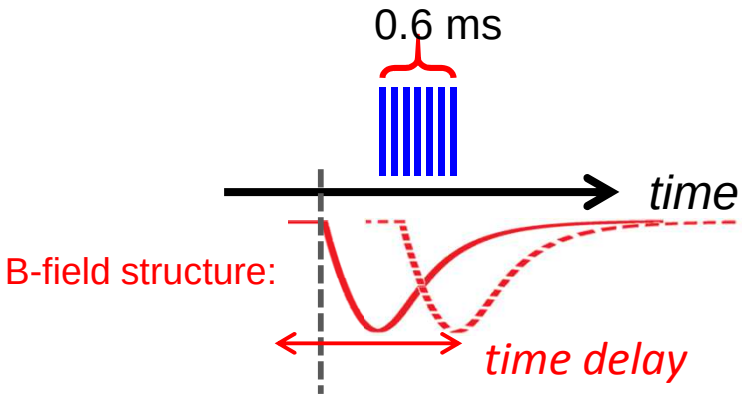
THz collinear with XFEL

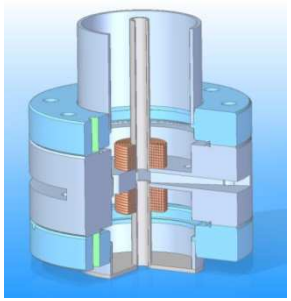
See talk: Robert Carley

R&D, B-field setup:

See talk: James Moore

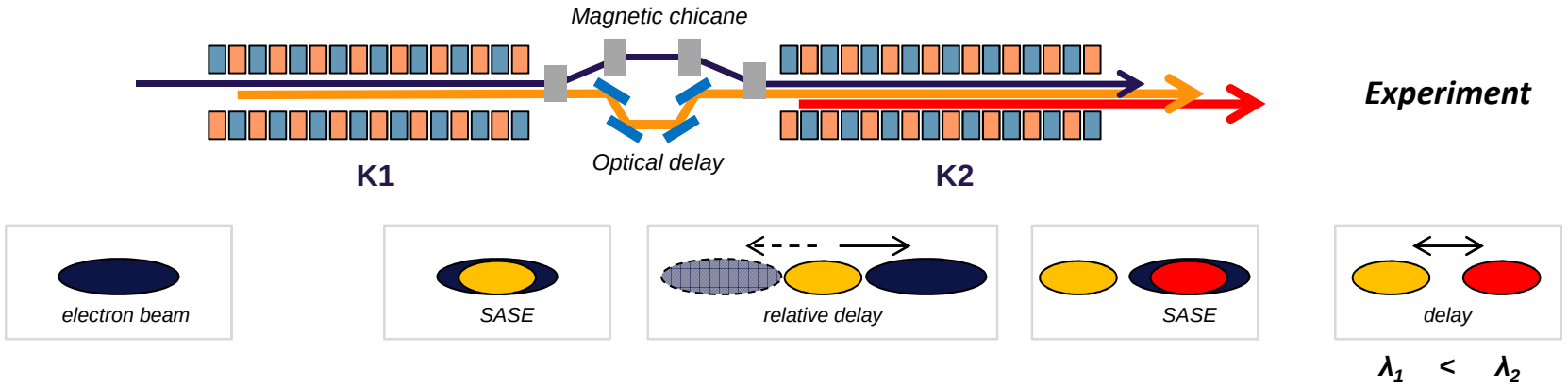
- Simple setup, easily adaptable for specific user requirements
- Special feature: pulsed magnet, fields up to **15 T**
- Temperature range: **4–300 K**
- Field direction: initially vertical, later also horizontal
- Sample degrees of motion: X, Y, Z, θ
- Sample transfer system
- Planned for 2018



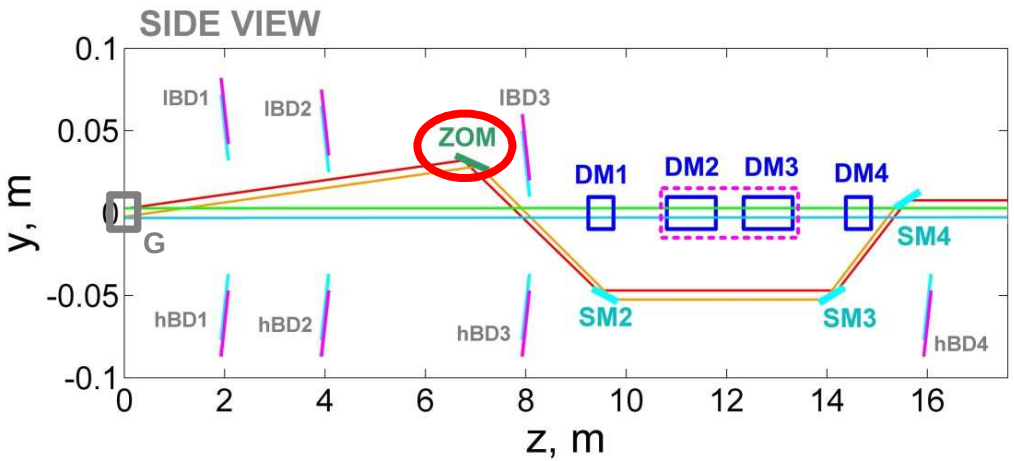


Two-color SASE3 operation

See talk: Svitozar Serkez



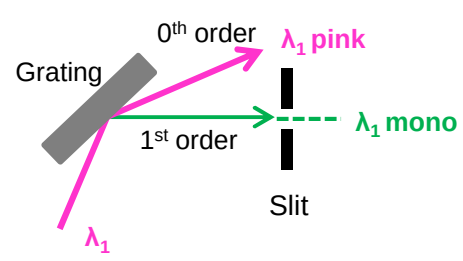
Concept of optical X-ray split and delay device for SASE3

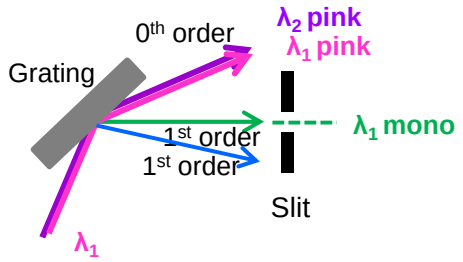


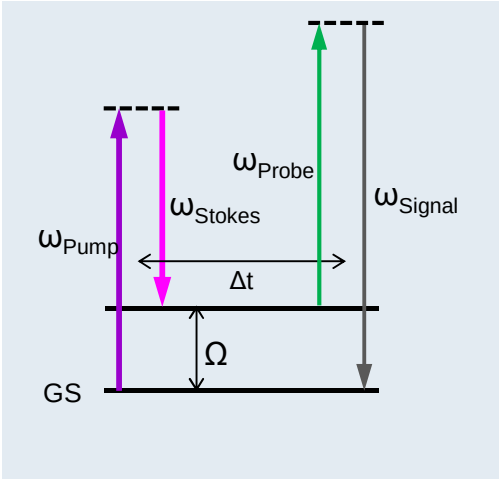
(by AlexanderYaroslavtsev)

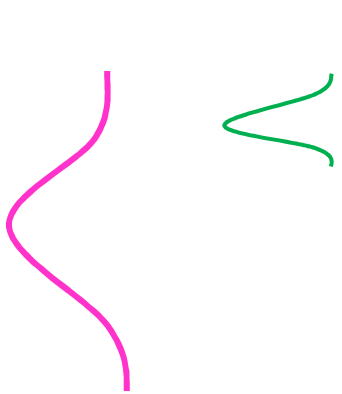
- Recombination of different grating reflection orders at the optical axis

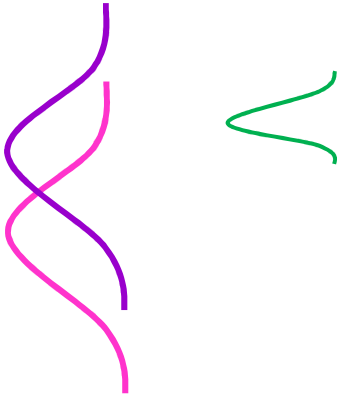
Nonlinear studies: Time-resolved CARS

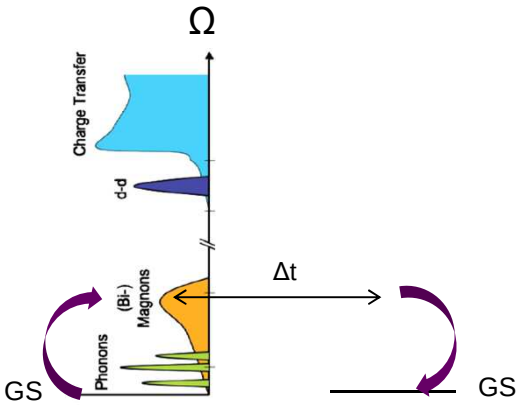


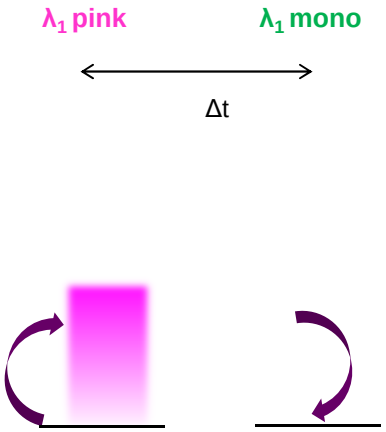


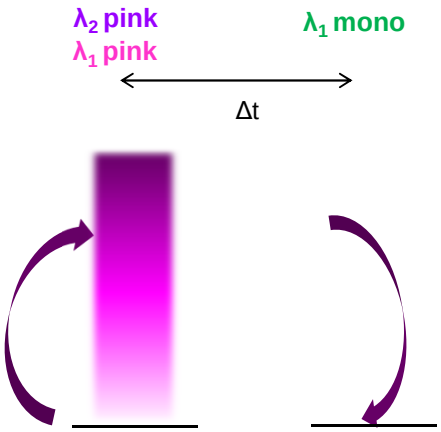












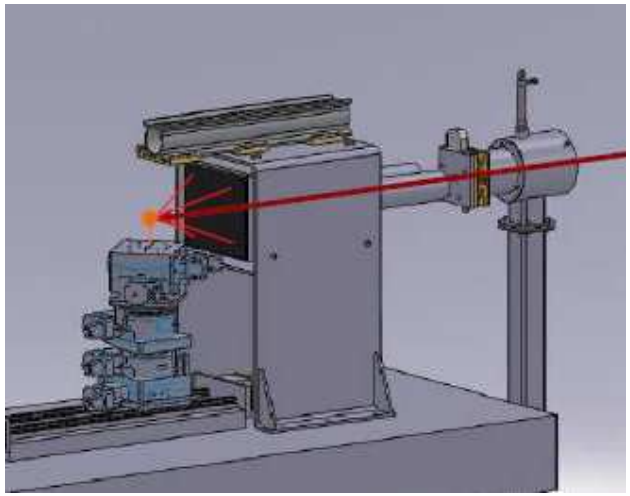
User lab

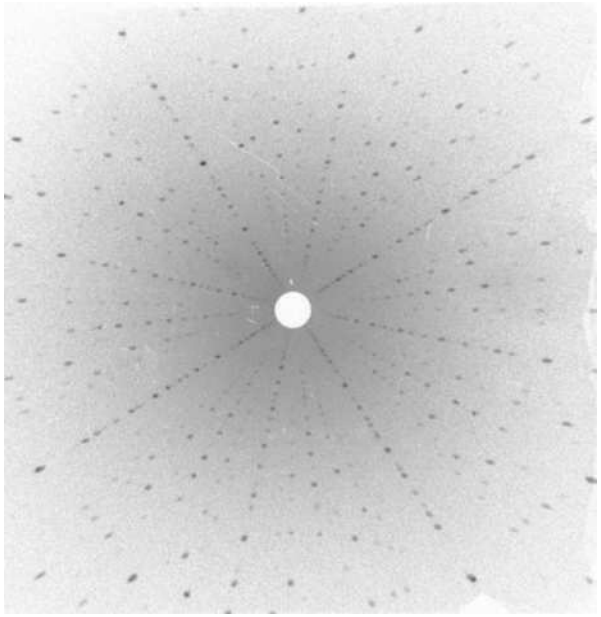
Possibility to determine the **orientation of pre-oriented** crystals.

See talk: Carsten Deiter

Are there further demands from users?, e.g.:

- alignment of crystals of unknown orientation (Laue setup)
- sample preparation
- ??





Summary

- XRD setup for spectroscopy, resonant diffraction and RIXS
- Energy extends to tender x-rays: additional resonances + structural studies accessible
- Pump laser: tunable wavelengths ranging from THz to UV
- R&D setup for special requirements and for B-field studies
- Two-color operation and split&delay line: novel experimental opportunities at SASE 3
- Sample preparation: user requirements?

Thank you !

Acknowledgements:

SCS group (WP-86)

Sample environment (WP-79)

Simulation of Photon fields (WP-72)