Principles of Non-Relativistic Scattering Applications to Quantum Matter

06.02-10.02 (2023)

Lectures by: Prof. Thomas Gehrmann, Prof. Johan Chang and Dr. Artur Gregor

Practical Information

	Monday	Tuesday	Wednesday	Thursday	Friday
Room	Y36J33	Y36J33	Y36J33	Y36J33	Y36J33
	Lecture 1 10-10h45 Johan	**Lecture 4** 10-10h45 Thomas	**Lecture 7** 10-10h45 Thomas	**Lecture 10** 10-10h45 Artur	**Lecture 13** 10-10h45 Johan
	Lecture 2 11-11h45 Johan	**Lecture 5** 11-11h45 Thomas	**Lecture 8** 11-11h45 Artur	**Lecture 11** 11-11h45 Artur	**Lecture 14** 11-11h45 Johan
	Lunch - Mensa	**Lunch - Mensa**	**Lunch - Mensa**	**Lunch - Mensa**	**Lunch - Mensa**
	Lecture 3 13h30-14h15 Thomas	**Lecture 6** 13h30-14h15 Thomas	**Lecture 9** 13h30-14h15 Artur	**Lecture 12** 13h30-14h15 Johan	**Lecture 15** 13h30-14h15 Johan
			Exercise Class 14h30-16		Exercise Class 14h30-16

Exam

Course Outline

Monday 06.02	Tuesday 07.02	Wed. 08.02	Thurs. 09.02	Friday 10.02
Lecture 1 10-10h45 Johan	**Lecture 4** 10-10h45 Thomas	**Lecture 7** 10-10h45 Thomas	**Lecture 10** 10-10h45 Artur	**Lecture 13** 10-10h45 Johan
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Lecture 3 13h30-14h15 Thomas	**Lecture 6** 14-14h45 Thomas	**Lecture 9** 13h30-14h15 Artur	**Lecture 12** 13h30-14h15 Johan	**Lecture 15** 13h30-14h15 Johan
		Exercise Class 14h30-16		Exercise Class 14h30-16

Introduction & overview. Why is scattering experiments important?

Theoretical background for scattering experiments

Scattering on condensed matter systems + Neutron scattering experiments

X-ray diffraction and spectroscopy techniques

Exercise 1 [*Yukawa and Coulomb potential*]

a) The Yukawa potential

$$V(r) = V_0 \frac{e^{-\mu r}}{\mu r}$$

describes the nucleon-nucleon interactions in the atomic nucleus. Its typical reach is $1/\mu$. Derive the scattering amplitude in the Born approximation and show that the scattering cross section is

$$\frac{d\sigma}{d\omega} = \left(\frac{2mV_0}{\mu 4\pi^2 h}\right)^2 \frac{1}{[2k^2(1-\cos\Theta)+\mu^2]^2}$$

b) Derive the scattering cross section for the Coulomb potential by considering the limit $\mu \to 0$ with

$$\frac{V_0}{\mu} = \frac{Ze^2}{4\pi\epsilon_0}$$

fixed.

Exercise 2 [*Born Approximation*]

a) Consider a spherically symmetric potential $V(\vec{r}) = g\delta(\vec{r})$, with g constant, and show that the Born approximation for the scattering amplitude is given by

$$f(\theta) = -\frac{m}{2\pi\hbar}g$$

b) Derive an expression for g if this potential is used to describe the scattering of thermal neutrons with scattering length b.

Exercise 3 [*Time evolution operator*]

The time evolution operator $U(t,t_0)$ fulfils the differential equation:

$$i\partial_t U(t,t_0) = H_I(t)\, U(t,t_0)\ .$$

Show that

a) $U(t,t_0)$ is unitary.

b) $U(t,t_0)$ can be expressed as Neumann series (use equivalent integral equation):

$$\begin{aligned} U(t,t_0) &= \mathbf{1} + (-i)\int_{t_0}^{t} dt_1 H_I(t_1) \\ &\quad + (-i)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, H_I(t_1) H_I(t_2) \\ &\quad + \dots \\ &\quad + (-i)^n \int_{t_0}^{t} dt_1 \dots \int_{t_0}^{t_{n-1}} dt_n\, H_I(t_1) H_I(t_2) \dots H_I(t_n) \\ &\quad + \dots \end{aligned}$$

c) $U(t,t_0)$ is given by the time-ordered product (insert into differential equation):

$$U(t,t_0) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^{t} dt_1 \dots \int_{t_0}^{t} dt_n\, T\left(H_I(t_1) \dots H_I(t_n)\right)\ .$$

Exercise 4 *Width of the diffraction maximum*

We assume that in a linear crystal on every lattice point $\vec{\rho} = m\vec{a}$, $m \in \mathbb{Z}$, there is an identical point-like scattering centre. The total amplitude of the scattered radiation is proportional to $F = \sum \exp\left(-im\vec{a} \cdot \Delta\vec{k}\right)$. The sum over M lattice points has the value

$$F = \frac{1 - \exp\left(-iM\vec{a} \cdot \Delta\vec{k}\right)}{1 - \exp\left(-i\vec{a} \cdot \Delta\vec{k}\right)} \tag{1}$$

when we use the series expansion

$$\sum_{m=0}^{M-1} x^m = \frac{1 - x^M}{1 - x}. \tag{2}$$

a) The scattered intensity is proportional to $|F|^2$. Show that

$$|F|^2 \equiv F^* F = \frac{\sin^2\left(\frac{1}{2}M\vec{a} \cdot \Delta\vec{k}\right)}{\sin^2\left(\frac{1}{2}\vec{a} \cdot \Delta\vec{k}\right)}. \tag{3}$$

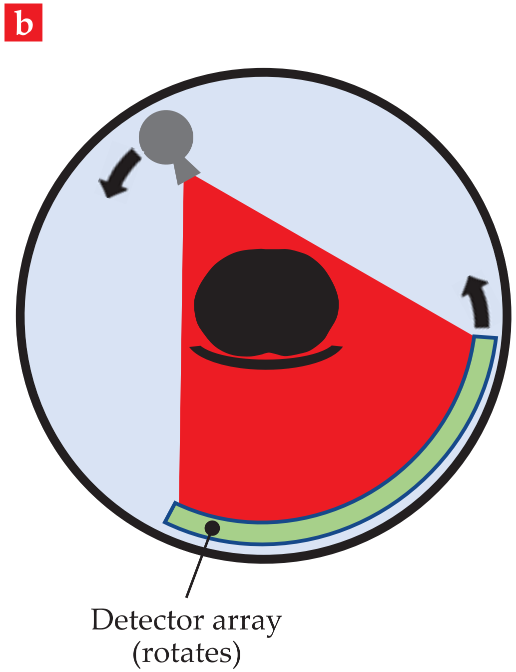
b) For $\vec{a} \cdot \Delta\vec{k} = 2\pi h$, $h \in \mathbb{Z}$, a diffraction maximum appears. We change $\Delta\vec{k}$ slightly and define ε in $\vec{a} \cdot \Delta\vec{k} = 2\pi h + \varepsilon$ such that ε gives the first zero-crossing of the function $\sin\left(\frac{1}{2}M\vec{a} \cdot \Delta\vec{k}\right)$. Show that $\varepsilon = 2\pi/M$. What does this mean for the width of the diffraction maximum?

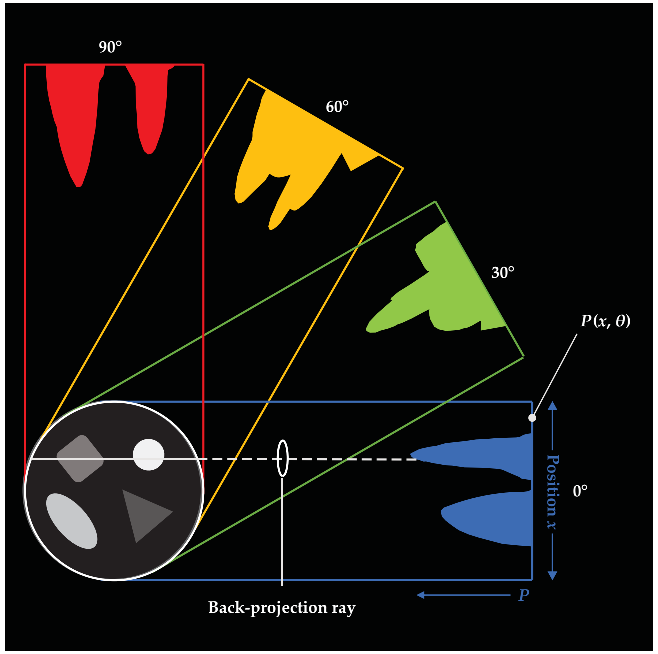
From Kittel

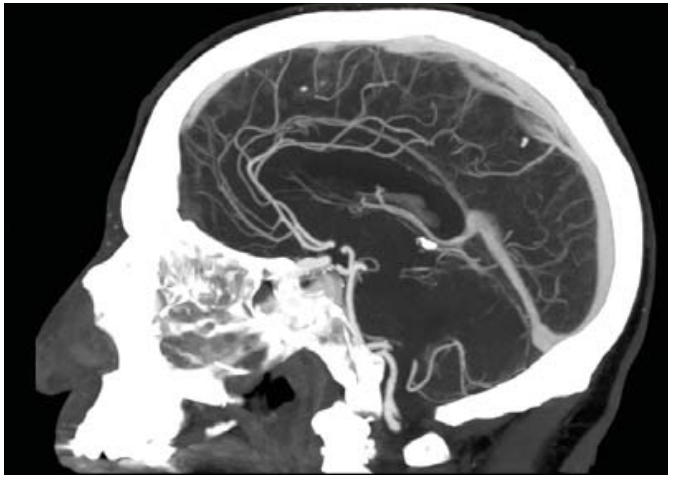
Computed tomography turns 50

John M. Boone and Cynthia H. McCollough

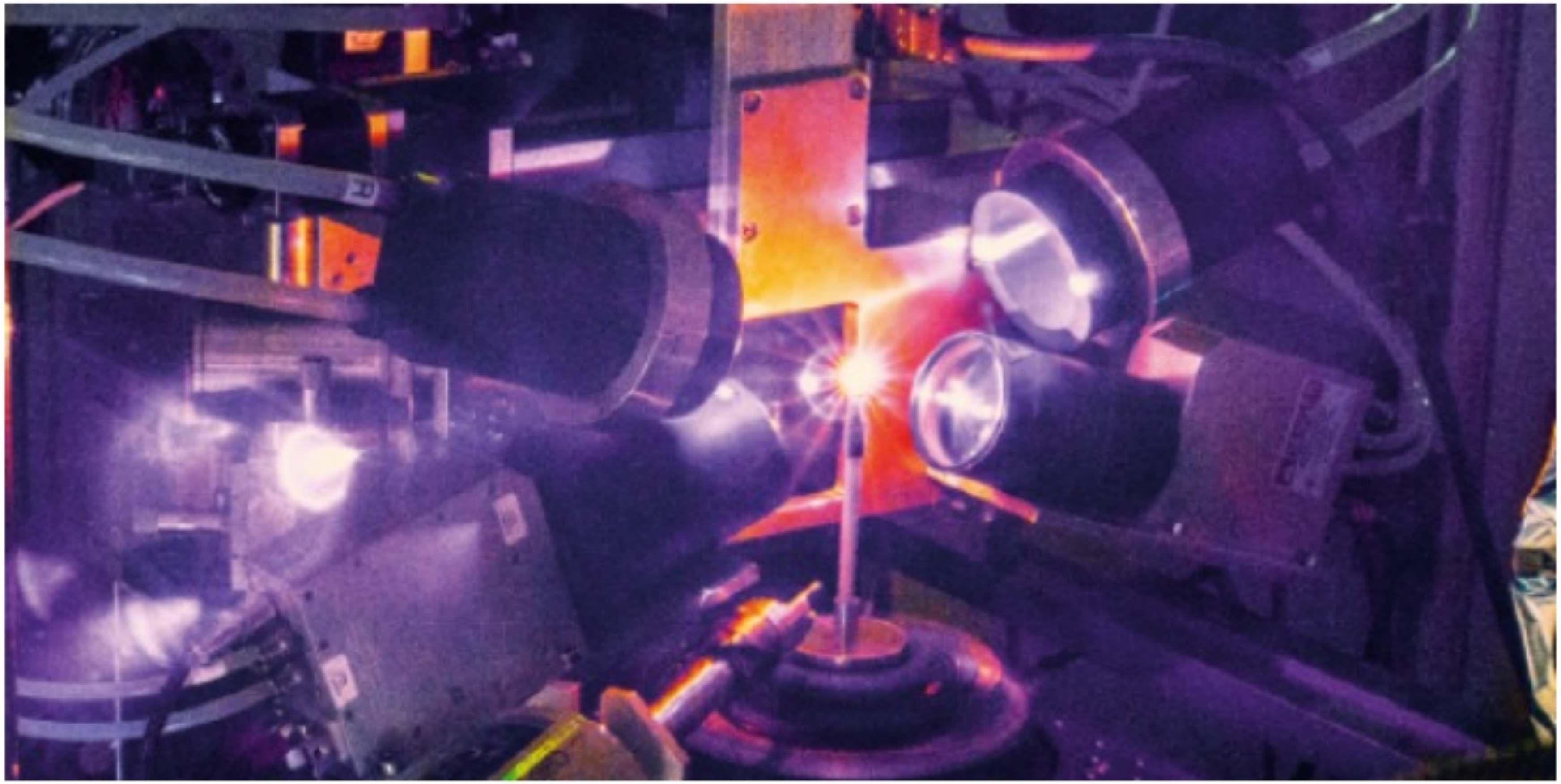
Physics Today **74**, 9, 34 (2021)







Nobel price in Medicine 1979
Allan Cormack & Godfrey Hounsfield

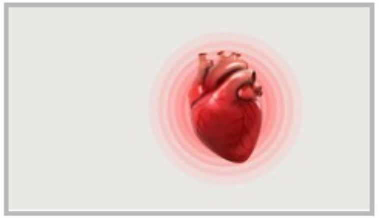


TOMCAT - X02DA: Tomographic Microscopy

A beamline for TOmographic Microscopy and Coherent rAdiology experimenTs

31 January 2023

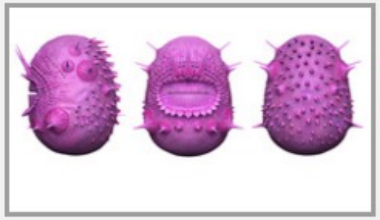
X-ray tomography helps understand how the heart beats



Researchers at the Swiss Light Source SLS use X-ray phase contrast imaging to study a heart in action as it beats.

17 August 2022

Weird fossil is not our ancestor

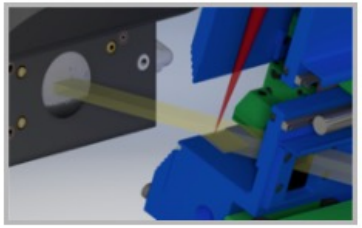


Research Using Synchrotron Light

X-ray light solves puzzle of human ancestry

17 January 2022

Direct observation of crack formation mechanisms with operando Laser Powder Bed Fusion X-ray radiography



Operando high-speed X-ray radiography experiments reveal the cracking mechanism during 3D laser printing of a Ni superalloy.

24 September 2021

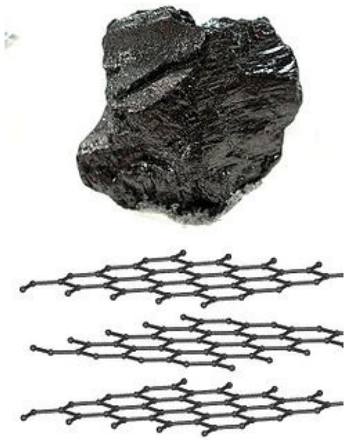
X-ray microscopy with 1000 tomograms per second

Research Using Synchrotron Light | Materials Research | Future Technologies

A team at the Swiss Light Source SLS have set a new record using an imaging method called tomoscopy.

Scattering - highlights

Nobel Prizes
1914 & 1915 Physics
Laue, Bragg & Bragg

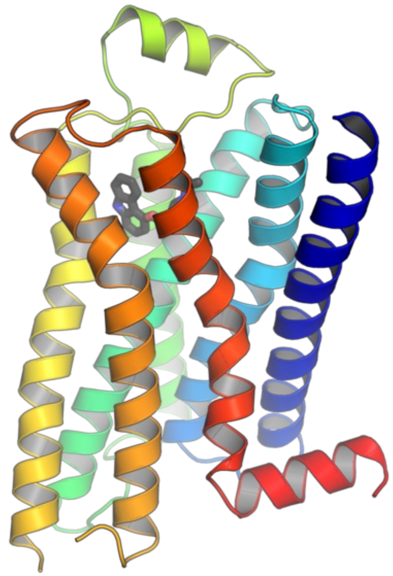


Structures solved
1917 Graphite
1919 $NaNO_3$ & $CsICl_2$

Nobel Prize
1962 Medicine
Watson, Crick & Wilkins

DNA structure solved

Nobel Prize
2012 Chemistry
Watson, Crick & Wilkins



Protein structures

X-ray Scattering Methodology

LAUE

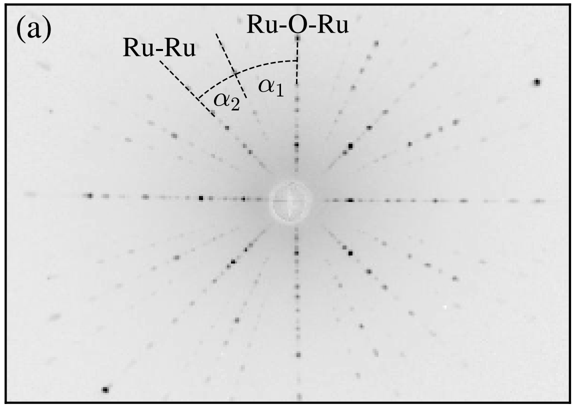
Rotating Crystal

Powder

Scherrer & Debye

Poly-chromatic Light

Mono-chromatic Light



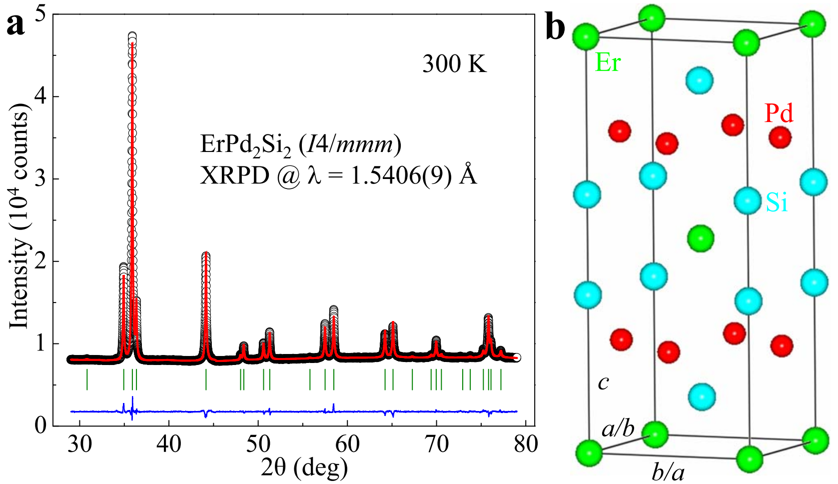
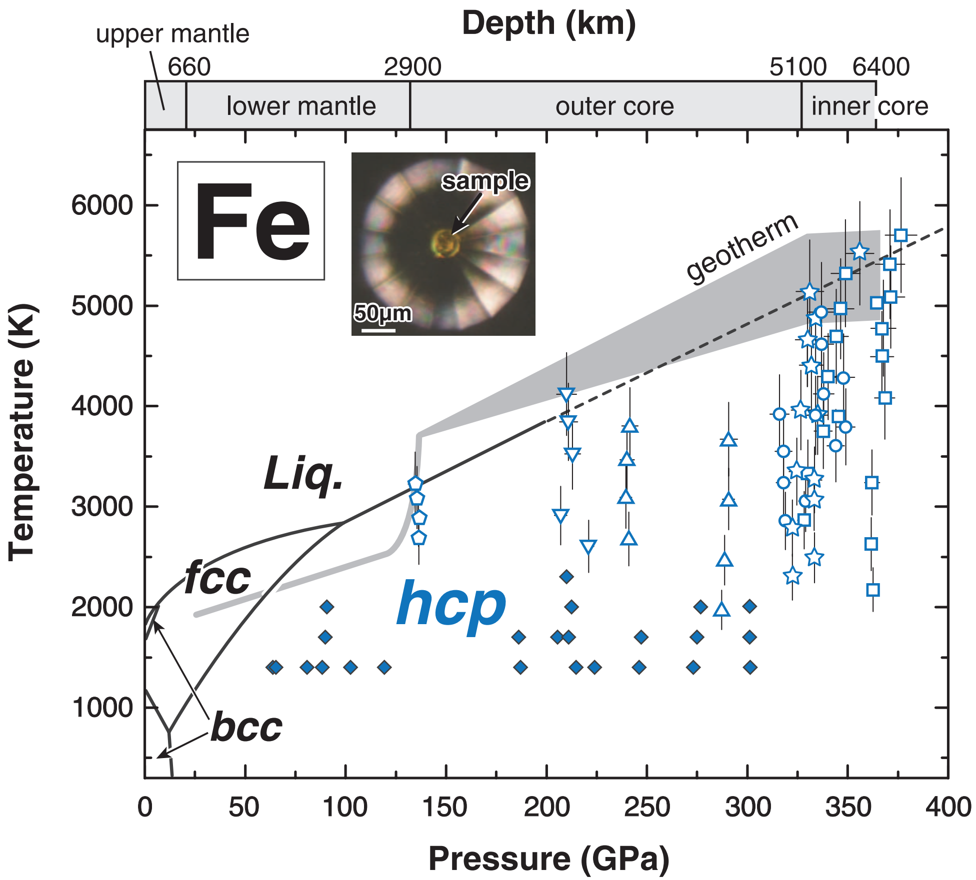


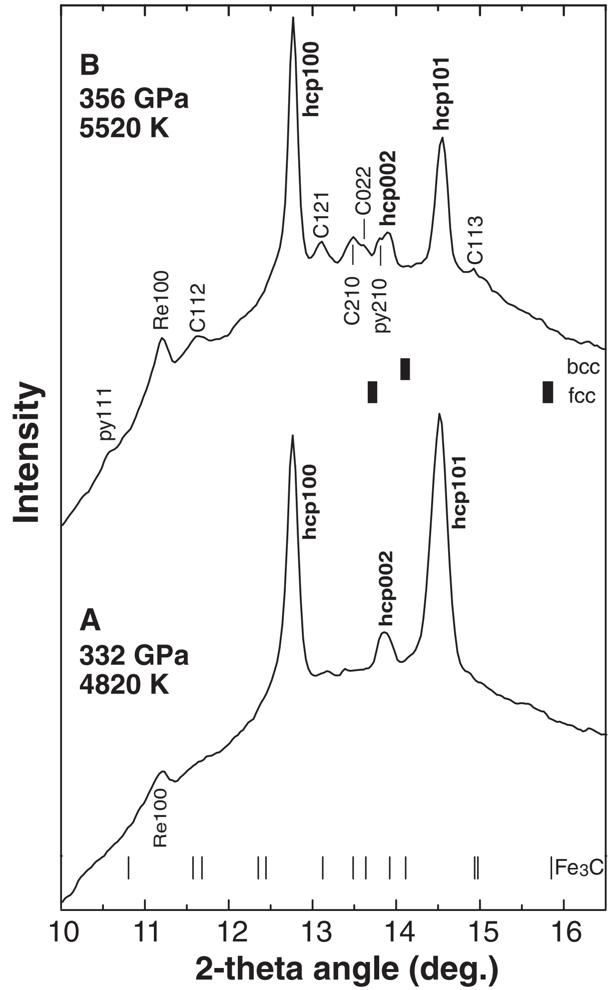
Figure 1 | Powder X-ray diffraction data and crystal structure of single-crystal $ErPd_2Si_2$ at 300 K. (a) Observed (circles) and calculated (solid

The Structure of Iron in Earth's Inner Core

Shigehiko Tateno,[1,2]* Kei Hirose,[1,2]* Yasuo Ohishi,[3] Yoshiyuki Tatsumi[2]

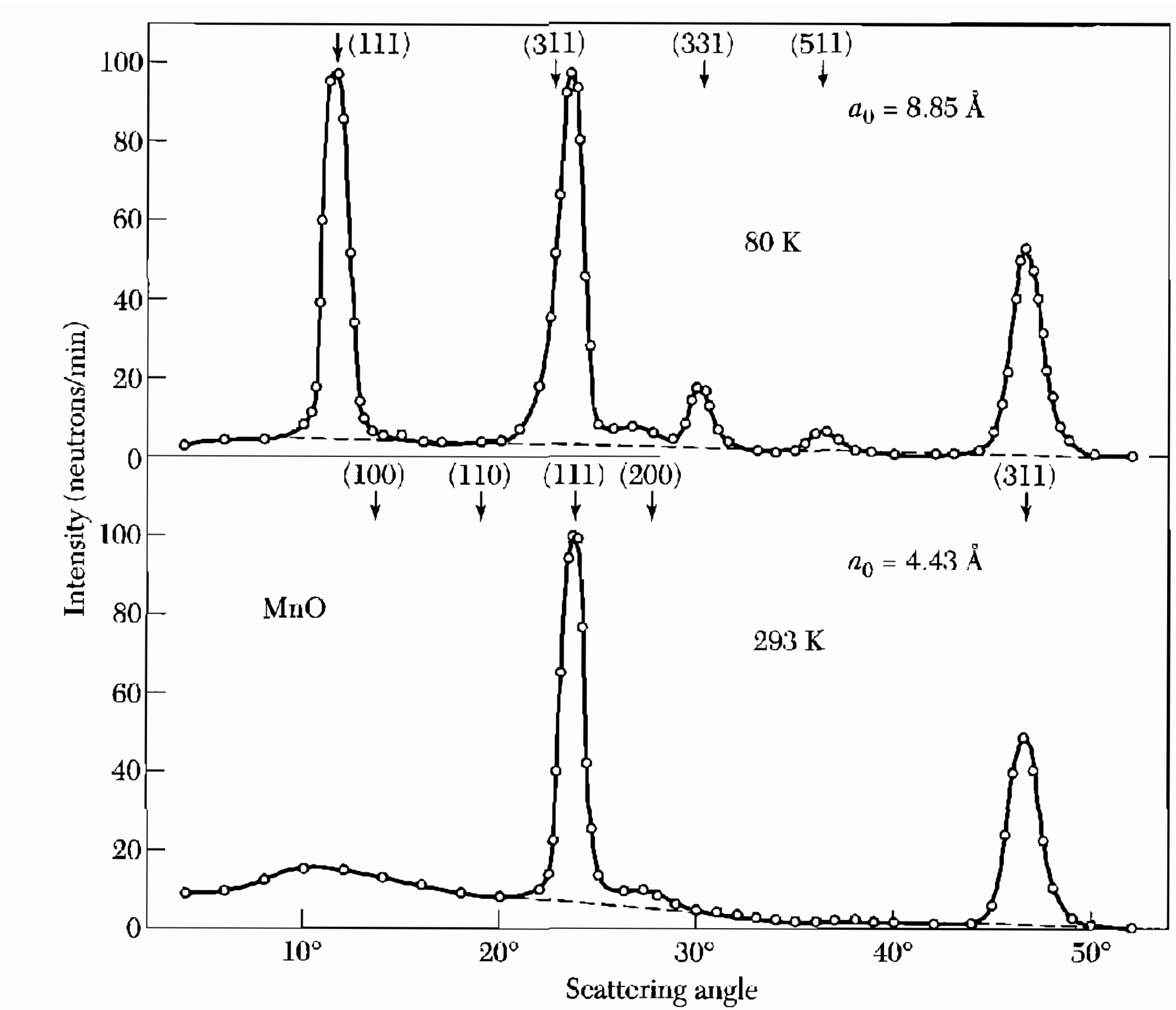
www.sciencemag.org SCIENCE VOL 330 15 OCTOBER 2010





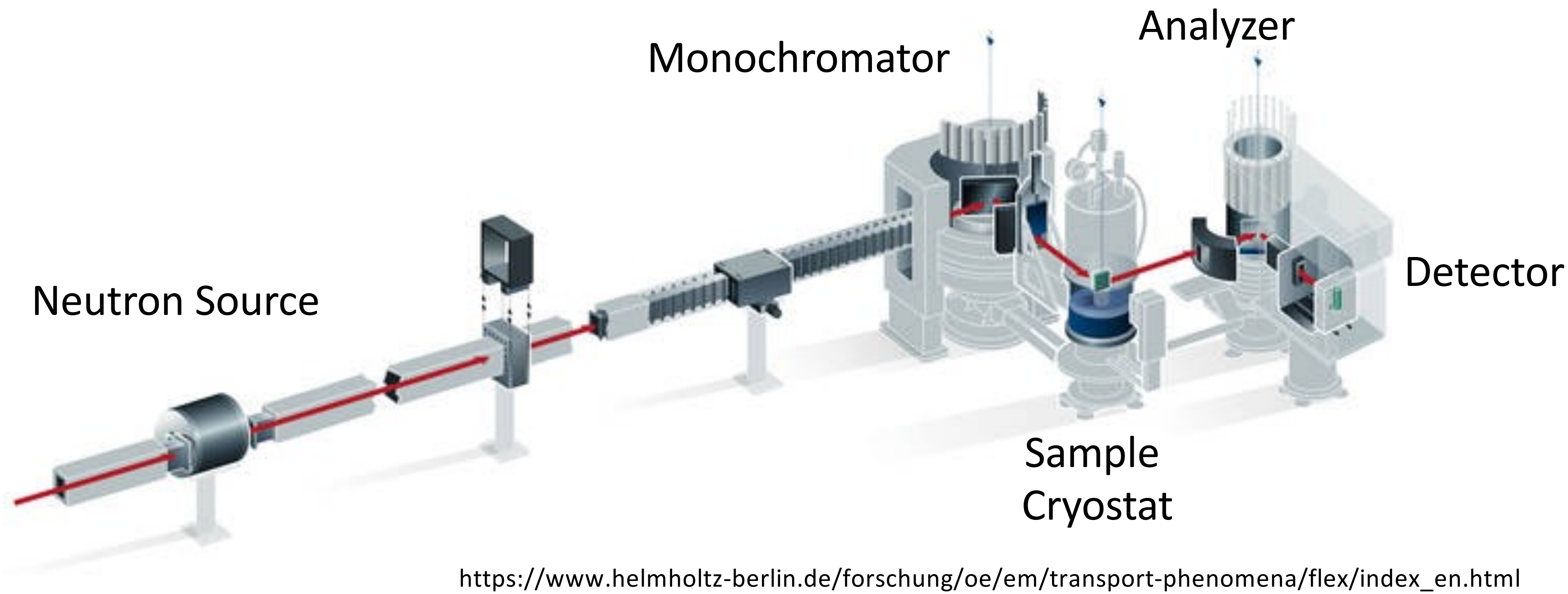
Antiferro-magnetism:

Neutron Diffraction



From Kittel

Triple axis spectrometer



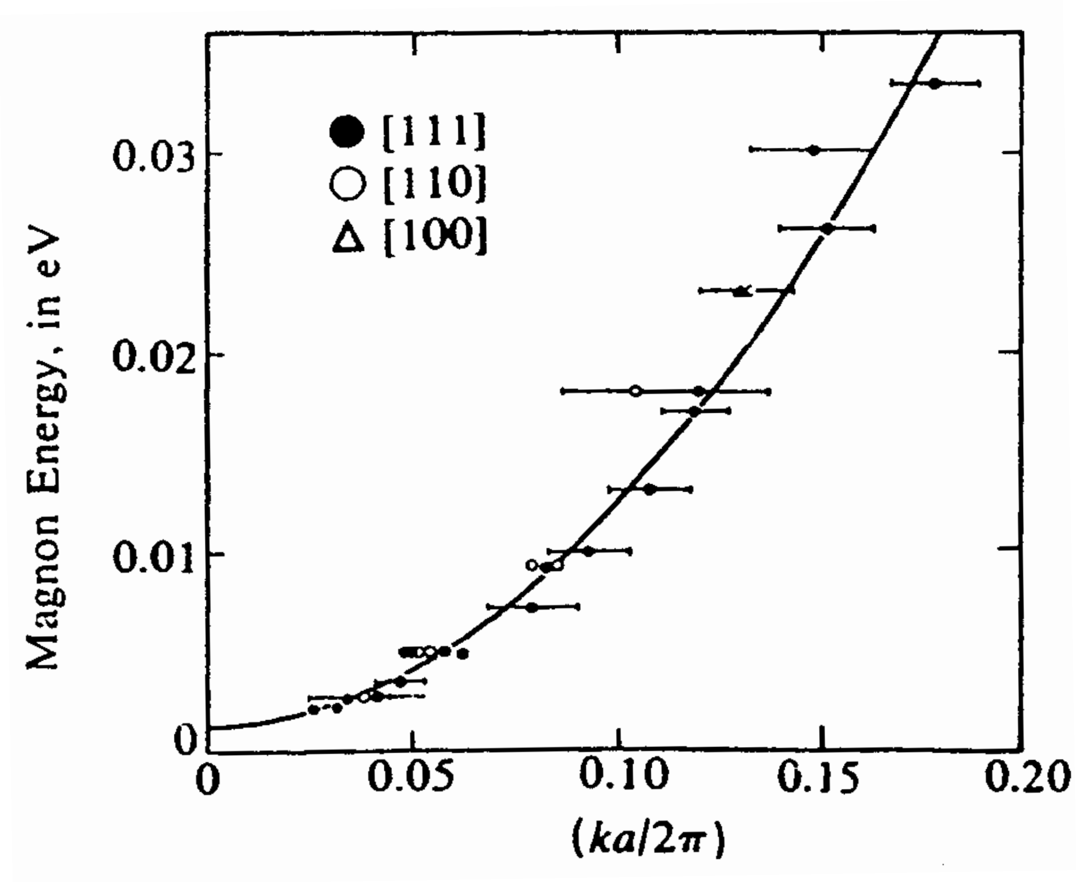
https://www.helmholtz-berlin.de/forschung/oe/em/transport-phenomena/flex/index_en.html

The Nobel Prize in Physics 1994
Bertram N. Brockhouse, Clifford G. Shull

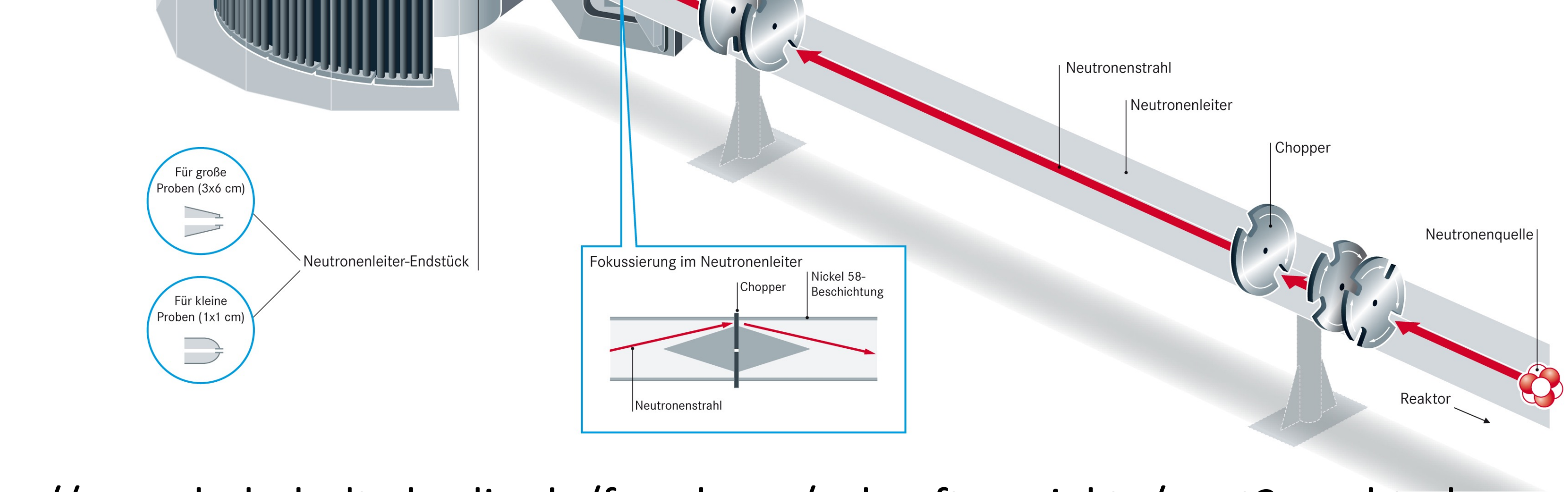
Ferromagnetic magnons:

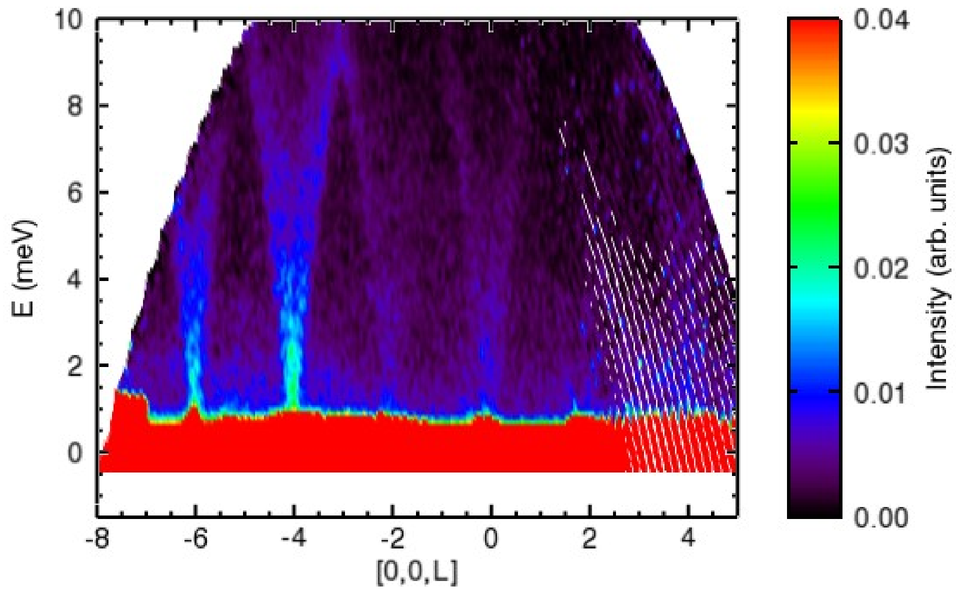
Neutron Spectroscopy

Brockhouse 1960



Time-of-flight spectrometry



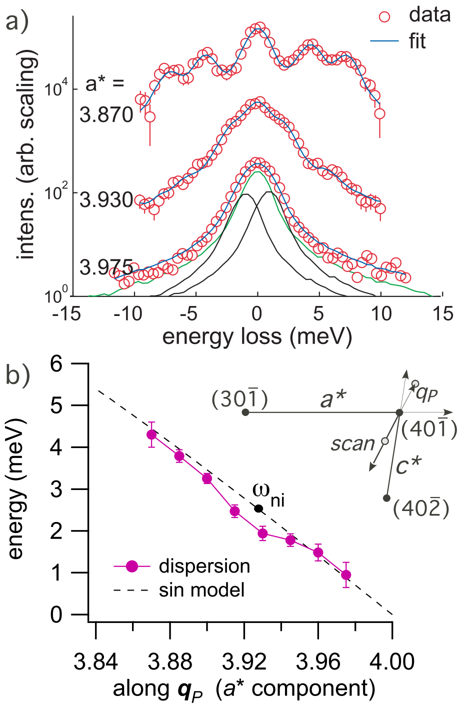


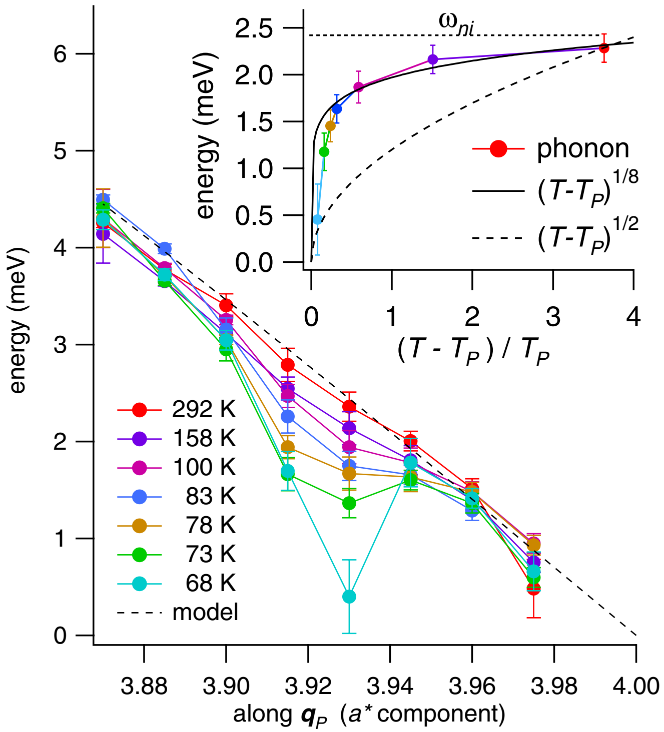
https://www.helmholtz-berlin.de/forschung/zukunftsprojekte/neat2_en.html

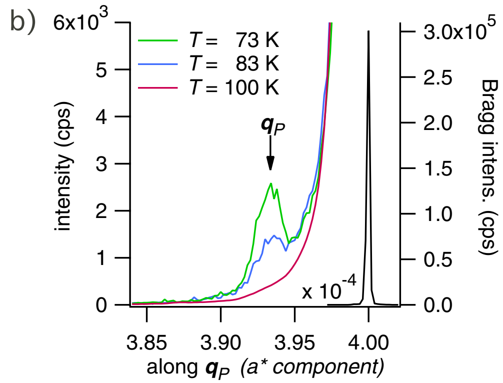
Giant Kohn Anomaly and the Phase Transition in Charge Density Wave $ZrTe_3$

Moritz Hoesch,[1] Alexey Bosak,[1] Dmitry Chernyshov,[2] Helmuth Berger,[3] and Michael Krisch[1]
[1]*European Synchrotron Radiation Facility, 6 rue Jules Horowitz, 38043 Grenoble Cedex, France*
[2]*Swiss-Norwegian Beam Lines at the ESRF, 6 rue Jules Horowitz, 38043 Grenoble Cedex, France*
[3]*Ecole Polytechnique Federale de Lausanne, Institut de Physique de la Matiere Complexe, 1015 Lausanne, Switzerland*

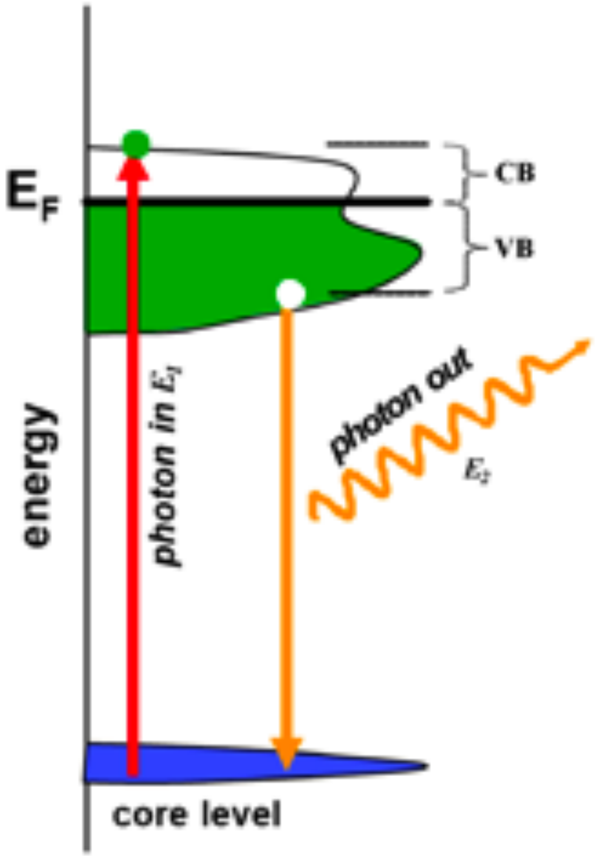
(Received 28 November 2008; published 25 February 2009)







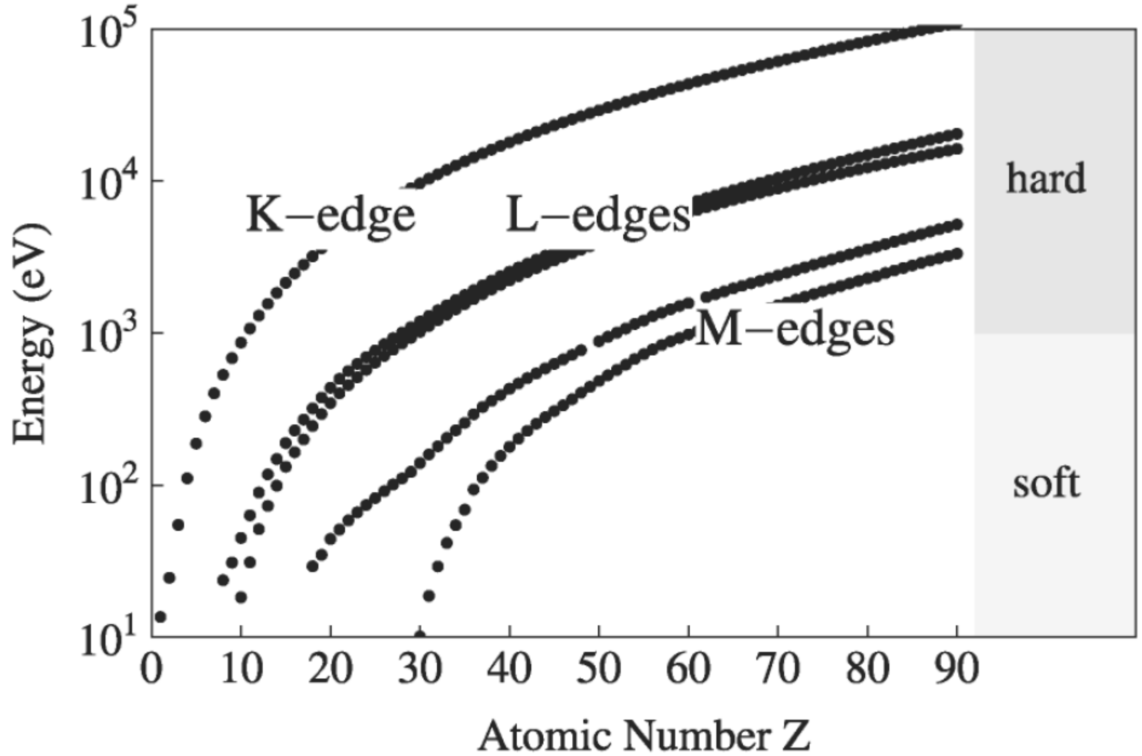
Resonant inelastic x-ray scattering (RIXS)



http://physics.usask.ca/~chang/homepage/xray/xray.html

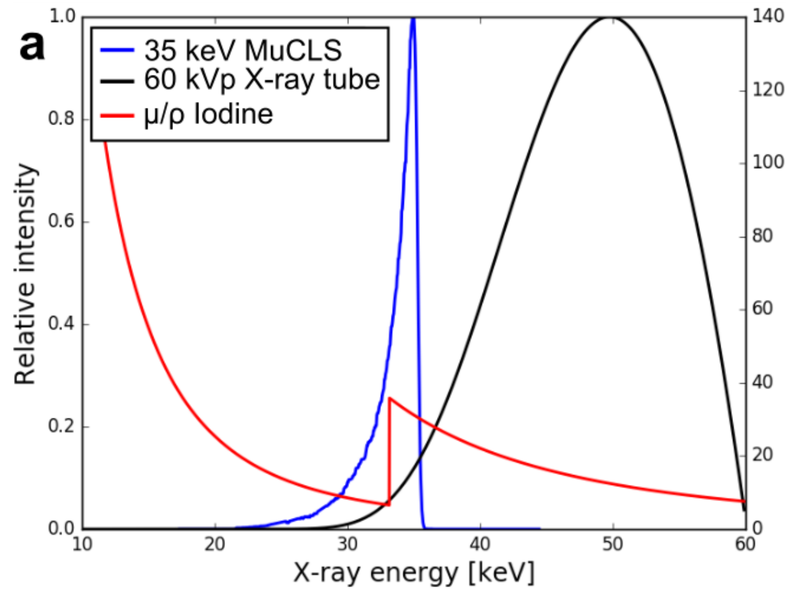
2017

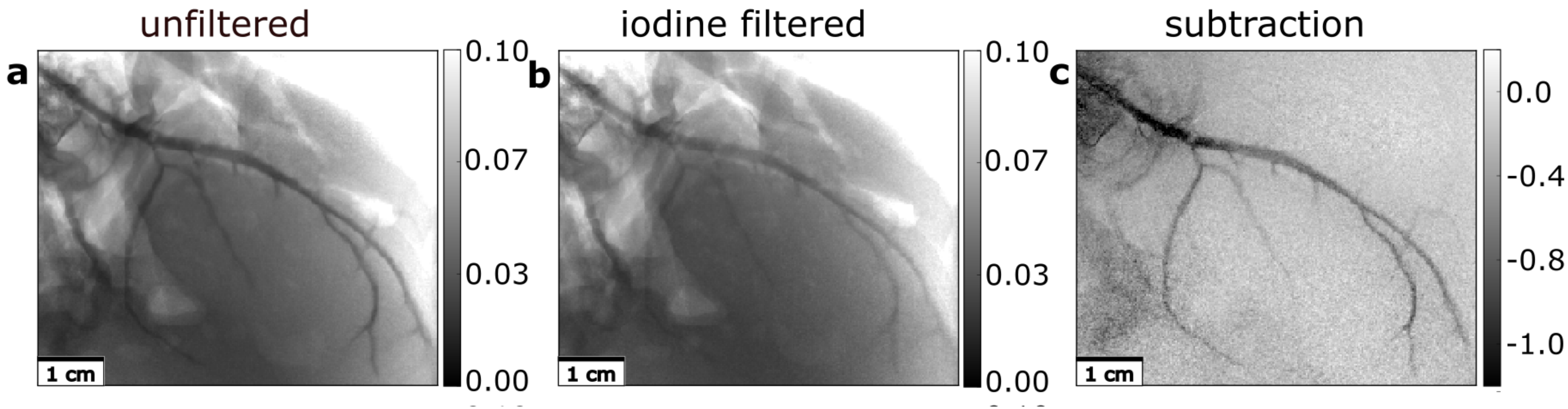
K-edge: 1s
L-edge: 2s or 2p
M-edge: 3s …



Rev. Mod. Phys. 83, 705 (2011)

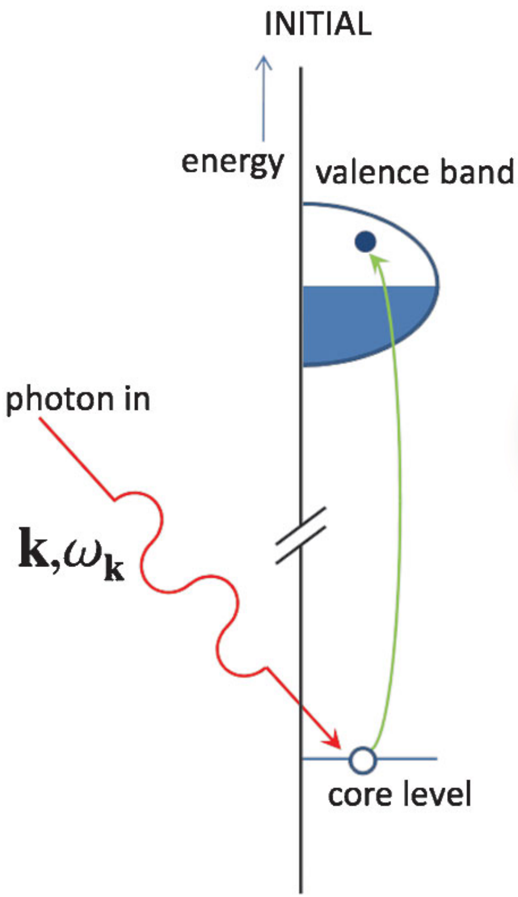
“Resonant imaging”



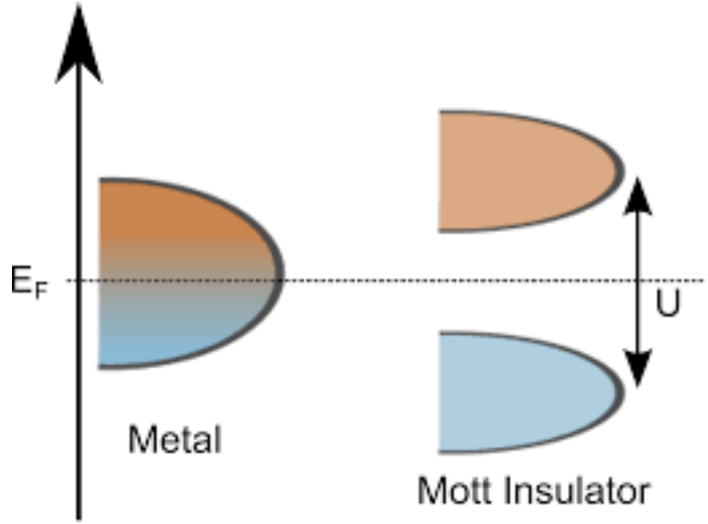


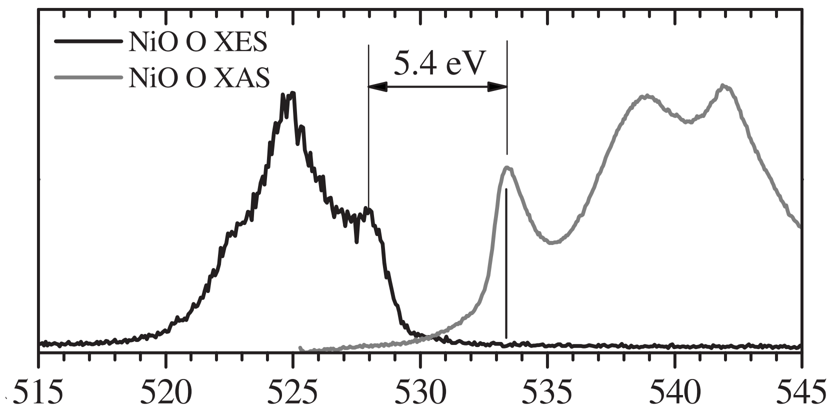
https://mediatum.ub.tum.de/doc/1575090/1575090.pdf

X-ray Absorption Spectroscopy (XAS)
Mott Insulator – Oxygen K-edge



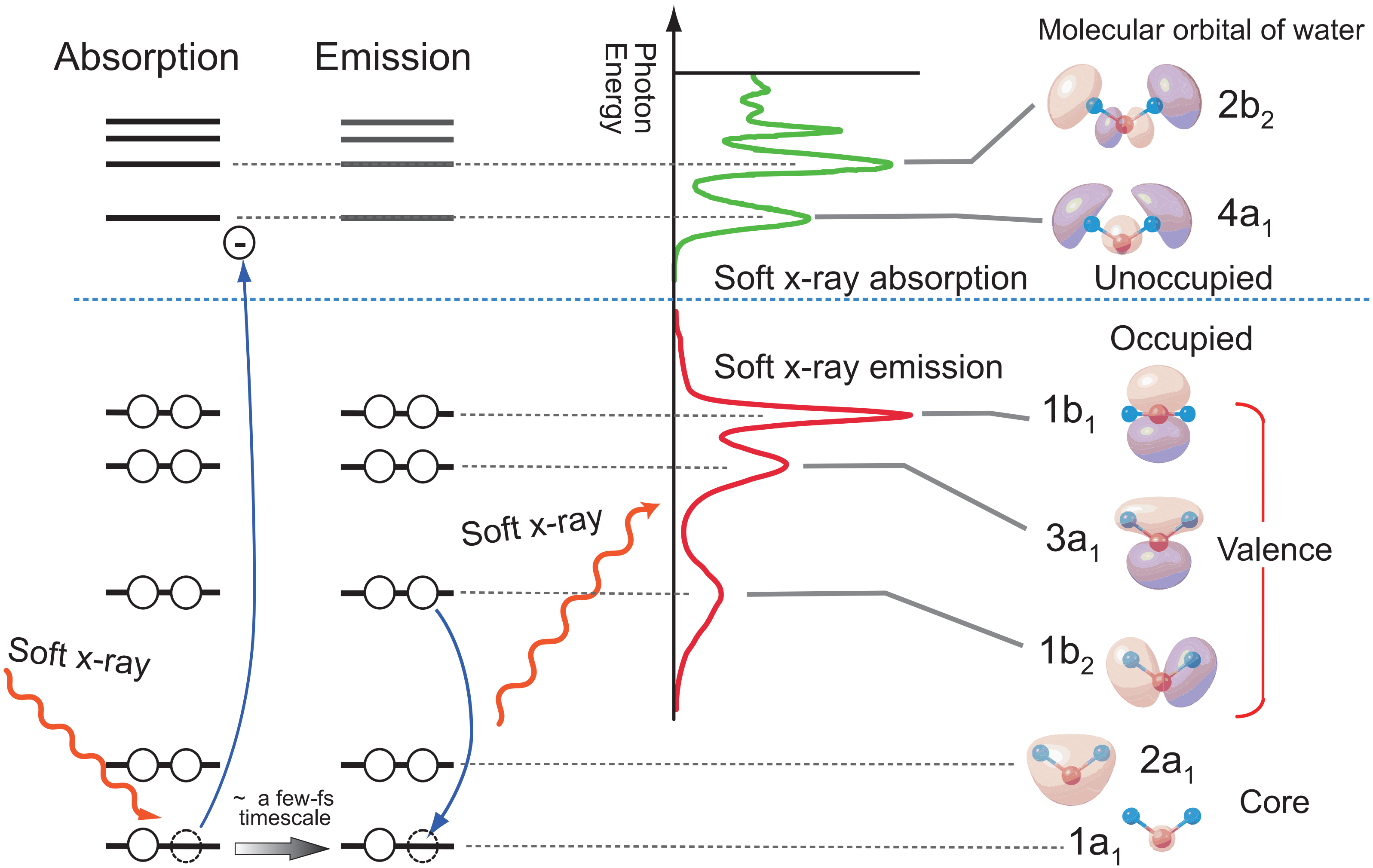
Synchrotron



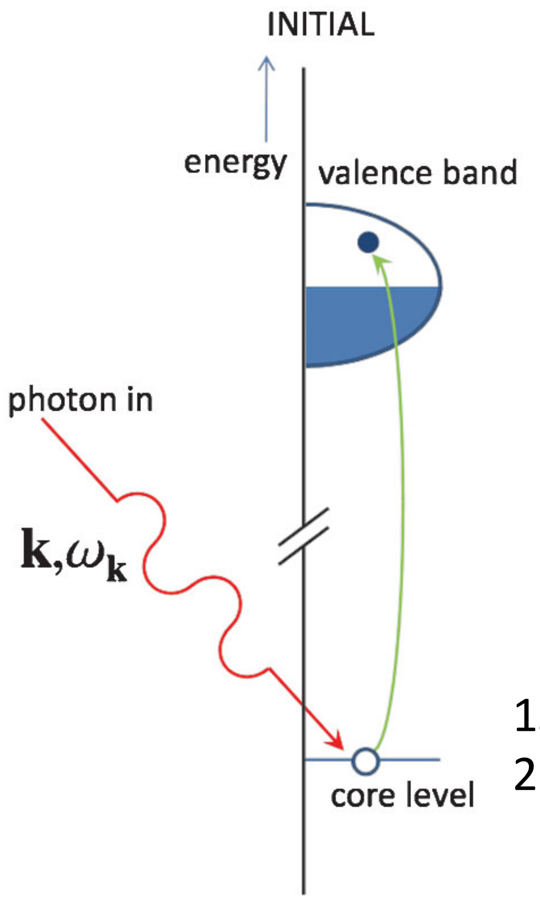


PHYSICAL REVIEW B **77**, 165127 (2008)

X-ray Absorption Spectroscopy (XAS)

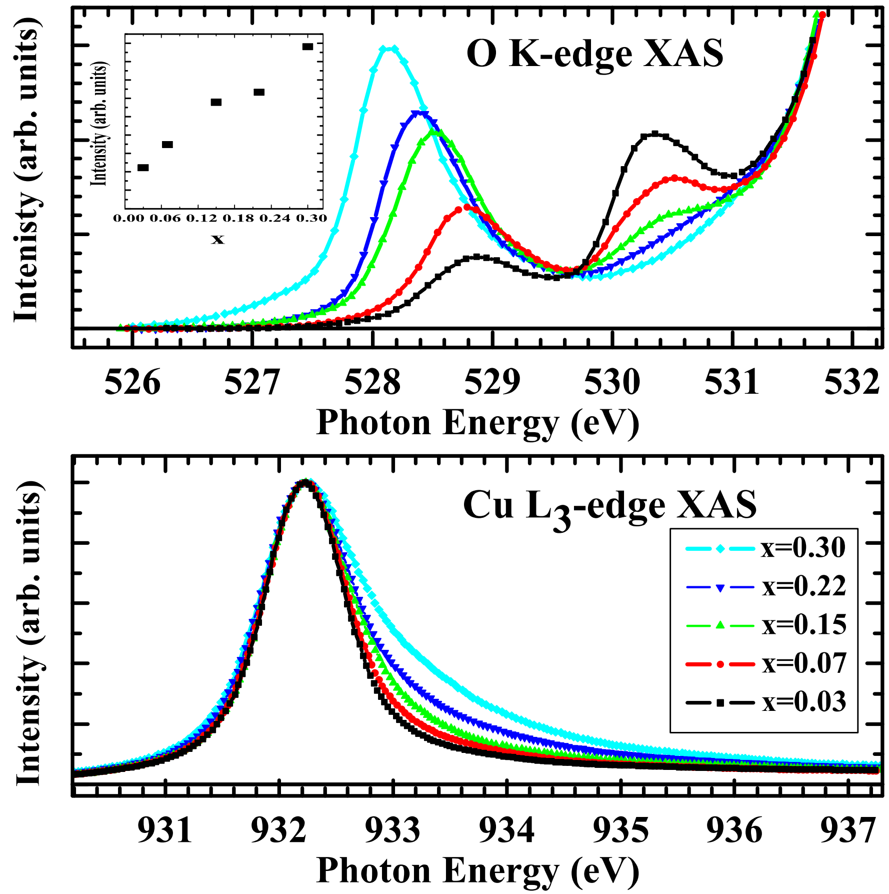


X-ray Absorption Spectroscopy (XAS) Different Edges



1s = K-edge
2p = L-edge

$La_{2-x}Sr_xCuO_4$

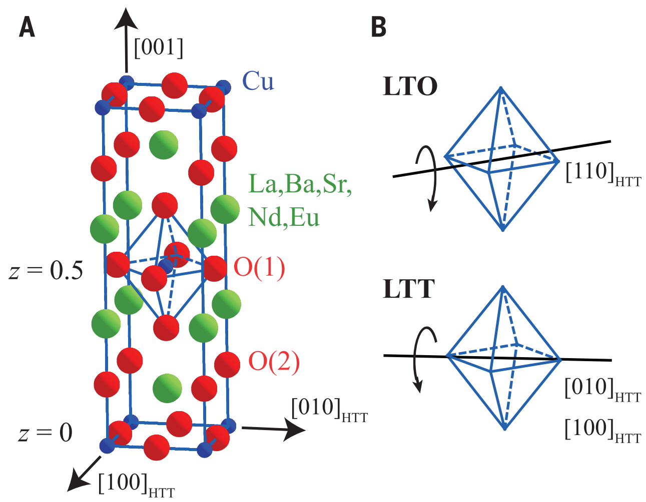


SUPERCONDUCTIVITY

Nematicity in stripe-ordered cuprates probed via resonant x-ray scattering

A. J. Achkar,[1] M. Zwiebler,[2] Christopher McMahon,[1] F. He,[3] R. Sutarto,[3] Isaiah Djianto,[1] Zhihao Hao,[1] Michel J. P. Gingras,[1,4,5] M. Hücker,[6] G. D. Gu,[6] A. Revcolevschi,[7] H. Zhang,[8] Y.-J. Kim,[8] J. Geck,[2,9] D. G. Hawthorn[1,4]*

Science **351**, 576 (2016)



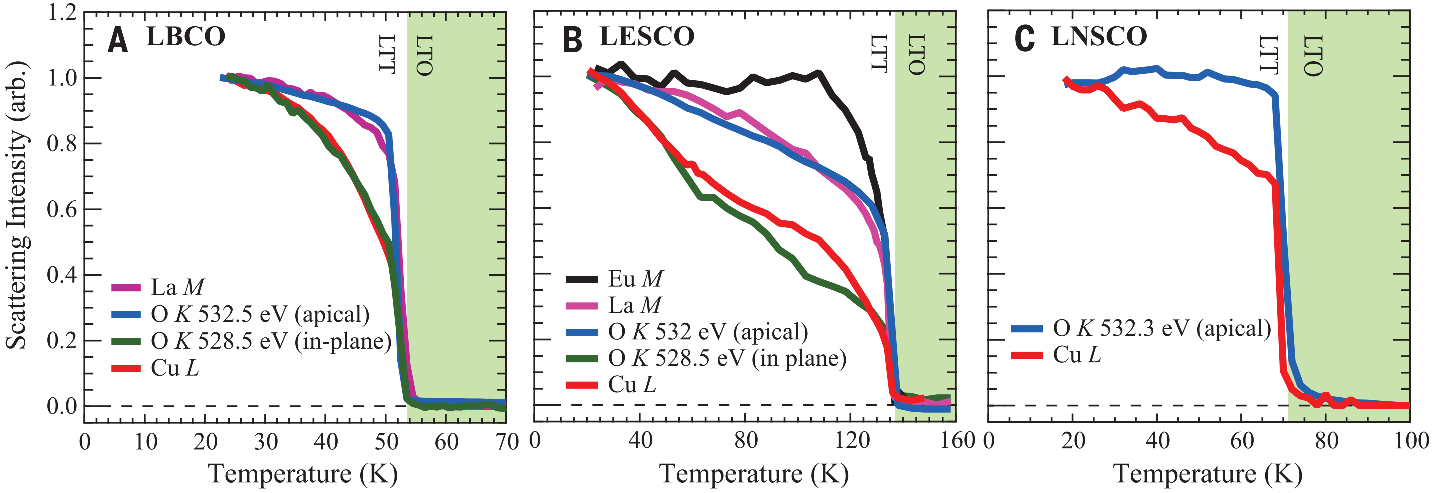
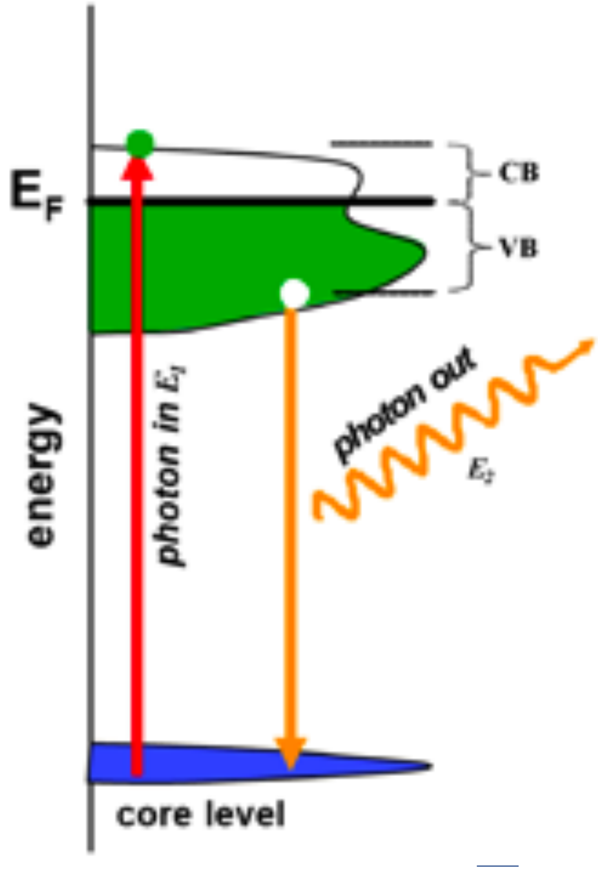
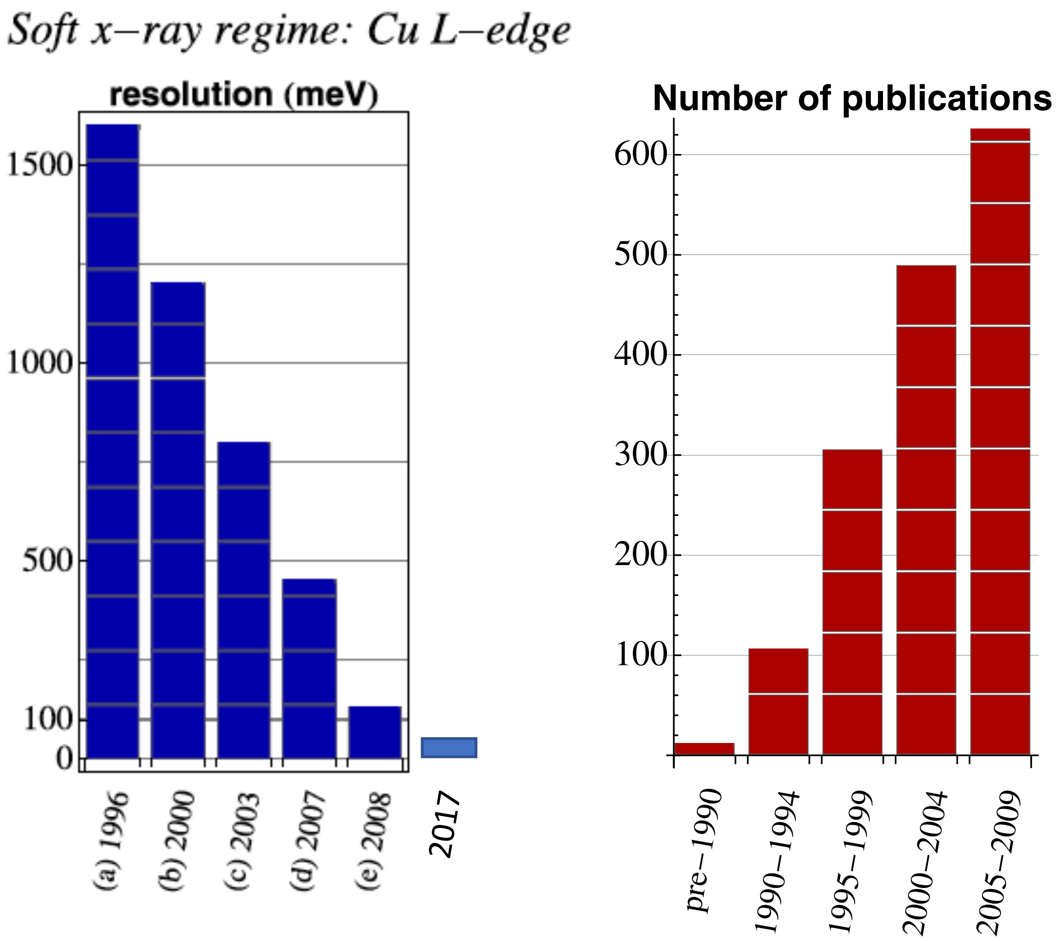


Fig. 2. Temperature dependence of the (001) Bragg peak intensity. The intensities are normalized by the corresponding low-temperature values, $I_{001}(T)/I_{001}(\sim 20K)$, with photon energy tuned to the La *M*-, Eu *M*-, O *K*-, and Cu *L*-edges for (**A**) LBCO, (**B**) LESCO, and (**C**) LNSCO. In all cases, the (001) peak has a more gradual temperature dependence for Cu and O in the CuO_2 planes than for atoms in the $(La,M)_2O_2$ layer.

Resonant inelastic x-ray scattering (RIXS)

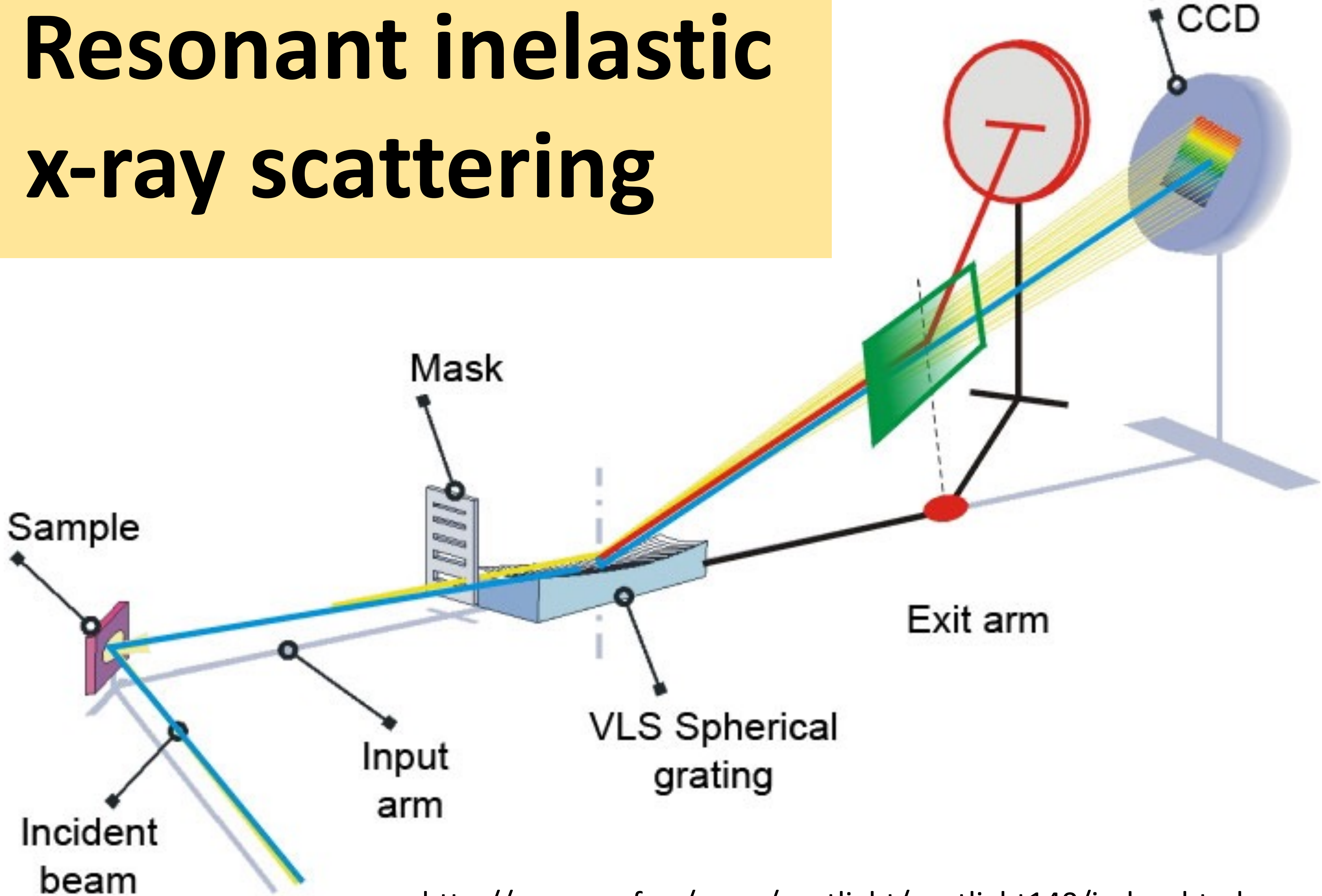


http://physics.usask.ca/~chang/homepage
/xray/xray.html



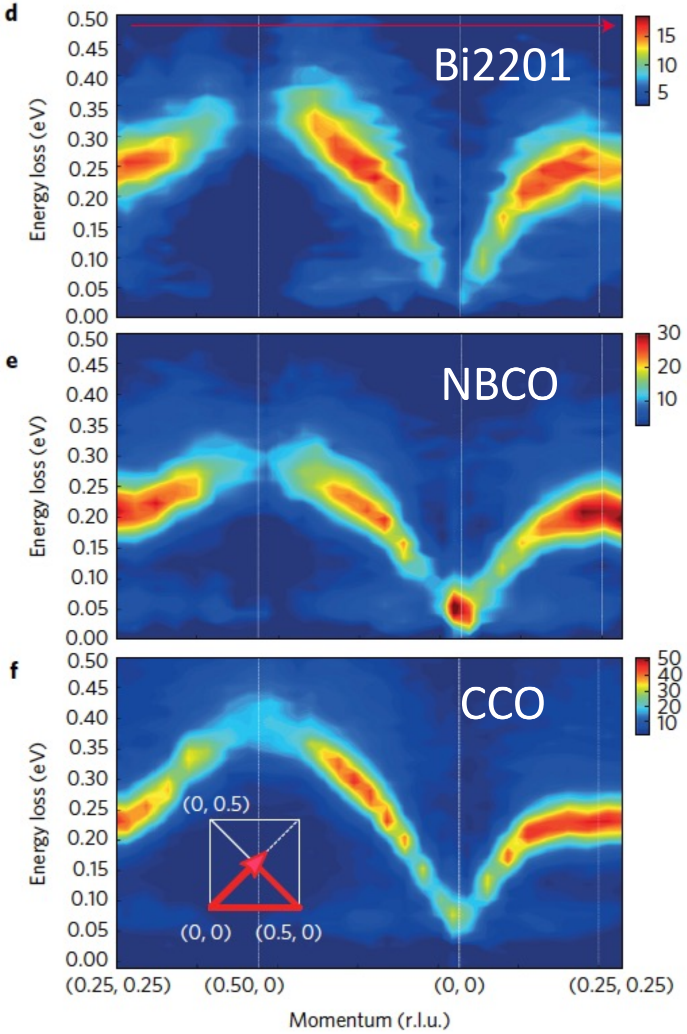
Rev. Mod. Phys. 83, 705 (2011)

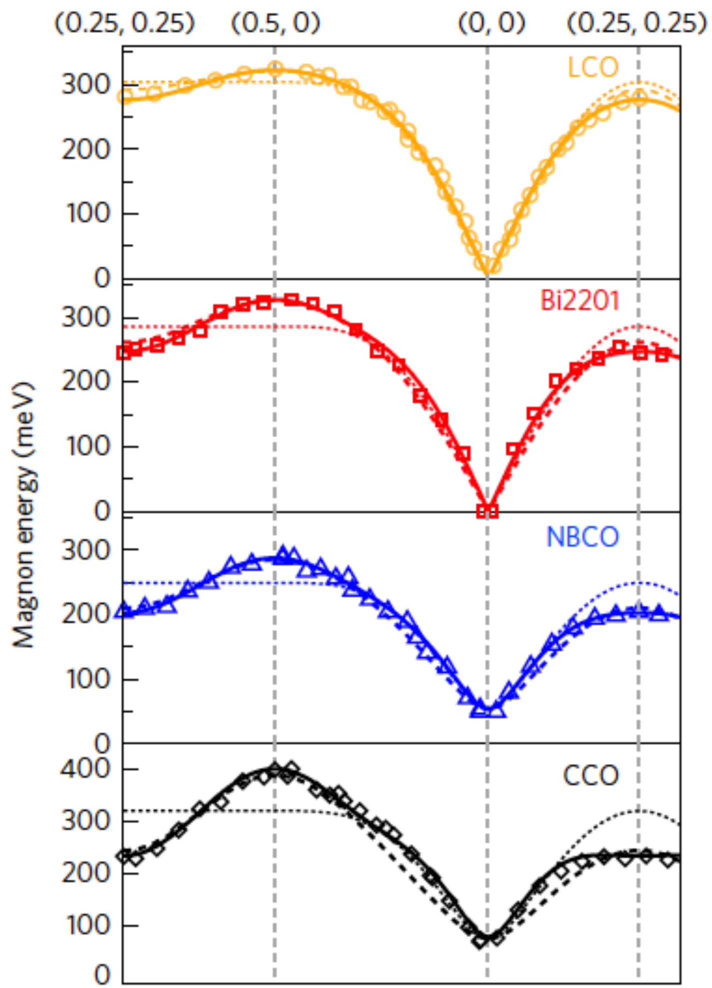
Resonant inelastic x-ray scattering



http://www.esrf.eu/news/spotlight/spotlight140/index_html

Antiferromagnetic magnons

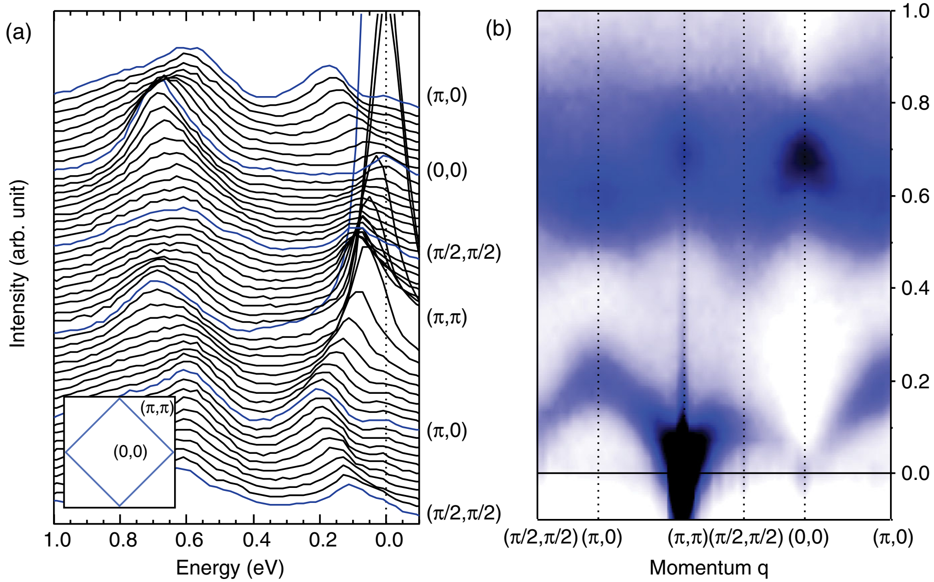


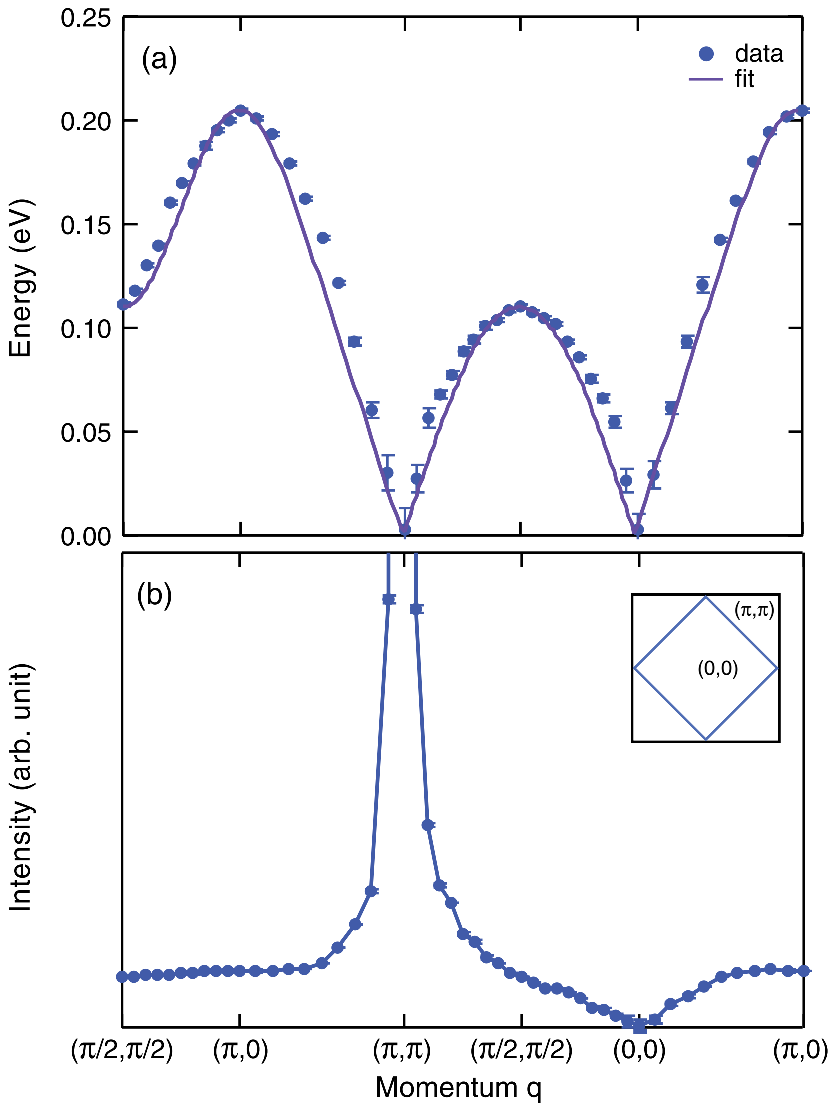


Nature Physics (2017) doi:10.1038/nphys4248

Antiferromagnetic magnons

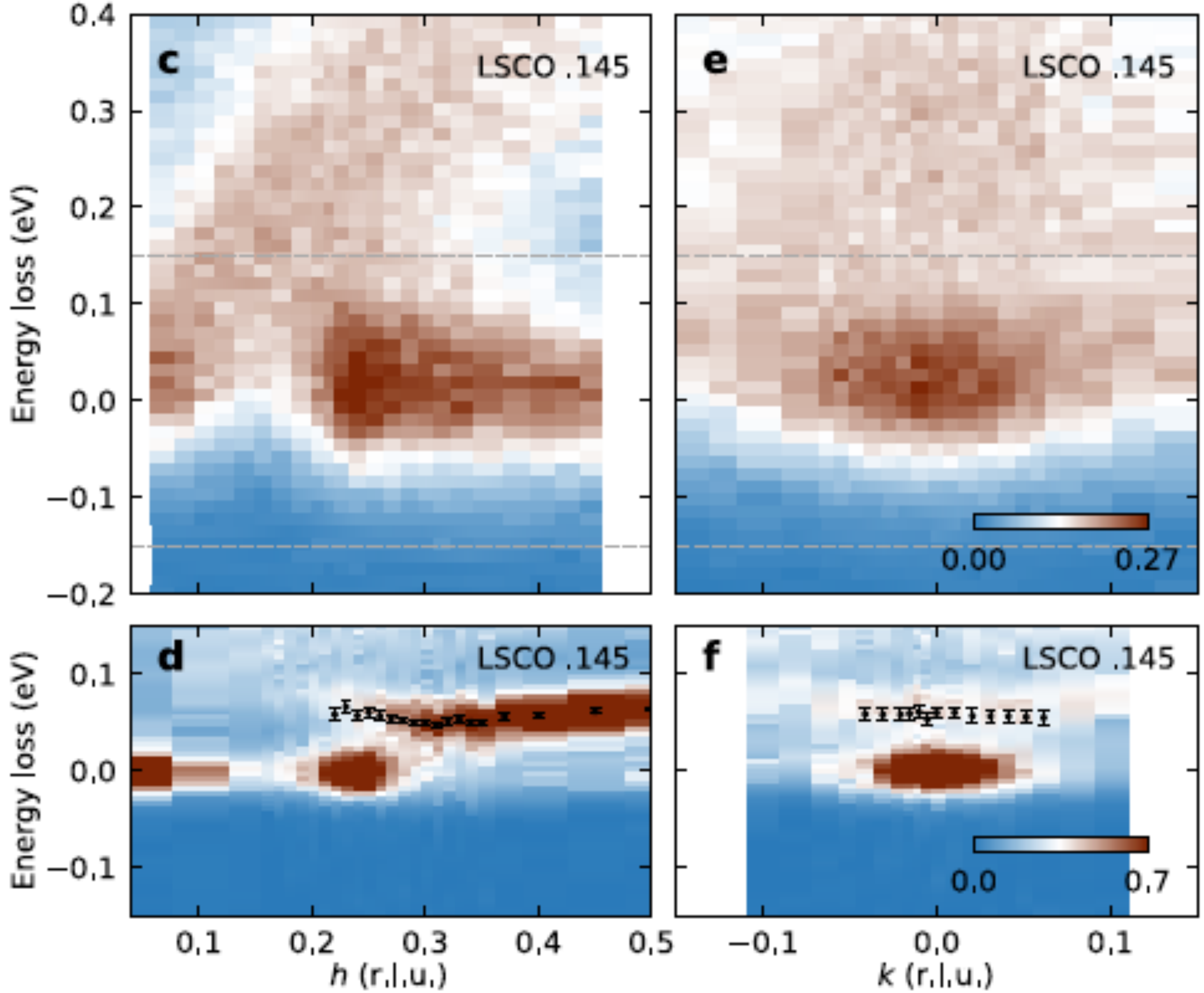
Sr_2IrO_4





PRL 108, 177003 (2012)

Phonons



Karin von Arx et al., npj Quantum Materials 8:7 (2023)

Course Outline

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		Exercise Class 14h30-16		Exercise Class 14h30-16

- (green) Introduction & overview. Why is scattering experiments important?
- (orange) Theoretical background for scattering experiments
- (blue) Scattering on condensed matter systems + Neutron scattering experiments
- (purple) X-ray diffraction and spectroscopy techniques