3rd ILSF Advanced School on Synchrotron Radiation and Its Applications

September 14-16, 2013

Study of High Tc Superconducting Properties by Using Synchrotron Radiation

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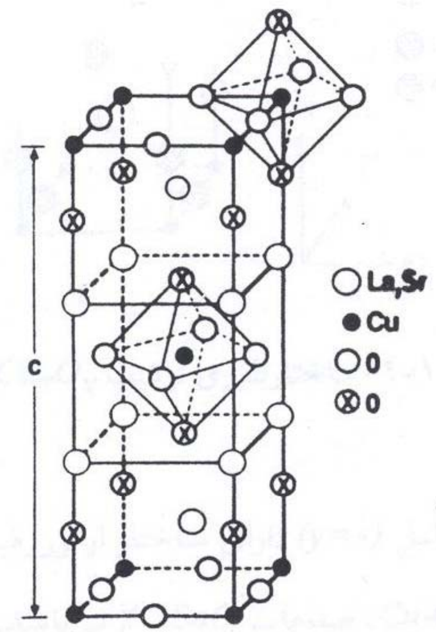
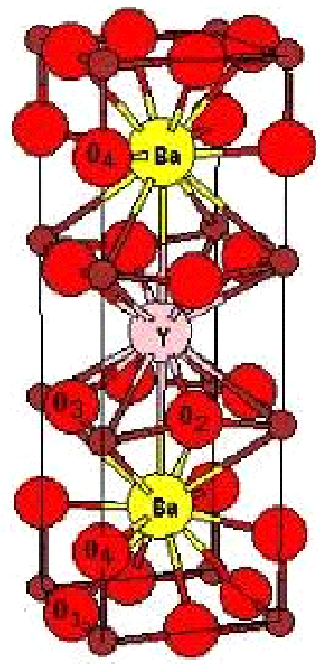
Sep 16, 2013

High Tc Cupper-Oxide Superconductors

- Bednorz-Muller (Noble prize1987)
- T_c=35-135 K



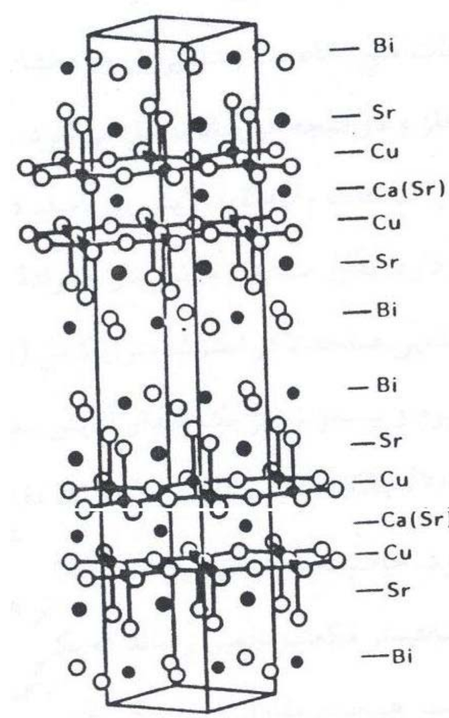
LSCO
T_c=38 K



Cu1

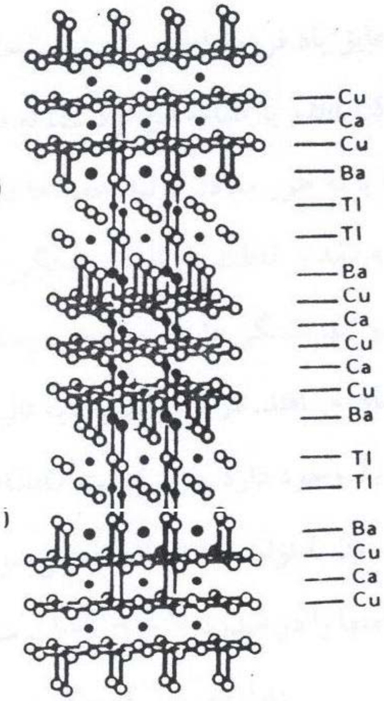
RBCO
T_c=90 K

MRL
Pr, O SIT problems



$Bi_2Sr_2CaCu_2O_8$

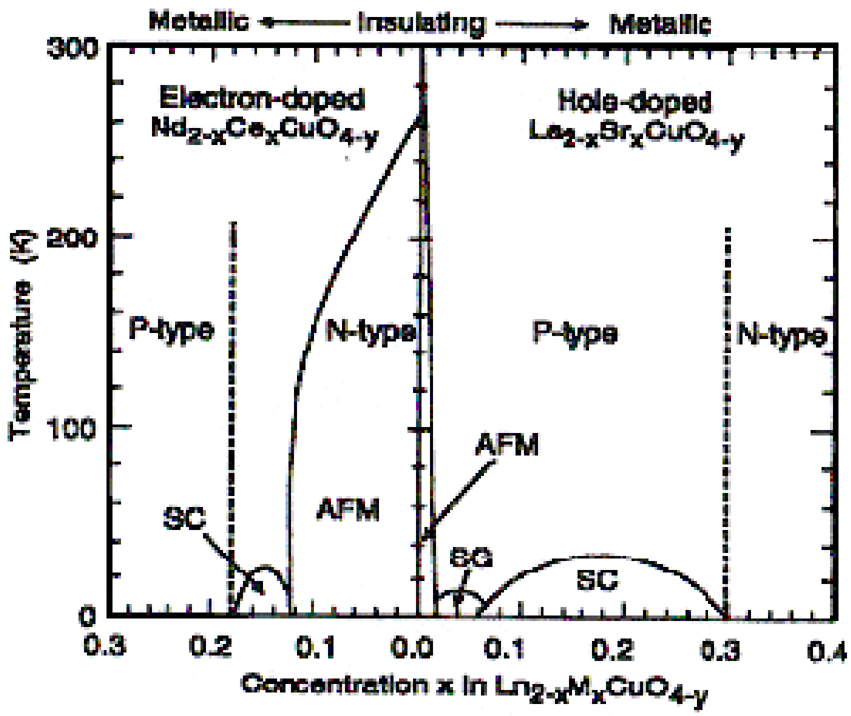
BSCCO
T_c=110 K

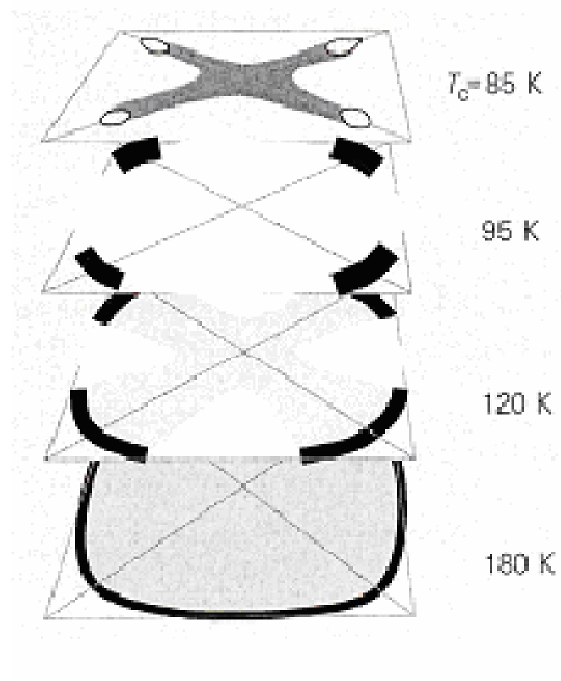


$Tl_2Ba_2Ca_2Cu_3O_{10}$

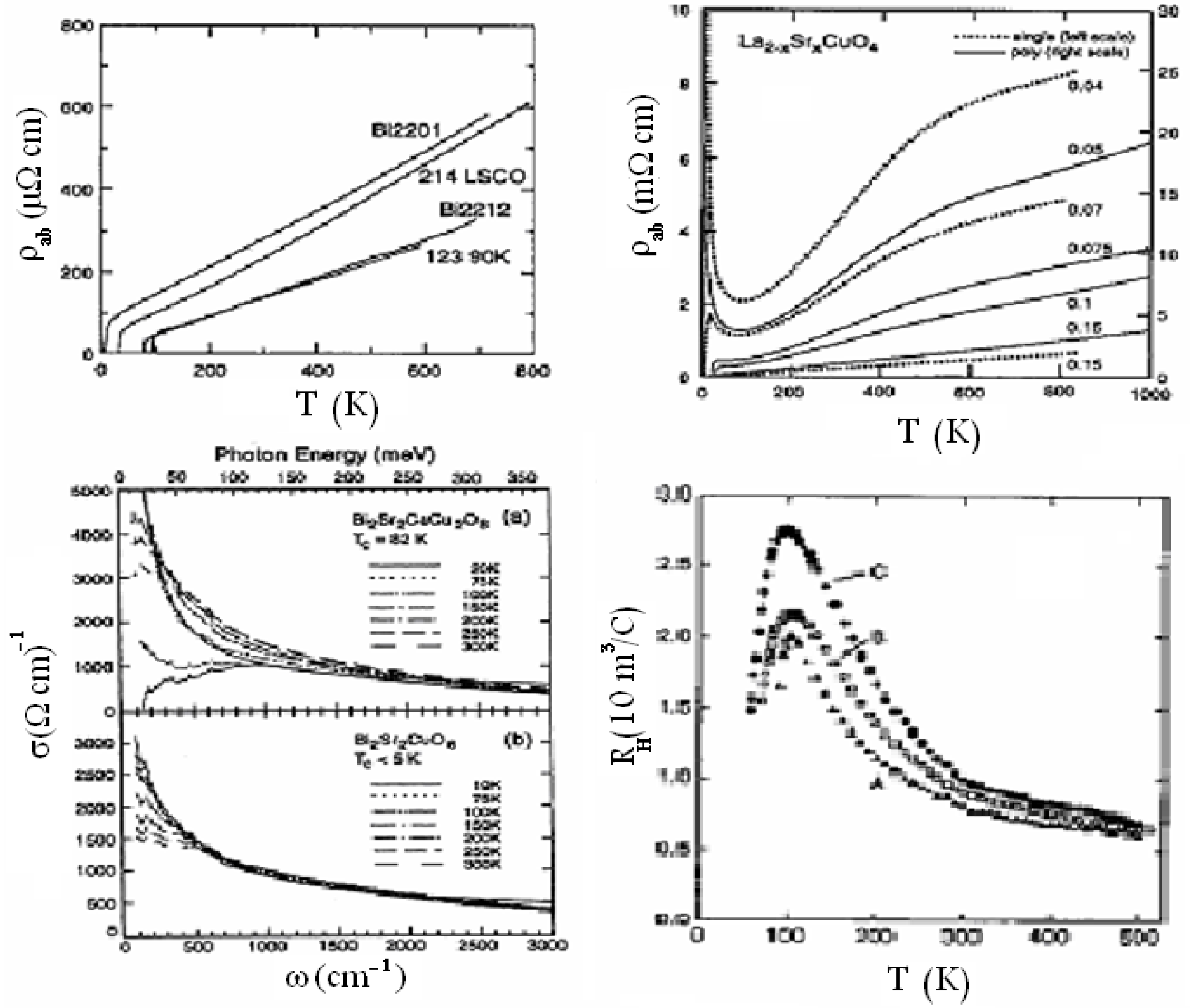
TlBCCO
T_c=125 K

HTSC Phase Diagram



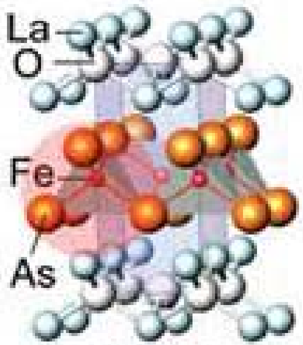


Unusual Electronic Properties of HTSCs in Normal Phase



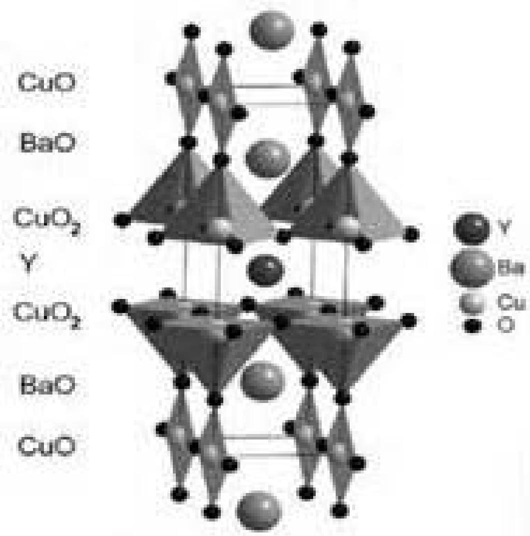
E. Dagotto, Rev. Mod. Phys. **66** (1994)763; D.N. Basov et al., Rev. Mod. Phys. **77** (2005)721.

New Superconductors

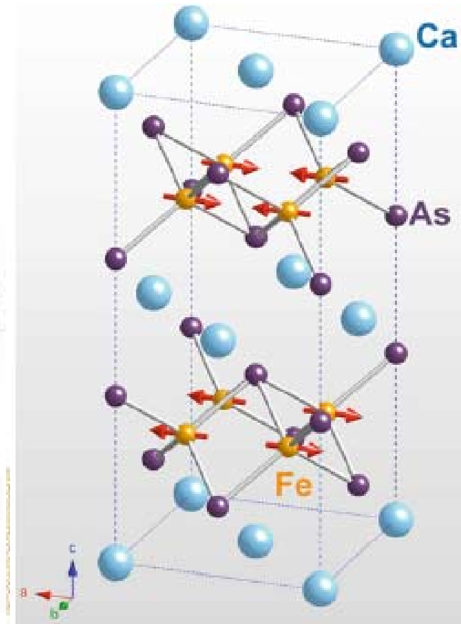


The unit cell of LaOFeP.

Kamihara, Y. *et al. J. Am. Chem. Soc. 128,* (2006).

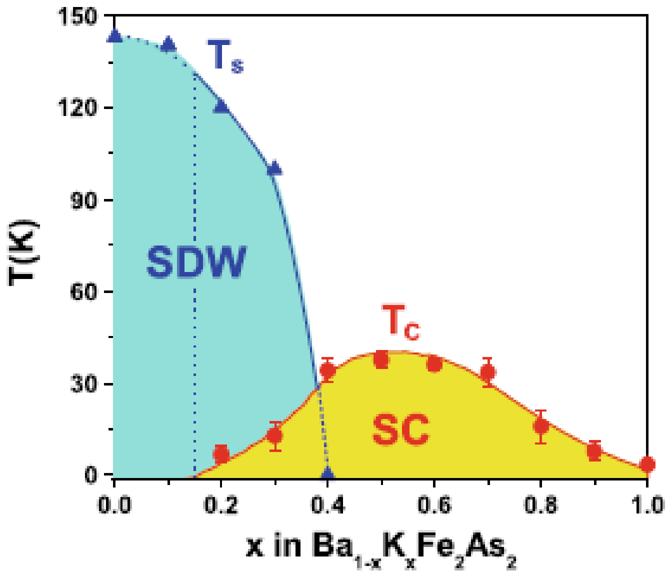


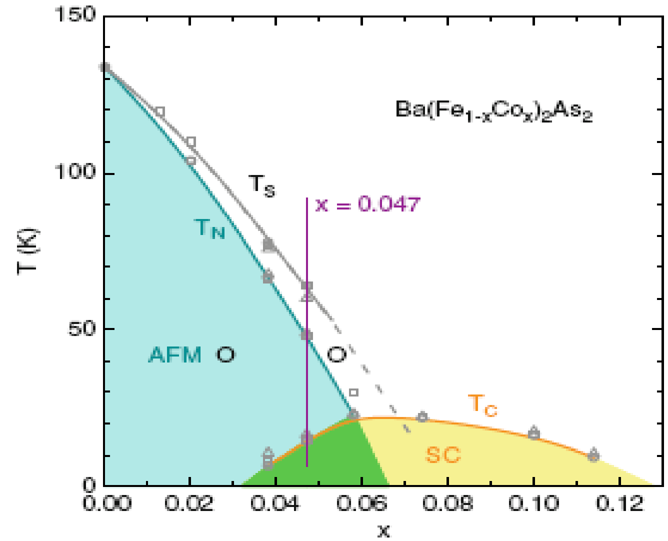
$YBa_2Cu_3O_7$



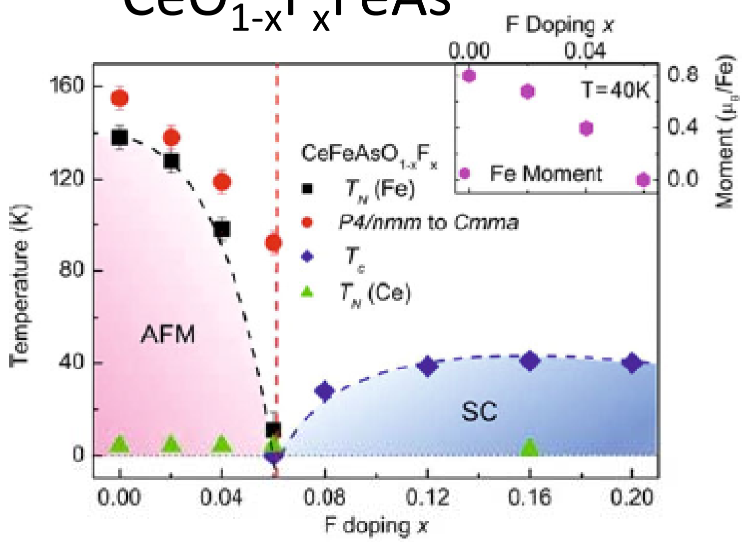
ReOFeAs	*La*	*Ce*	*Pr*	*Nd*	*Sm*	*Gd*
T_c, K	41	41	52	51.9	55	53.5
Reference	[27]	[9]	[10]	[28]	[11]	[29]
a, Å	4.035	3.996	3.925	3.940	3.940	
c, Å	8.740	8.648	8.595	8.496	8.496	

Phase Diagram





$CeO_{1-x}F_xFeAs$



FeAs Research Group

J Supercond Nov Magn
DOI 10.1007/s10948-012-1717-8

ORIGINAL PAPER

Electronic and Phonon Structures of $BaFe_2As_2$ Superconductor by *Ab*-initio Density Functional Theory

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M. Akhavan

Received: 28 May 2012 / Accepted: 29 June 2012

Abstract Electronic and phonon structures of the $BaFe_2As_2$ superconductor in the magnetic–orthorhombic phase have been investigated by the ab-initio density functional theory using the pseudopotential Quantum Espresso code. Density of state and electronic band structure for this phase

potassium doping at the Ba site changes the system from the spin-density wave (SDW) metal to the superconductor having T_c as much as 38 K at $x = 0.4$ [5]. The Hall effect measurement indicates that charge carriers are hole-like. The crystal structure of $BaFe_2As_2$ is tetragonal with the I4/mmm

Research Challenges

Problems of theory

- Strongly Correlated: LDA-DFT does not give reasonable results
- Many Body Hamiltonian is diagonalized only for small lattice
- Complete Hamiltonian?
- doping, temperature, interactions, etc?

How Experiments can help?

Determination of crystal structure

…. Superconducting properties

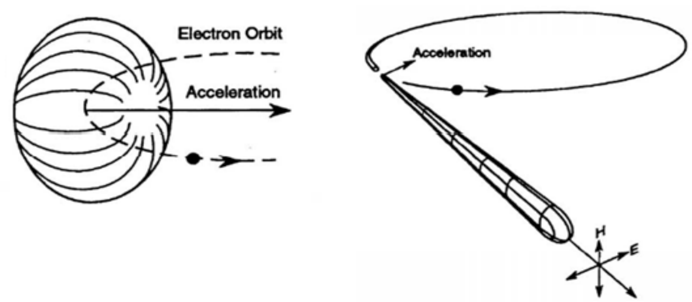
…. Phase diagram

…. Electronic structure

…. Phonons, magnetic excitations, etc

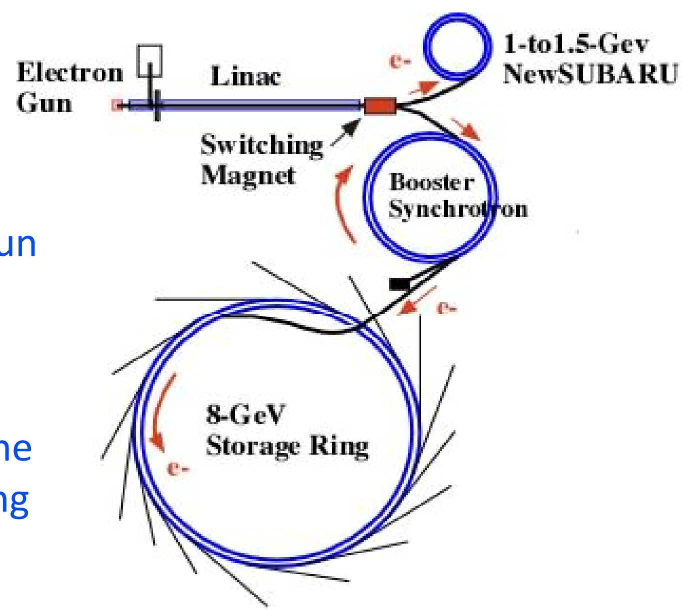
Light Source Accelerator

Relativistic forward focusing of Synchrotron Radiation



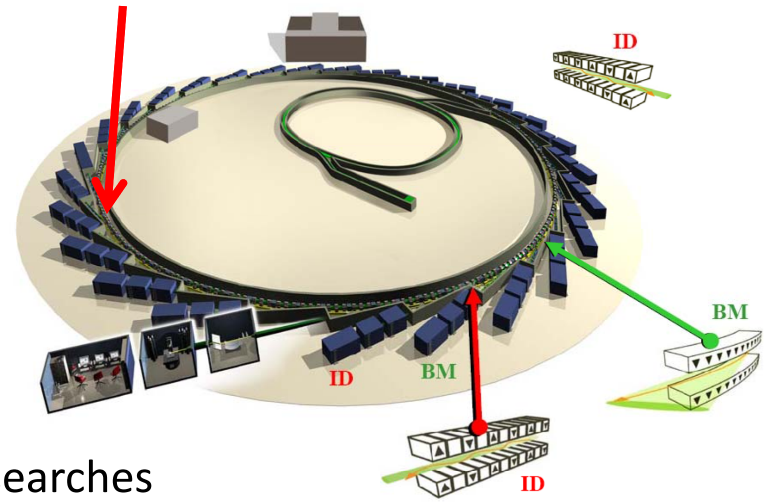
Non relativistic
Isotropic Radiation

Relativistic (v>99.999999 c)
Forward Cone Radiation (mrad)



- Electron Gun
- Buncher
- Linac
- Booster
- Transfer Line
- Storage Ring

Accelerated electrons



Researches

Light Sources

Light Source Examples

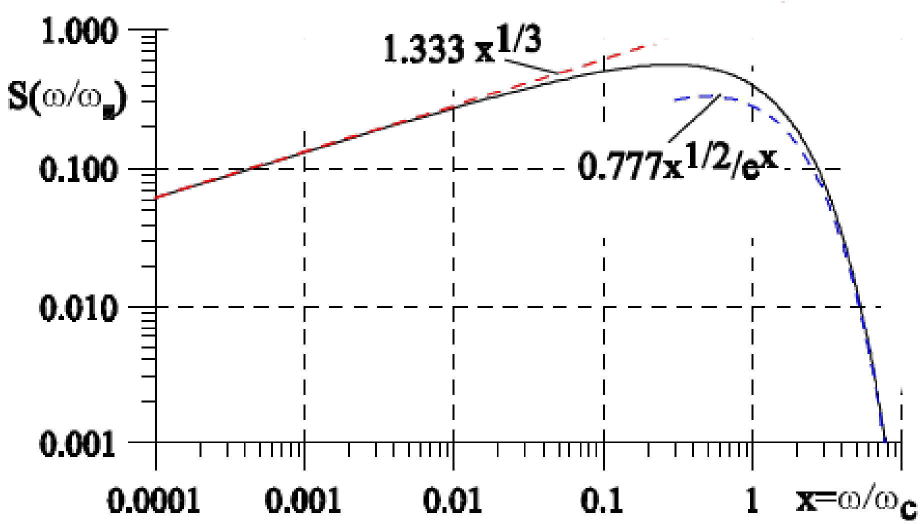
ALBA Spain 2011
3 Gev, 268.8 m

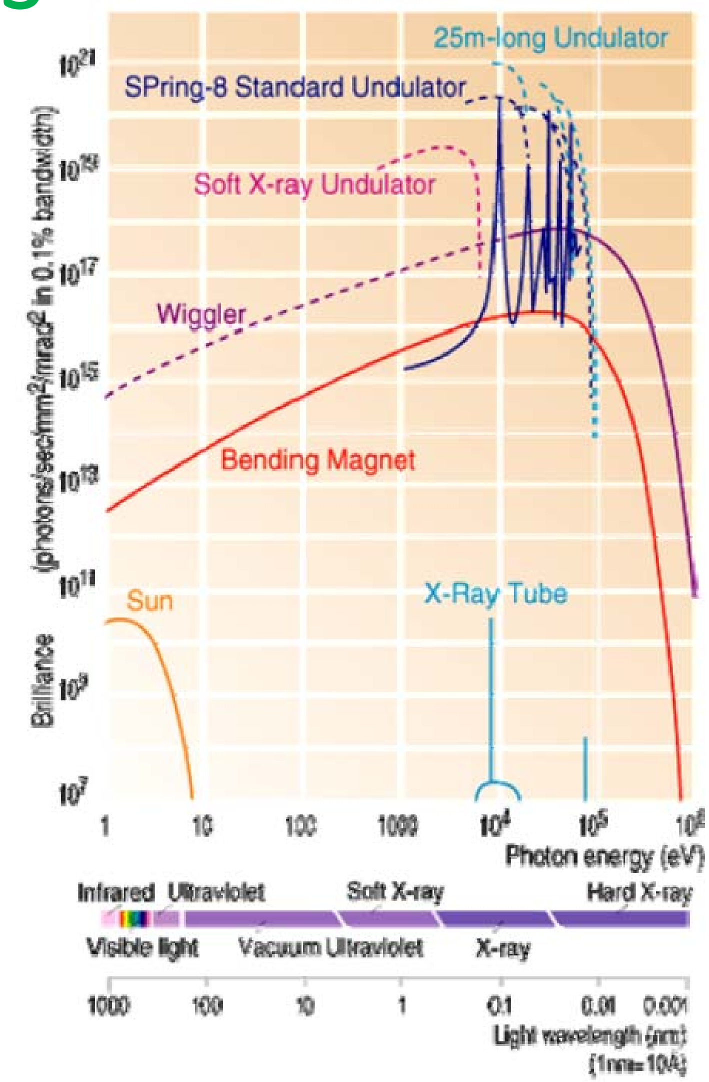
SPring-8 Japan 1997
8 Gev, 1436 m

APS, USA 1996
7 Gev, 1104 m

ESRF France, 1994
6 Gev, 844 m

Radiation Properties





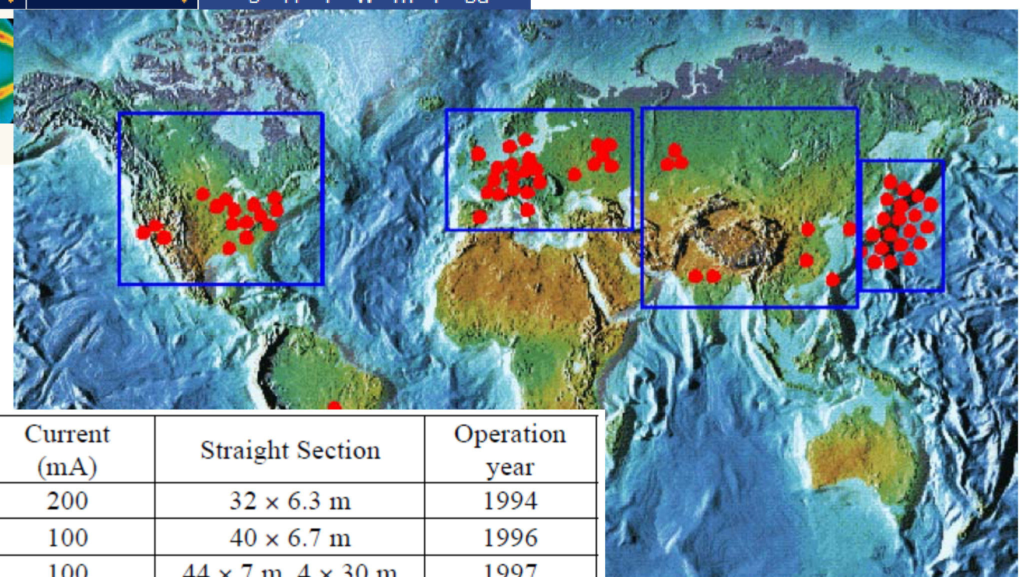
$$\frac{\mathrm{d}\dot{N}_{\mathrm{ph}}}{\mathrm{d}\psi} = C_\psi \, E \, I \, \frac{\Delta\omega}{\omega} \, S\left(\frac{\omega}{\omega_c}\right)$$

$$C_\psi = \frac{4\alpha}{9e\, mc^2} = 3.9614 \times 10^{19} \ \frac{\text{photons}}{\text{s rad A GeV}}$$

$$\varepsilon_c\,(\mathrm{keV}) = 2.2183 \frac{E^3\,(\mathrm{GeV}^3)}{\rho\,(\mathrm{m})} = 0.66503\, E^2\,(\mathrm{GeV}^2)\, B\,(\mathrm{T}$$

$$\mathcal{B} = \frac{N_{\mathrm{ph}}}{4\pi^2 \sigma_x\, \sigma_{x'}\, \sigma_y\, \sigma_{y'} \ \frac{\mathrm{d}\omega}{\omega}}$$

Statistics



3rd Generation SRF in 1990s

Light Source	Energy (GeV)	Circumference (m)	Emittance (nm-rad)	Current (mA)	Straight Section	Operation year
ESRF	6.0	844.4	4.0	200	32 × 6.3 m	1994
APS	7.0	1104	3.0	100	40 × 6.7 m	1996
SPring-8	8.0	1436	3.4	100	44 × 7 m, 4 × 30 m	1997
ALS	1.9	196.8	6.3	400	12 × 6.7 m	1993
TLS	1.5	120	25	240	6 × 6 m	1994
ELETTRA	2.4	259	7.0	300	12 × 6.1 m	1994
PLS	2.5	280.6	12.0	200	12 × 6.8 m	1995
LNLS	1.37	93.2	100	250	6 × 3 m	1997
MAX-II	1.5	90	9.0	280	10 × 3.2 m	1997
BESSY-II	1.7	240	6.1	200	8 × 4.9 m, 8 × 5.7 m	1999
Siberia-II	2.5	124	98	200	12 × 3 m	1999

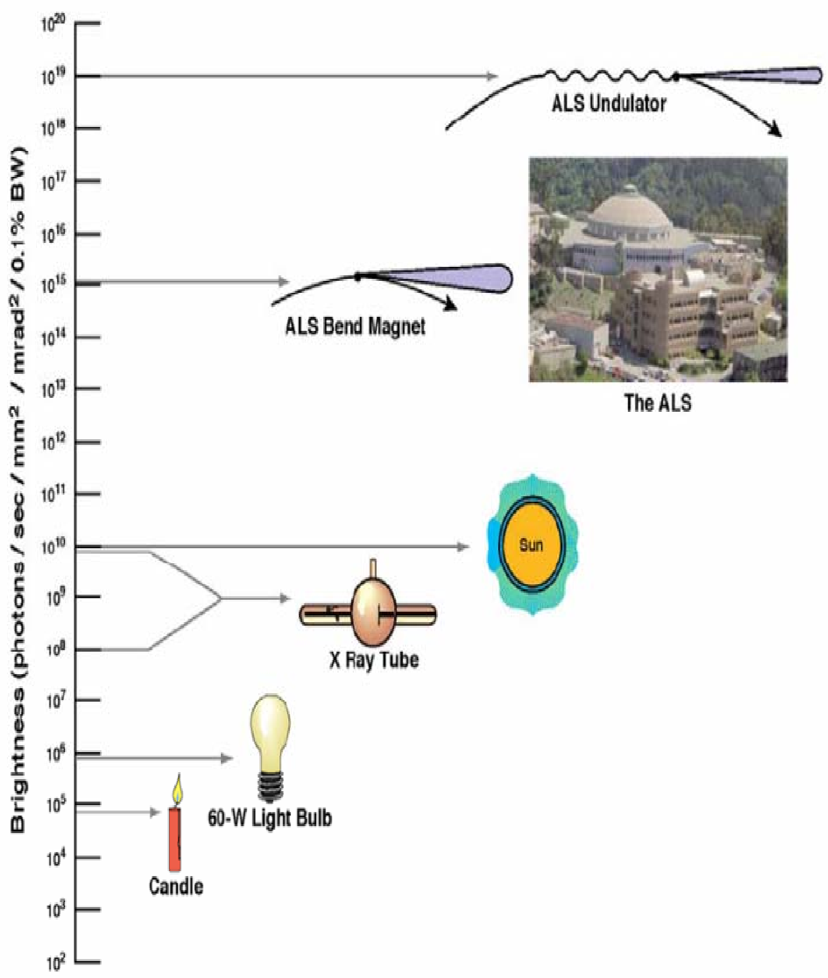
3rd Generation SRF in 2000s

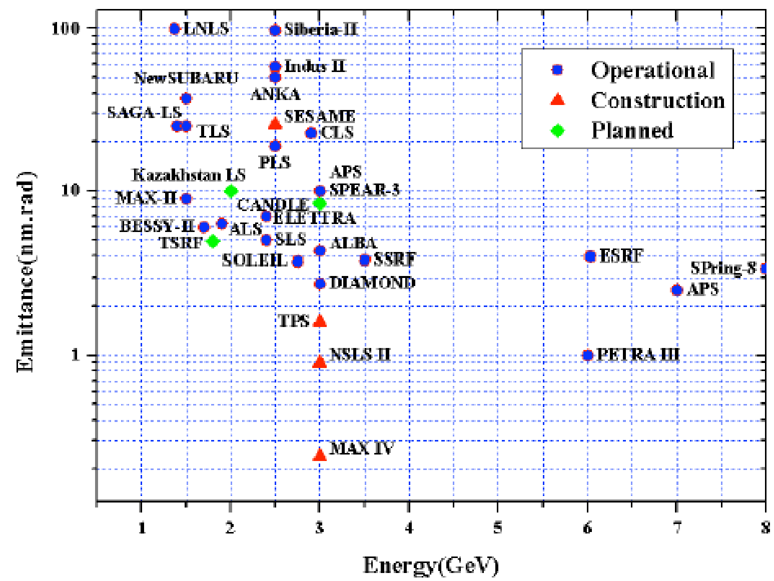
Light Source	Energy (GeV)	Circumference (m)	Emittance (nm-rad)	Current (mA)	Straight Section	Operation Year
New SUBARU	1.5	118.7	38	500	4 x 2.6 m, 2 x 14 m	2000
SLS	2.4-2.7	288	5.0	400	3 × 11.7 m, 3 × 7 m, 6 × 4 m	2001
ANKA	2.5	110.4	50	200	4 × 5.6 m, 4 × 2.2 m	2002
CLS	2.9	170.88	22.7	300	12 × 5.2 m	2003
SPEAR-3	3.0	234	18	500	12 × 3 m, 4 × 4.5 m, 2 × 7.5 m	2004
SAGA-LS	1.4	75.6	7.5	300	8 × 2.5 m	2006
SOLEIL	2.75	354.1	3.74	500	4 × 12 m, 12 × 7 m, 8 × 3.8 m	2007
DIAMOND	3.0	561.6	2.7	300	6 × 11.3 m, 18 × 8.3 m	2007
ASP	3.0	216	10	200	14 × 5.4 m	2008
INDUS II	2.5	172.5	58.1	300	8 × 4.5 m	2008
SSRF	3.5	432	3.9	300	4 × 12 m, 16 × 6.5 m	2009
ALBA	3.0	268.8	4.3	400	4 × 8 m, 12 × 4.2 m, 8 × 2.6 m	2010
PETRA III	6.0	2304	1.0	100	20 × 4 m	2010

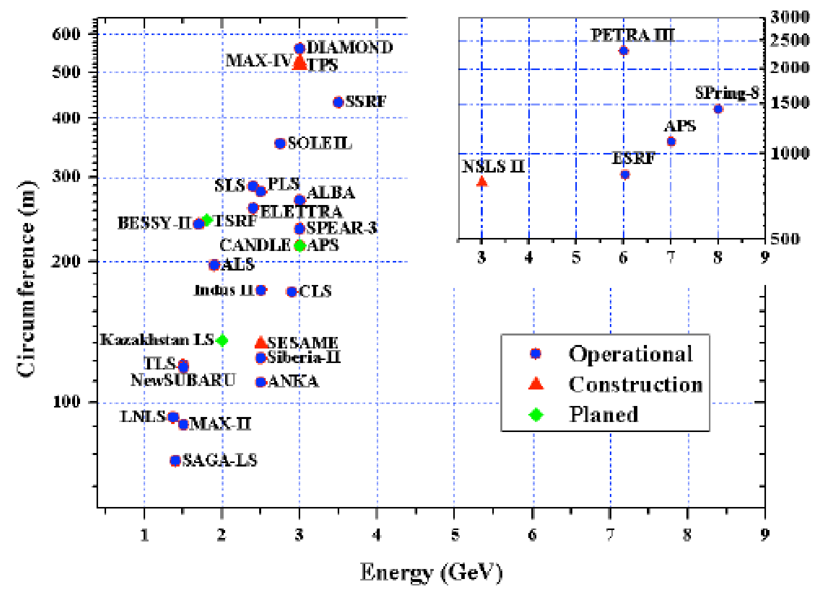
3 Generation Synchrotron Under construction

Light Source	Energy (GeV)	Circumference (m)	Emittance (nm-rad)	Current (mA)	Straight Section	Status
CANDLE	3.0	216	8.4	350	16 x 4.8 m	Planned
MAX IV	1.5/3.0	96 / 528	5.6 / 0.24	500	12 / 20 - straight sections	(2010)
PLS-II	3.0	281	5.8	400	12 X 6.8 m, 12 x 3.1 m	(2011)
TPS	3.0	518	1.7	400	18 x 7 m, 6 x 12 m	(2013)
NSLS-II	3.0	792	0.9	500	15 x 6 m, 15 x 9.3 m	(2014)
SESAME	2.5	133	26	400	4 x 5 m, 8 x 3.5 m, 4 x 1.9 m	(2014)

Characteristics

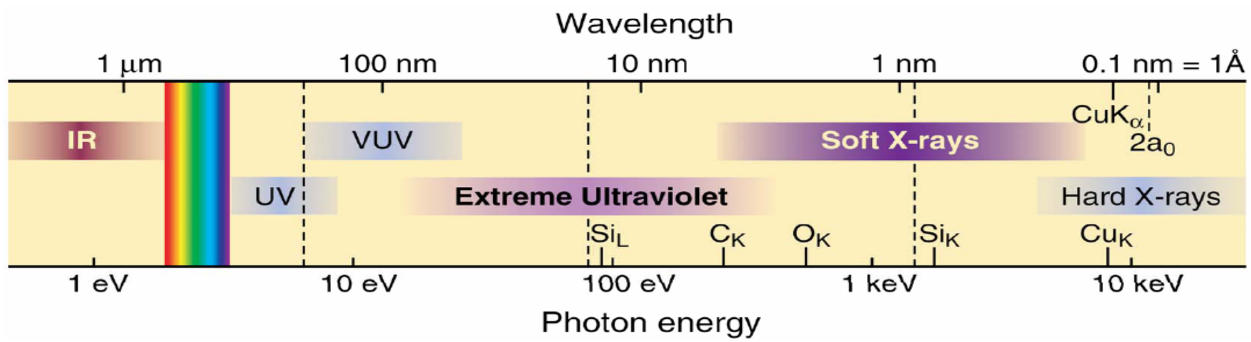


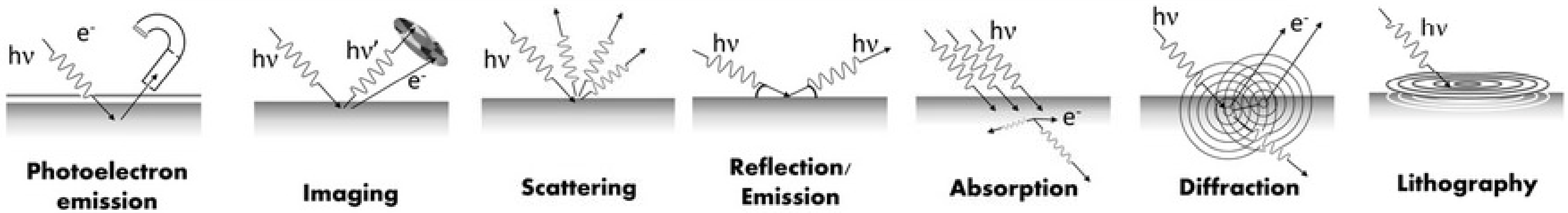


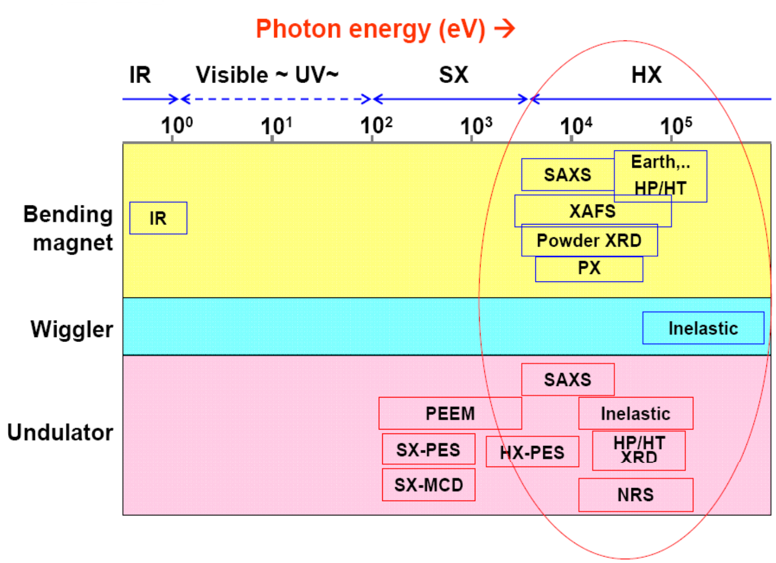


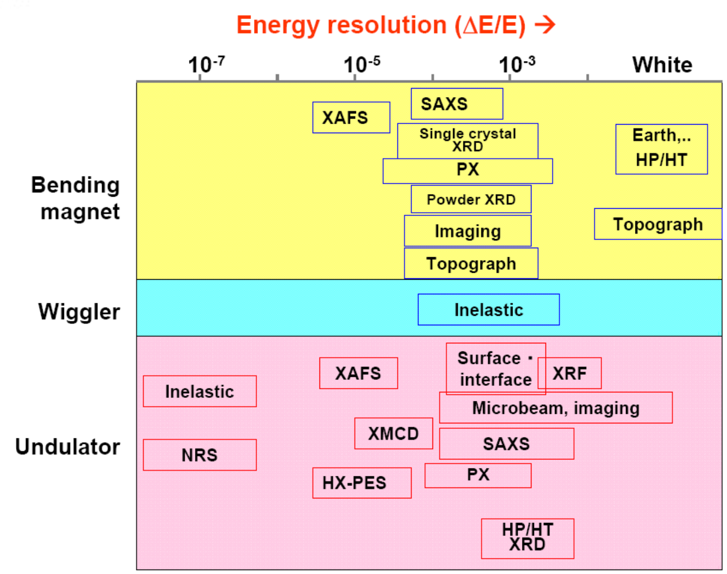
Iranian Light Source Facility

Experimental Techniques









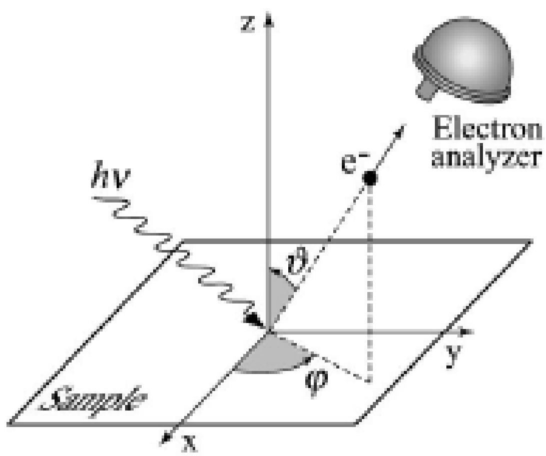
ARPES

- Angular Resolved PhotoEmission Spectroscopy

Electronic structure (bands, Fermi surface, ..)

Electron-phonon interaction

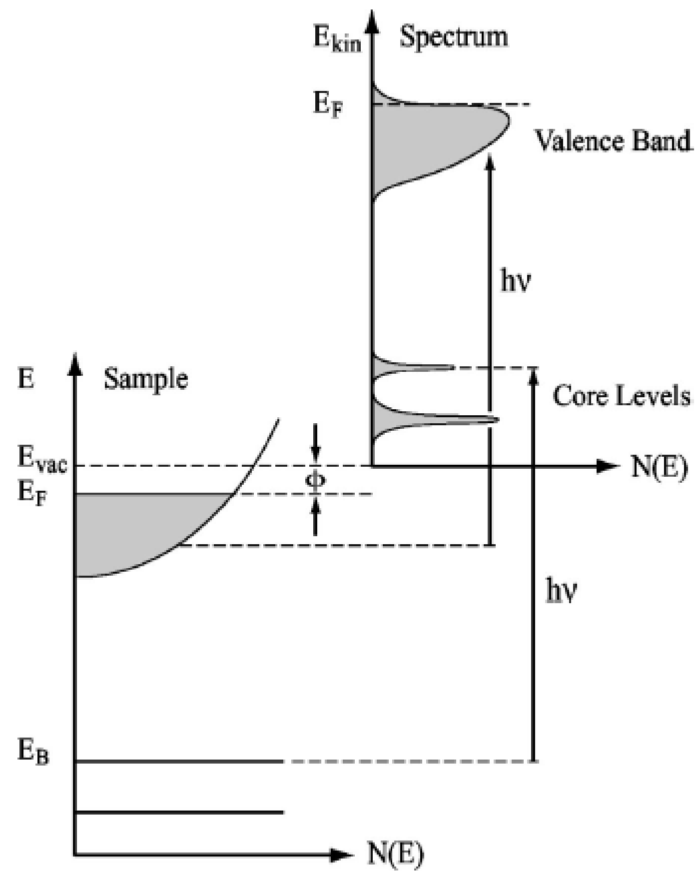
Superconducting Gap structure



Photoemission geometry

$$E_{kin} = h\nu - \phi - |E_B|,$$

$$\mathbf{p}_{\parallel} = \hbar \mathbf{k}_{\parallel} = \sqrt{2mE_{kin}} \cdot \sin\vartheta$$



REVIEWS OF MODERN PHYSICS, VOLUME 75, APRIL 2003

Angle-resolved photoemission studies of the cuprate superconductors

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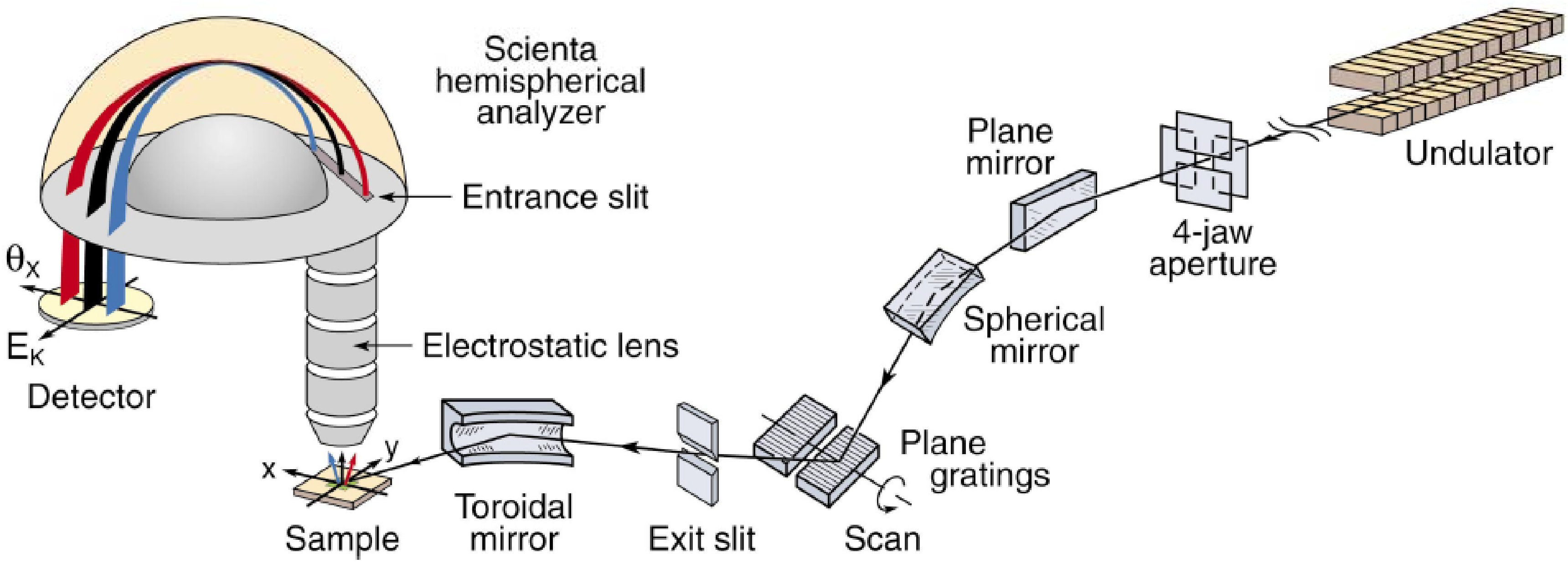
(Published 17 April 2003)

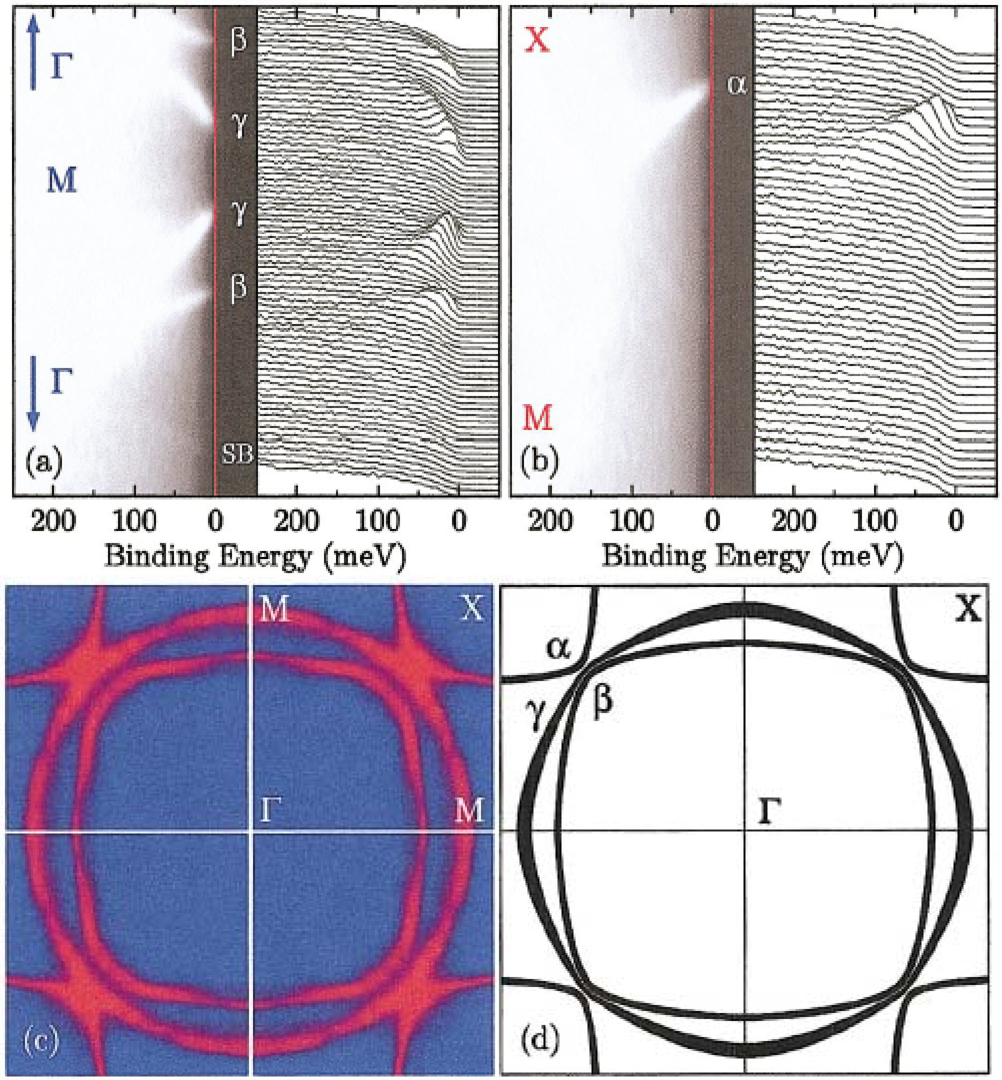
The last decade witnessed significant progress in angle-resolved photoemission spectroscopy (ARPES) and its applications. Today, ARPES experiments with 2-meV energy resolution and 0.2° angular resolution are a reality even for photoemission on solids. These technological advances and the improved sample quality have enabled ARPES to emerge as a leading tool in the investigation of the high-T_c superconductors. This paper reviews the most recent ARPES results on the cuprate superconductors and their insulating parent and sister compounds, with the purpose of providing an updated summary of the extensive literature. The low-energy excitations are discussed with emphasis on some of the most relevant issues, such as the Fermi surface and remnant Fermi surface, the superconducting gap, the pseudogap and d-wave-like dispersion, evidence of electronic inhomogeneity and nanoscale phase separation, the emergence of coherent quasiparticles through the superconducting transition, and many-body effects in the one-particle spectral function due to the interaction of the charge with magnetic and/or lattice degrees of freedom. Given the dynamic nature of the field, we chose to focus mainly on reviewing the experimental data, as on the experimental side a general consensus has been reached, whereas interpretations and related theoretical models can vary significantly. The first part of the paper introduces photoemission spectroscopy in the context of strongly interacting systems, along with an update on the state-of-the-art instrumentation. The second part provides an overview of the scientific issues relevant to the investigation of the low-energy electronic structure by ARPES. The rest of the paper is devoted to the experimental results from the cuprates, and the discussion is organized along conceptual lines: normal-state electronic structure, interlayer interaction, superconducting gap, coherent superconducting peak, pseudogap, electron self-energy, and collective modes. Within each topic, ARPES data from the various copper oxides are presented.

Experimental setup & condition



Energy Range: Ultraviolet (<100 eV)
Energy Resolution: a few meV
Angular Resolution: 0.2°
Pressure lower than $5*10^{-11}$ torr

Fermi Surface



Experiment

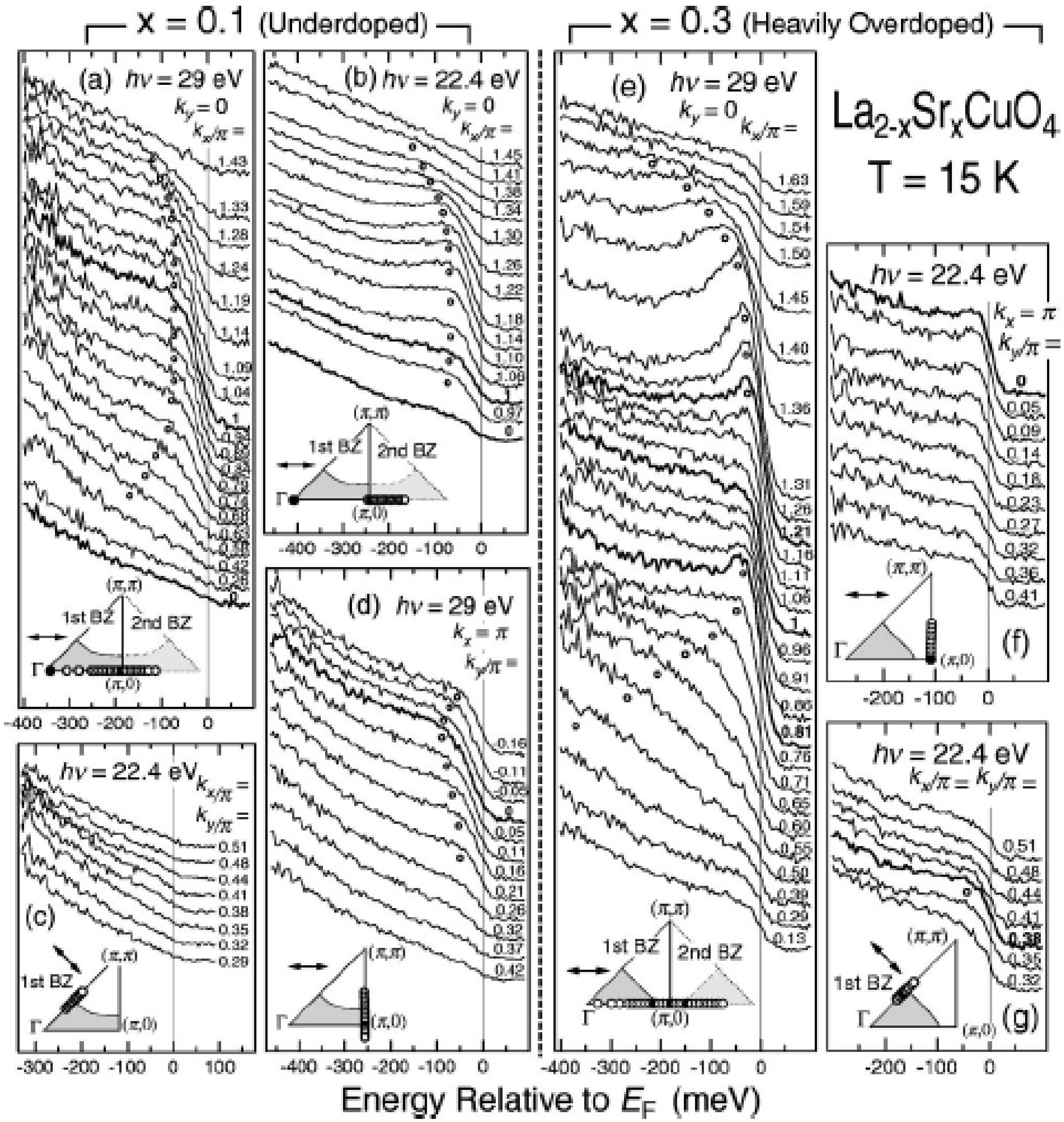
Sr_2RuO_4 cleaved at 180 K
T= 10 K hν=28 eV

Calculation

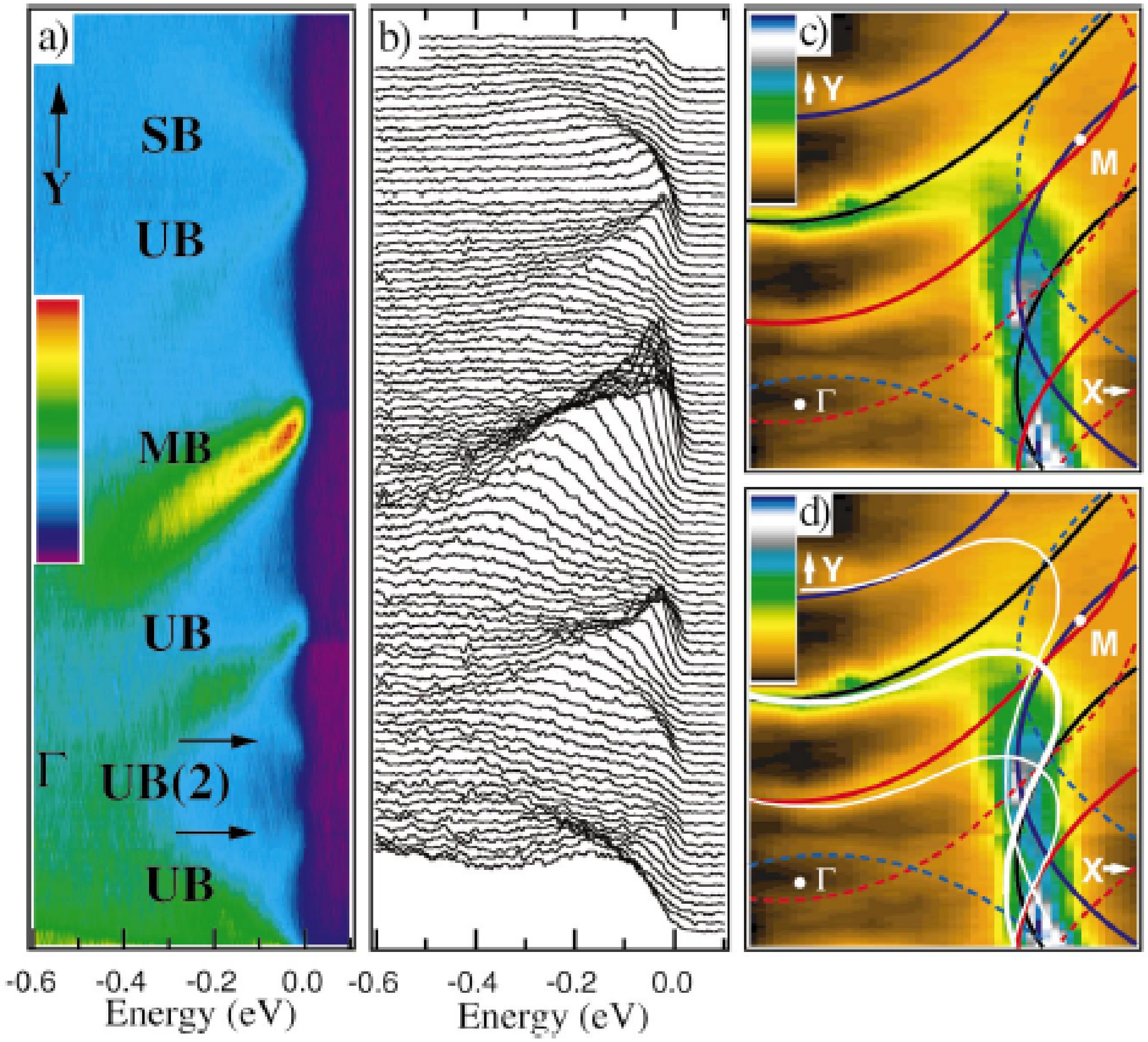
Local-density-approximation
band-structure calculation

Band structure & Fermi surface of new superconductor Sr2RuO4 (isostructure with La2CuO4)

Doping and Momentum dependence



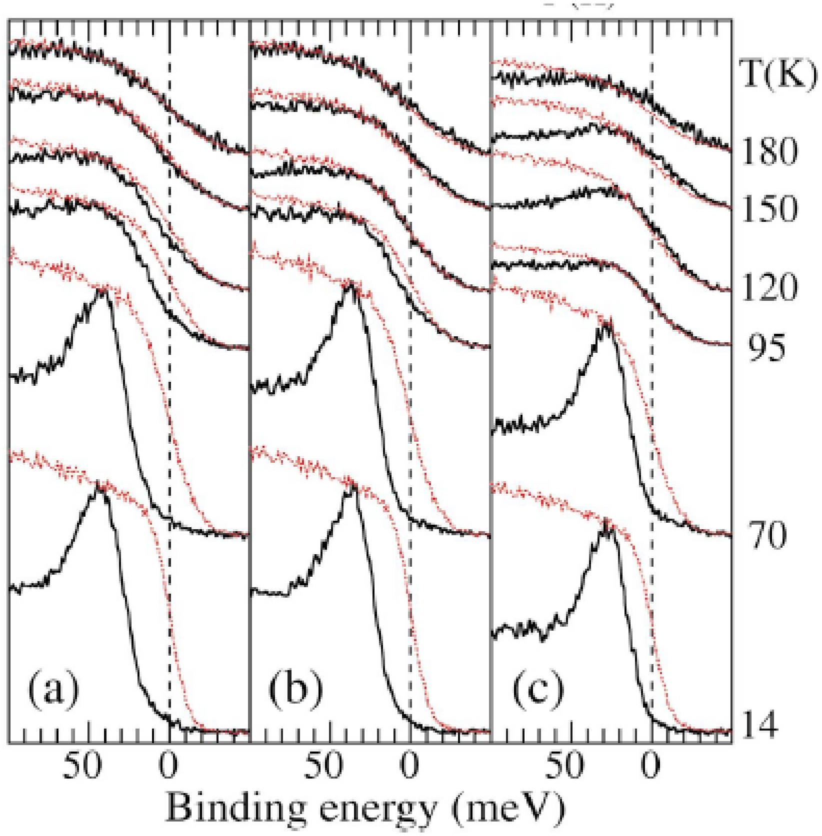
Band Structure & Fermi Surface

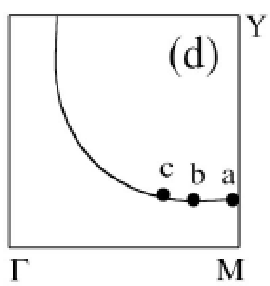


Integrated intensity map (±100 meV)

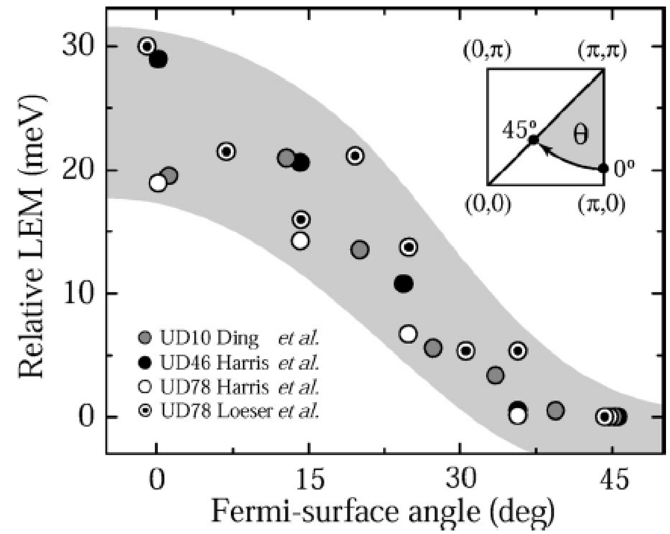
Optimally doped Bi2212 (Tc=90 K) at 40 K

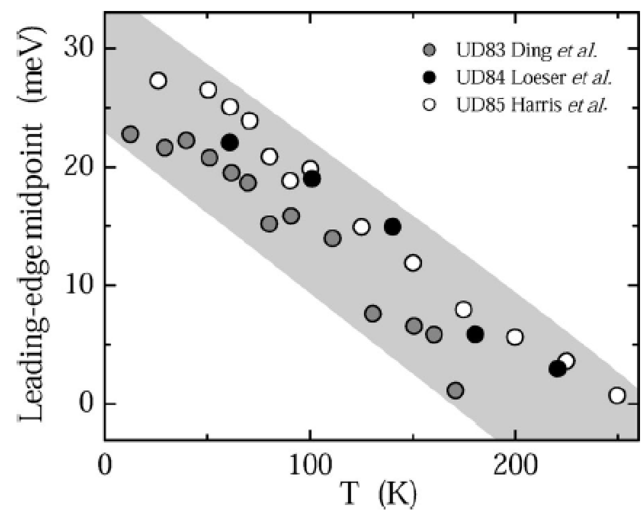
Pseudogap: T and k dependence



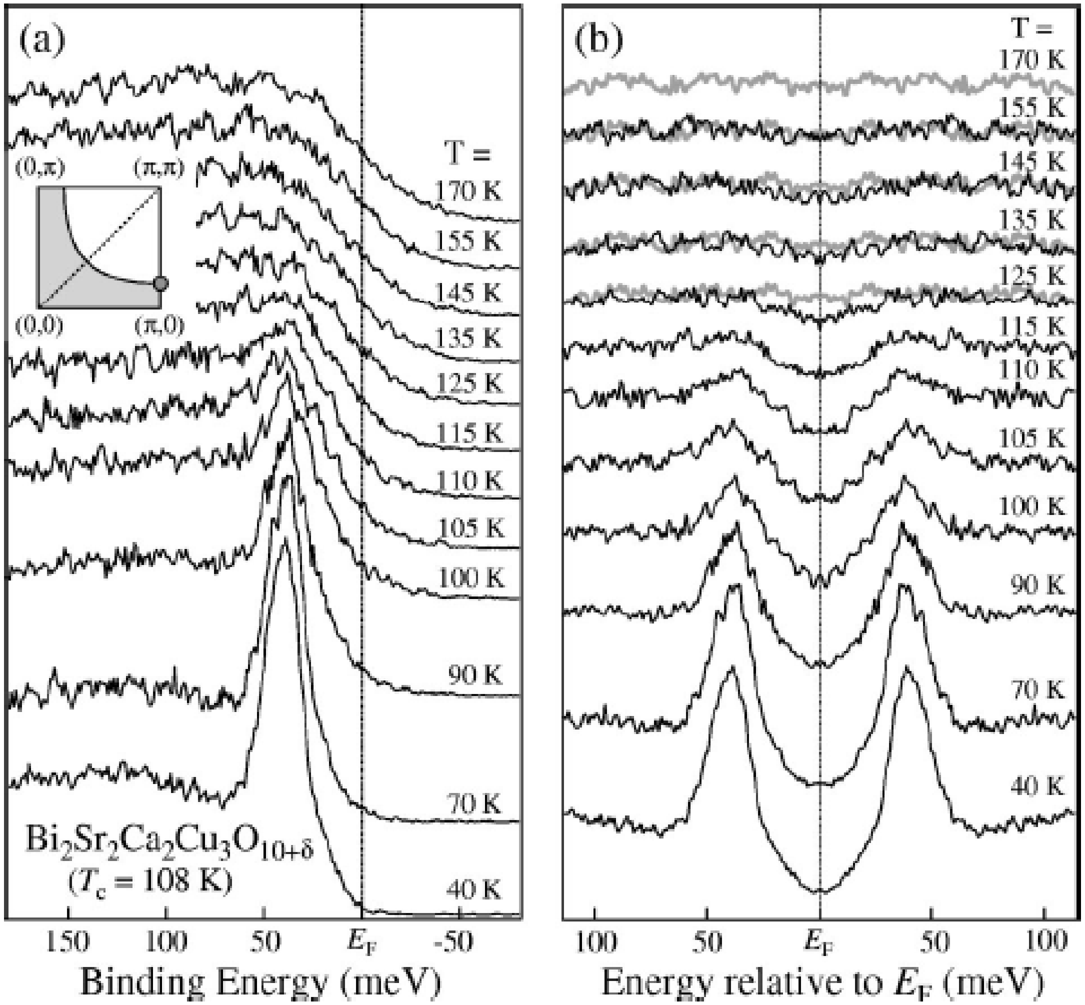


Bi2212 (T_c=85 K)

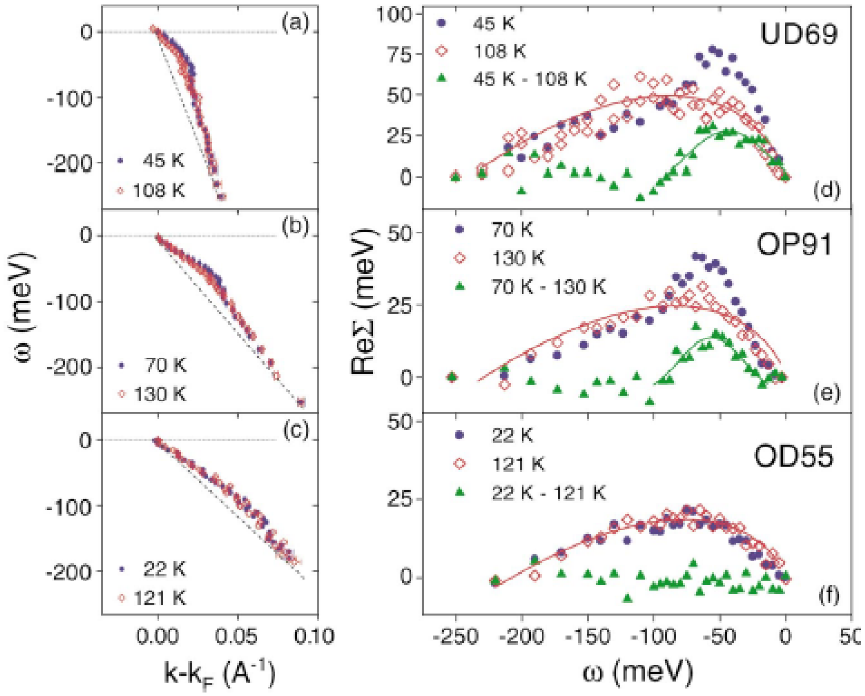


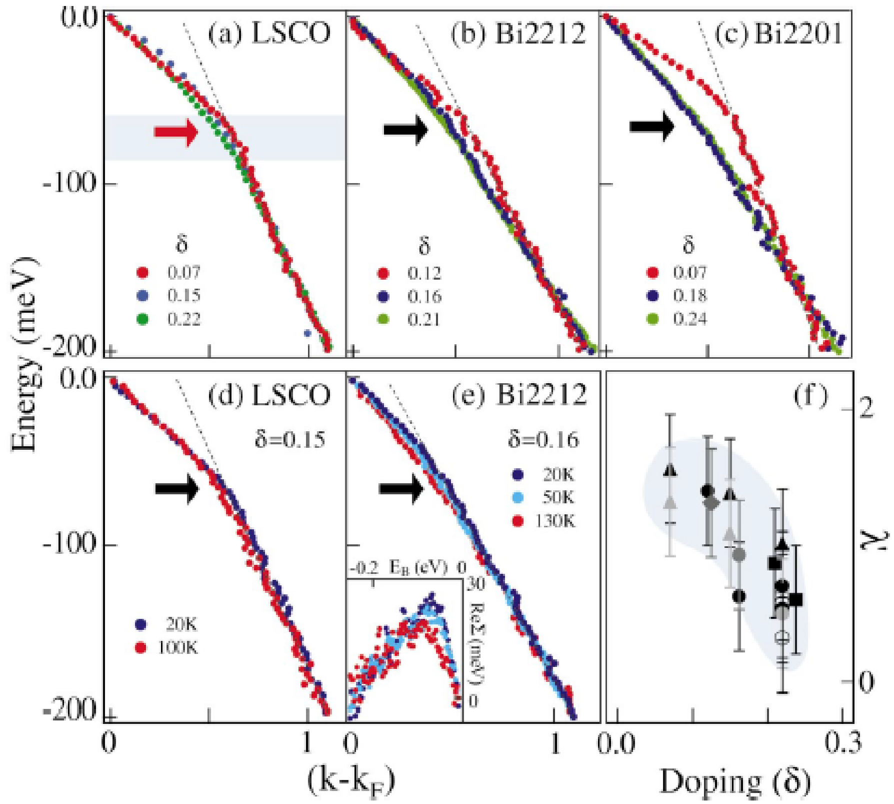


Peak-Deep-Hump structure and Superconducting Gap

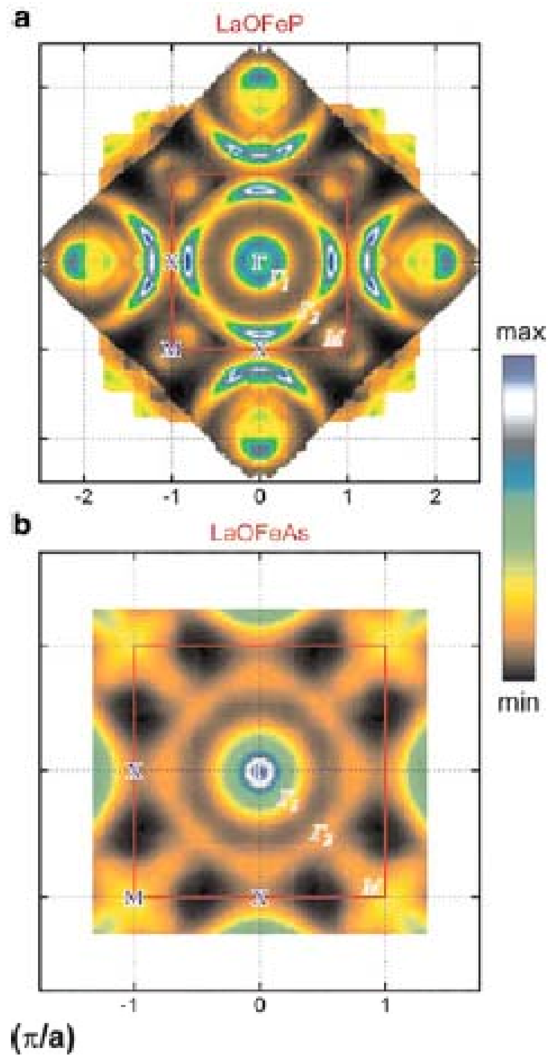


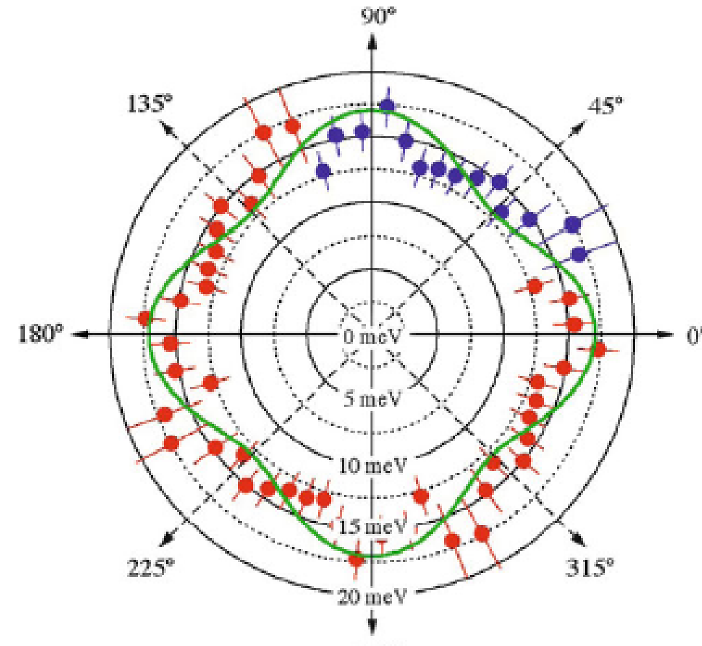
Electron-Phonon Interaction

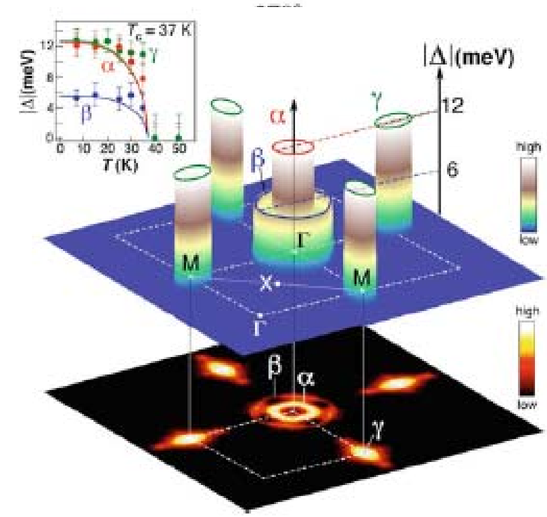




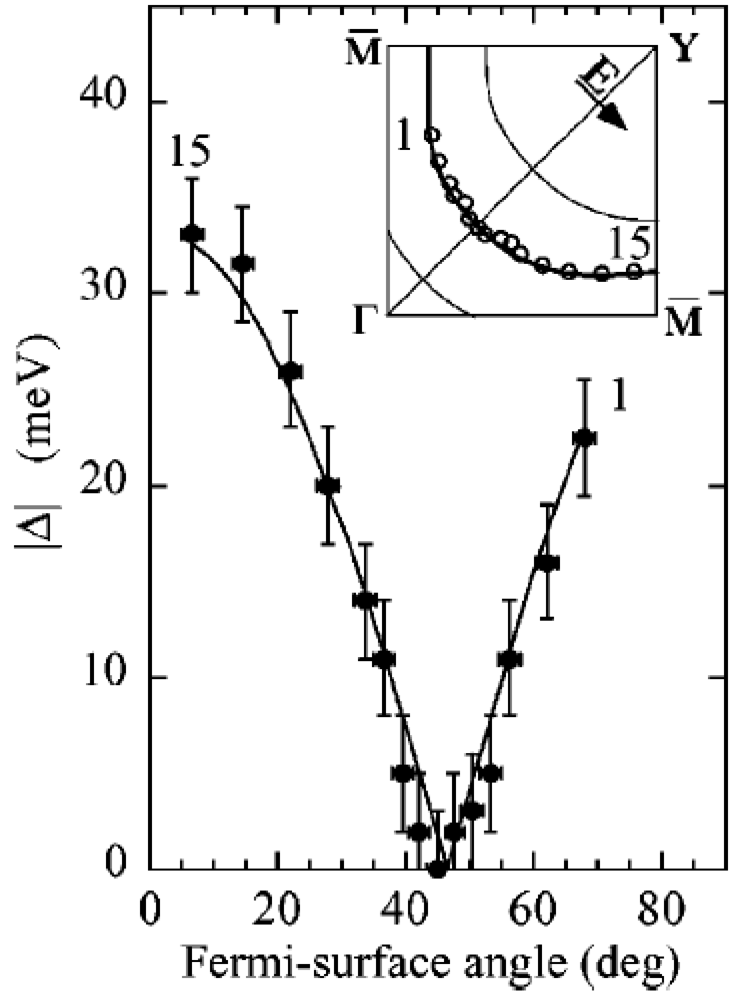
FeAs Superconductors

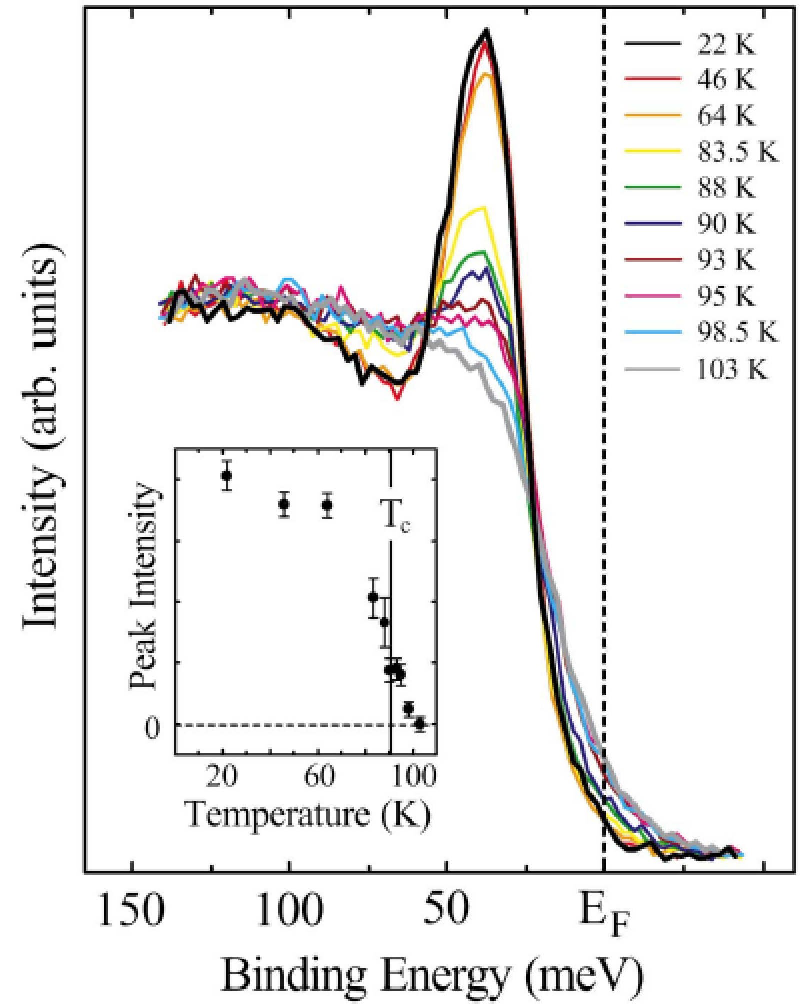






Pairing Symmetry





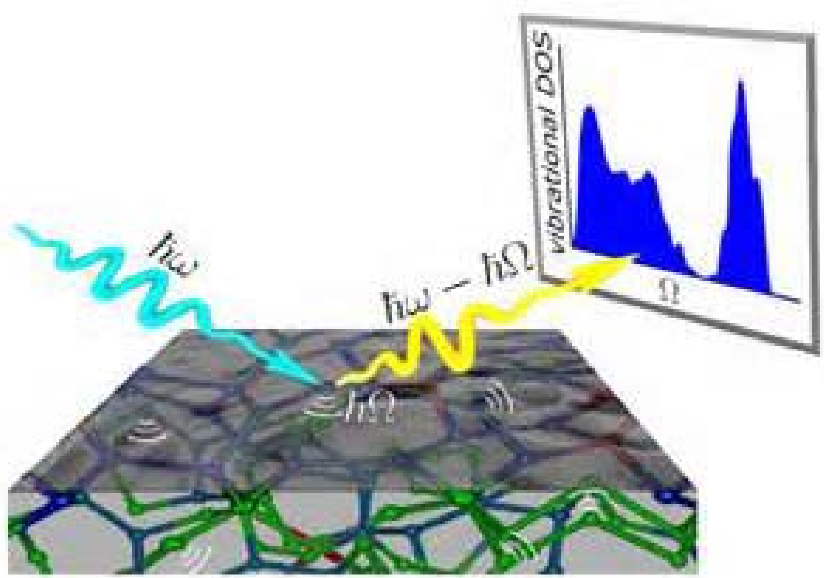
IXS

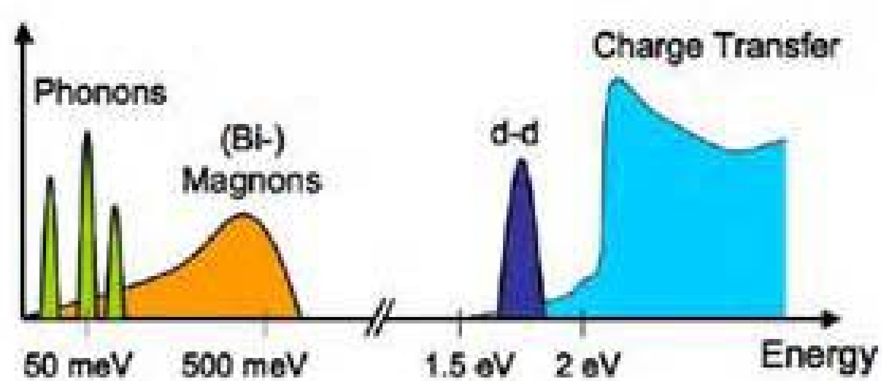
- Inelastic X-ray Scattering

Electronic and dynamic excitations

Phonon structure

Electron-phonon interaction





Rep. Prog. Phys. 63 (2000) 171–232. Printed in the UK PII: S0034-4885(00)88954-X

Phonon spectroscopy by inelastic x-ray scattering

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Received 24 May 1999, in final form 18 November 1999

Abstract

The present synchrotron sources with brilliant x-ray beams, due to high photon fluxes, small source sizes and high collimation, have revolutionized x-ray physics.

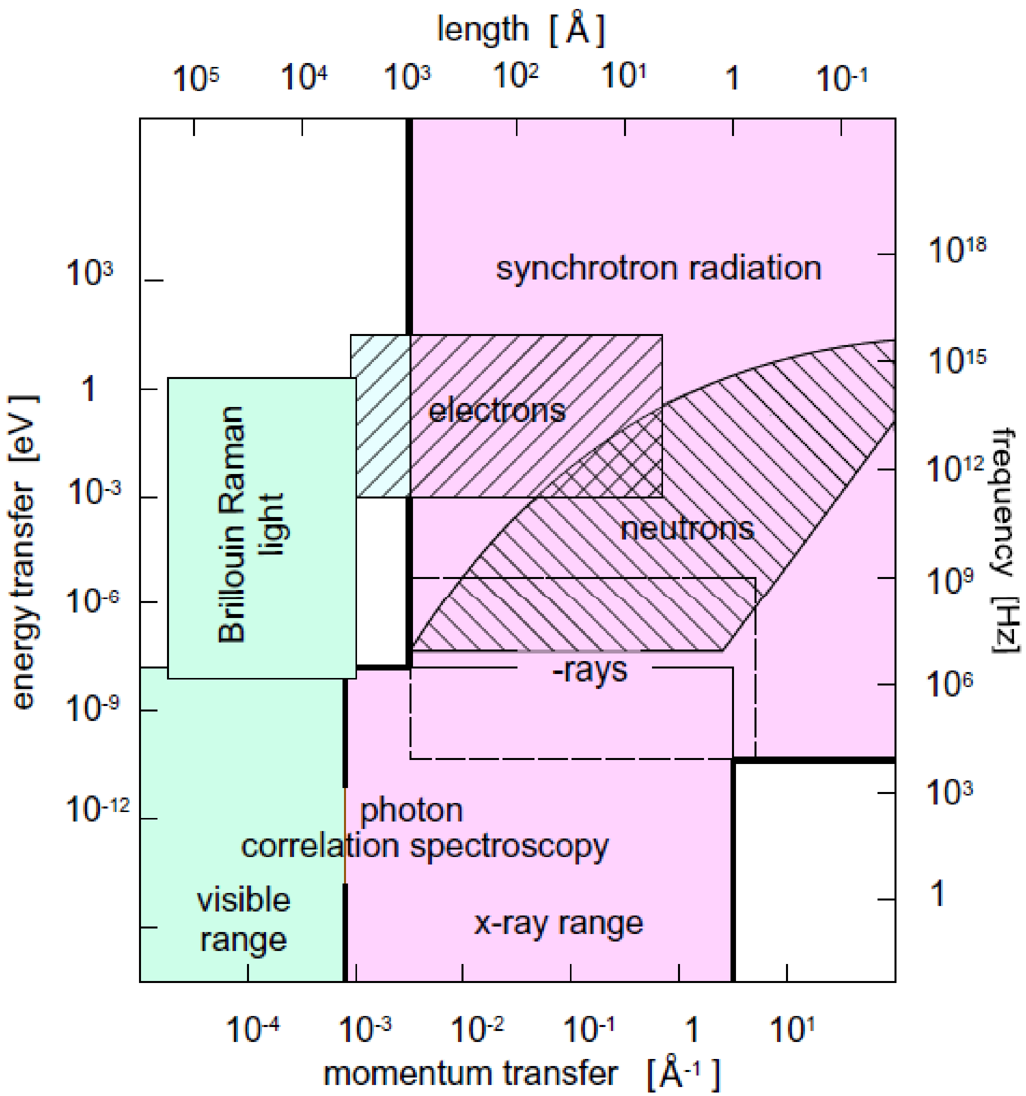
Enormous progress has been initiated in all established x-ray methods, with the aim of the development of new types of spectroscopy. This is particularly true for the spectroscopy of the dynamics in condensed matter. Meanwhile, there are two powerful x-ray methods with very high-energy resolution available for the study of low energetic excitations like phonons.

This review summarizes the developments of these methods focusing on these instrumental developments of the spectrometers using either crystal optics in close-to-backscattering geometry or nuclear resonant techniques.

Applications to measurements of phonon dispersion curves and of phonon density of states in ordered and disordered solids and in liquids are presented. It is shown how x-ray results are stimulating improvements in the theoretical approaches to the dynamics. New insights into the dynamics of liquids are discussed.

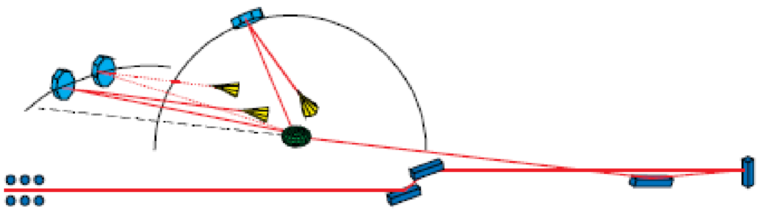
The sensitivities of the spectroscopies allow the study of vibrational behaviour in very small amounts of material even in nanometre-sized thin films or particles. We can already analyse the phonon spectrum of a monolayered nuclear resonant isotope. Prospects of the techniques are also demonstrated.

Energy-Momentum

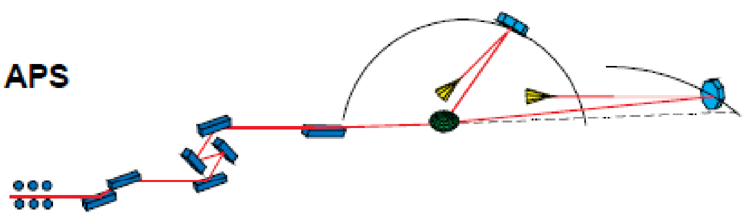


Experimental setup

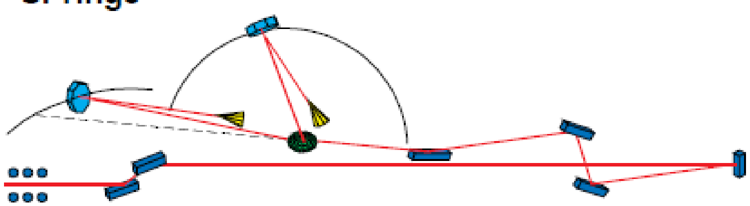
ESRF

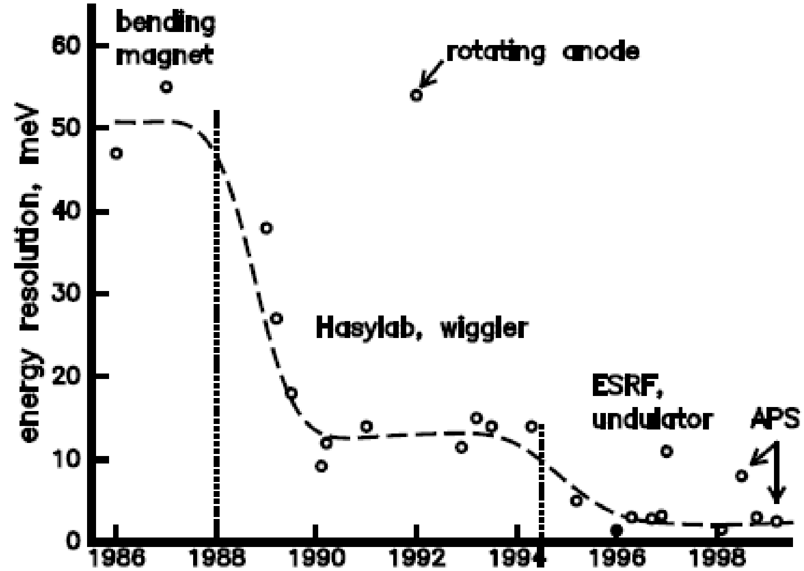


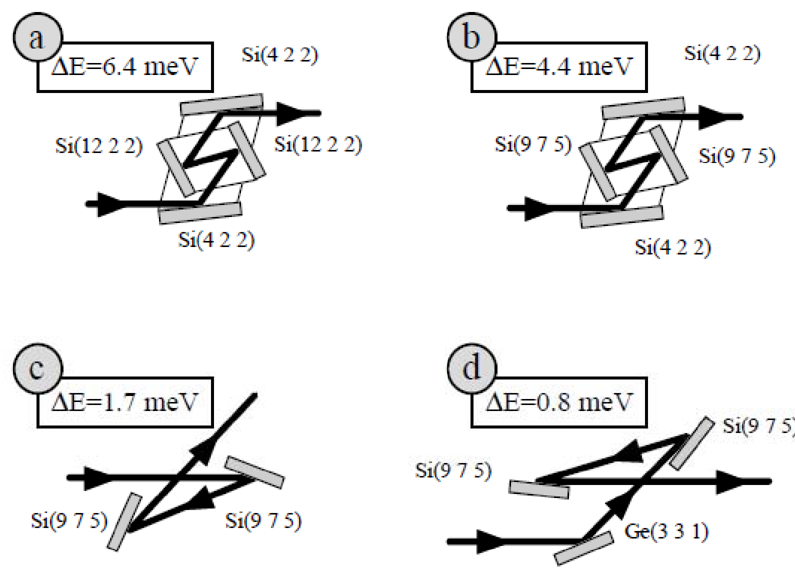
APS



SPring8







Experimental Condition

Table 2. Comparison of backscattering spectrometers at HASYLAB, at the ESRF, at APS and SPring-8.

Location	INELAX HASYLAB Hamburg, Germany	ID16 ESRF Grenoble, France	3ID APS Chicago, USA	BL35XU SPring-8 Kansai, Japan
Operational	1987	1994	1997	2000
Source characteristics				
Ring energy	4.5 GeV	6.0 GeV	7.0 GeV	8.0 GeV
Ring current	140 mA	200 mA	100 mA	100 mA
Insertion device	wiggler	2 undulators	undulator	undulator
Length	2.6 m	1.6 m each	2.5 m	4.5 m
Divergence:				
vertical	0.12 mrad	24 μrad	12 μrad	11 μrad
horizontal	2.6 mrad	40 μrad	42 μrad	35 μrad
X-ray optics				
Pre-monochromator	Si (1 1 1) 2-crystal setting room temperature	Si (1 1 1) channel-cut at 90–120 K	diamond 2-crystal setting room temperature	Si (1 1 1) 2-crystal setting cryogenically cooled
Main monochromator	Si (h h h) backscattering spherically bent	Si (h h h) backscattering flat focusing mirror	Si (4 4 0) + (15 11 3) nested channel-cut focusing mirror	Si (h h h) backscattering flat focusing mirror
Focus spot	3×1 mm^2	500×300 μm^2	600×500 μm^2	100×150 μm^2
Analyser	Si (h h h) spherically bent	Si (h h h) spherically bent	Si (h h h) spherically bent	Si (h h h) spherically bent

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Examples

Softening of Cu-O Bond Stretching Phonons in Tetragonal $HgBa_2CuO_{4+\delta}$

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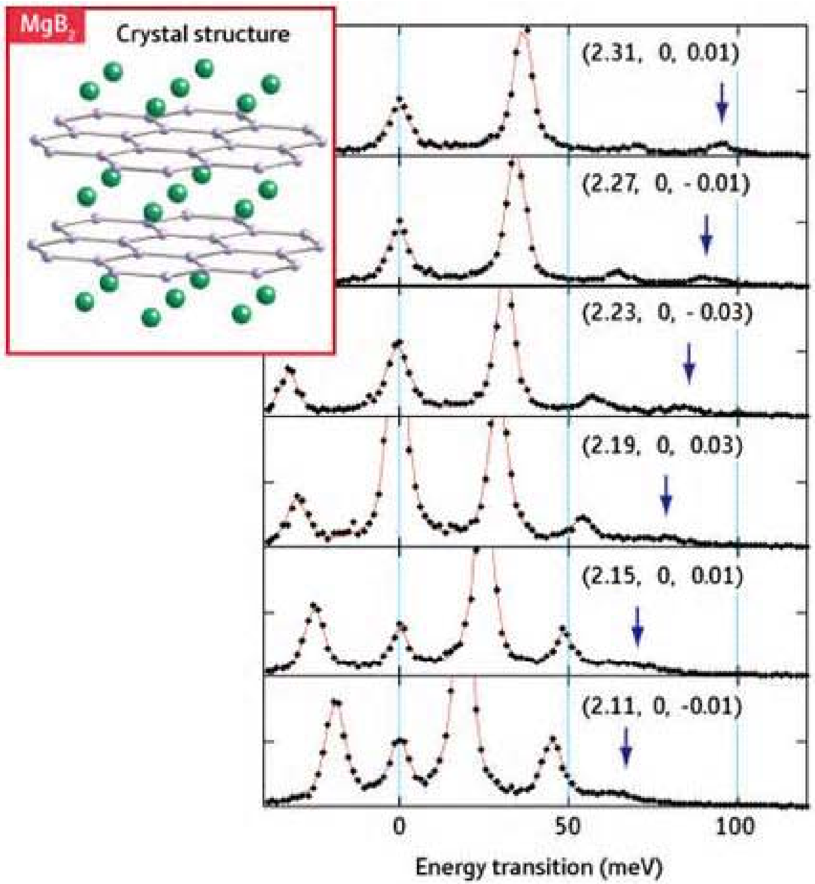
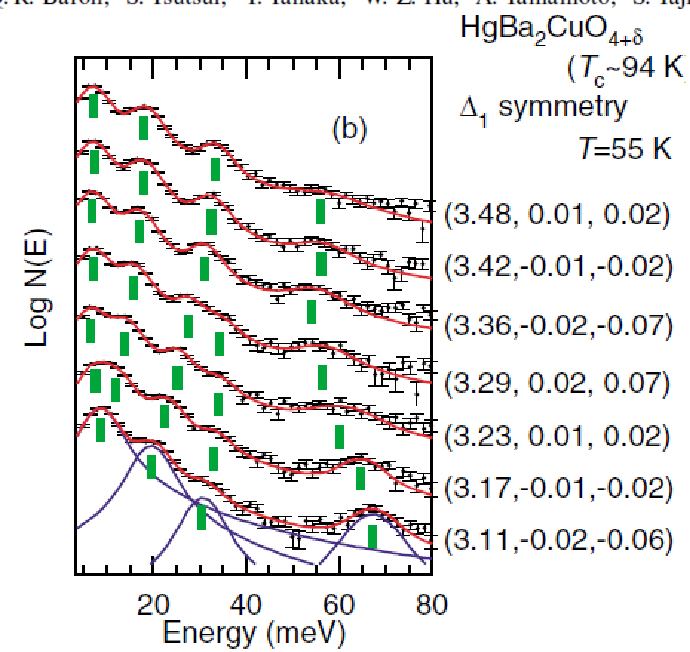
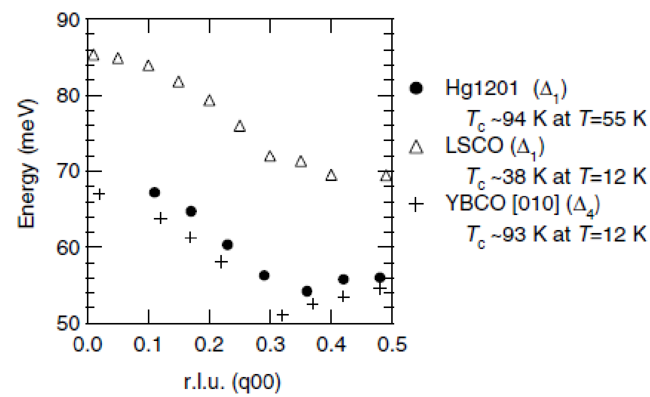
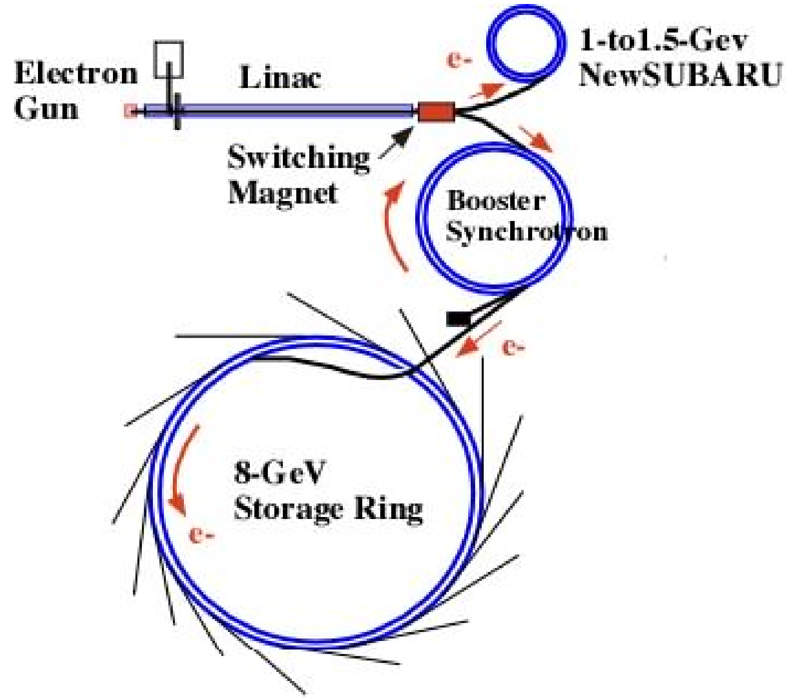






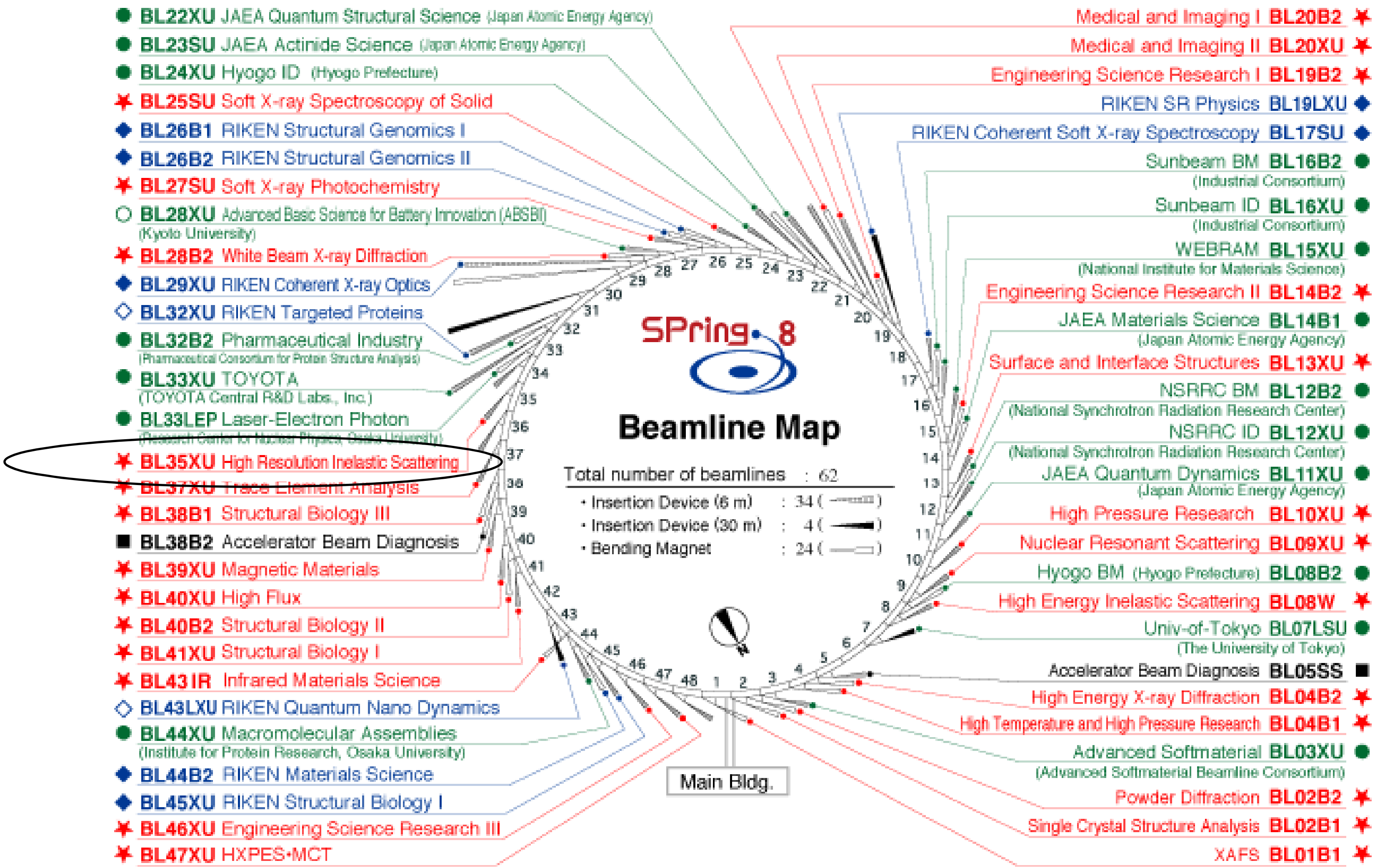
SPring8 Synchrotron



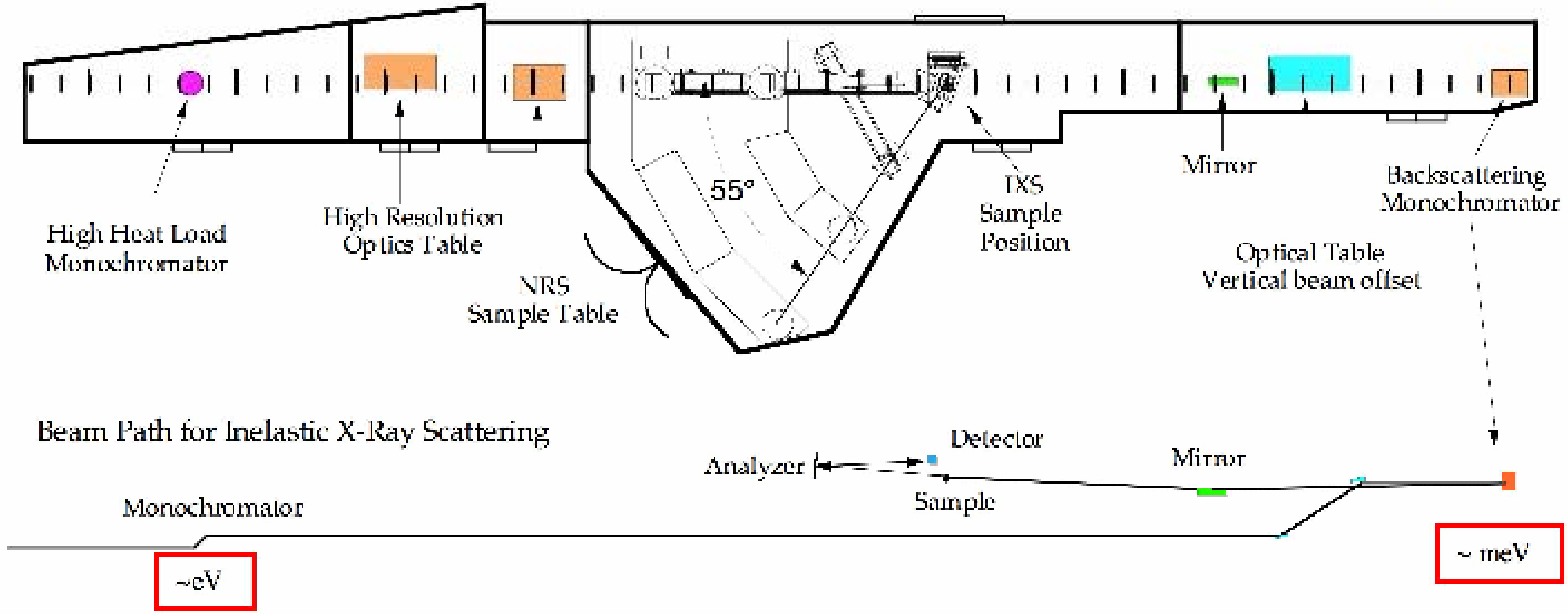
Iranian Light Source Facility

IPM

BL35- Inelastic X-ray Scattering

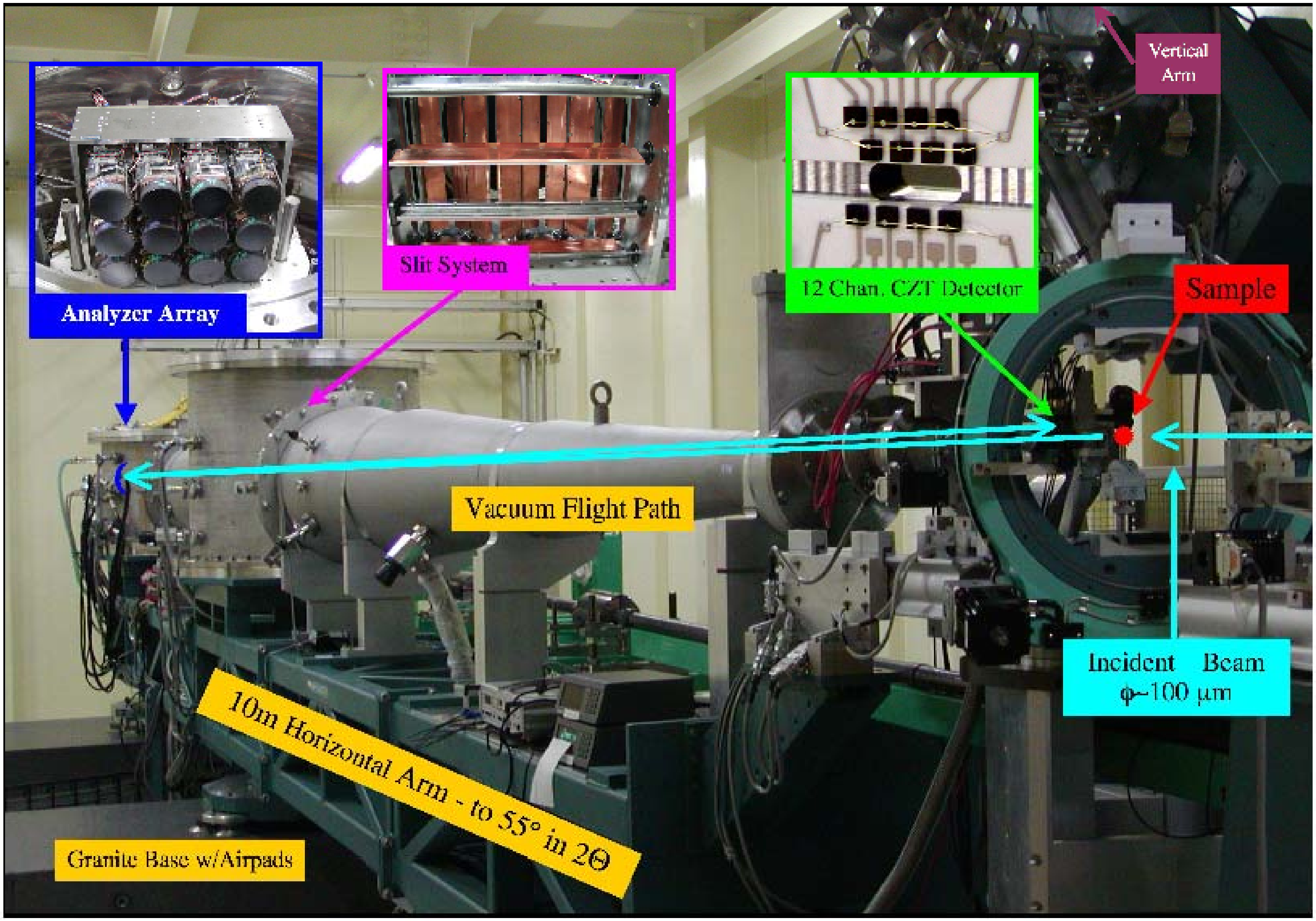


BL35XU Layout

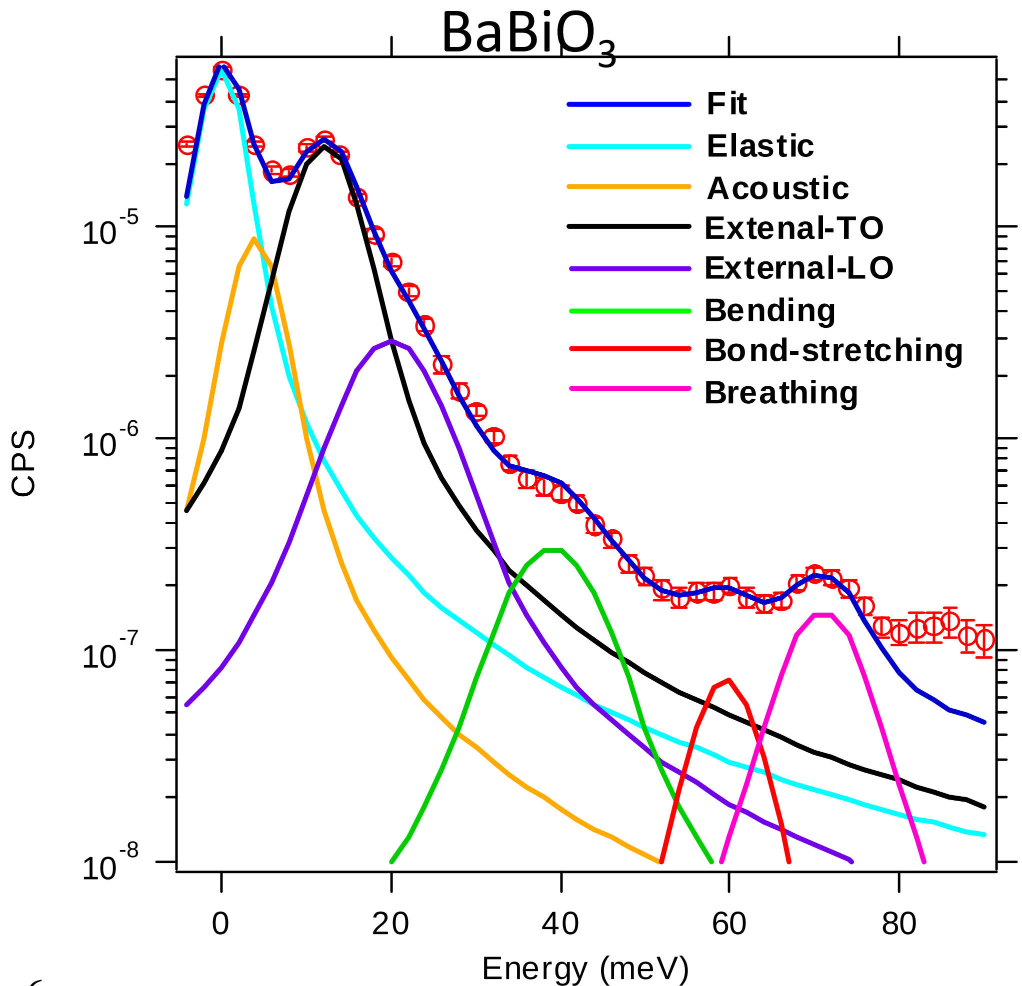


Energy (keV)	Si Order	Resolution (meV)	Flux at Sample (GHz)
15.816	(8 8 8)	6	30
17.794	(9 9 9)	3	10
21.747	(11 11 11)	1.5	3.5
25.702	(13 13 13)	1.0	0.8

Experimental Station

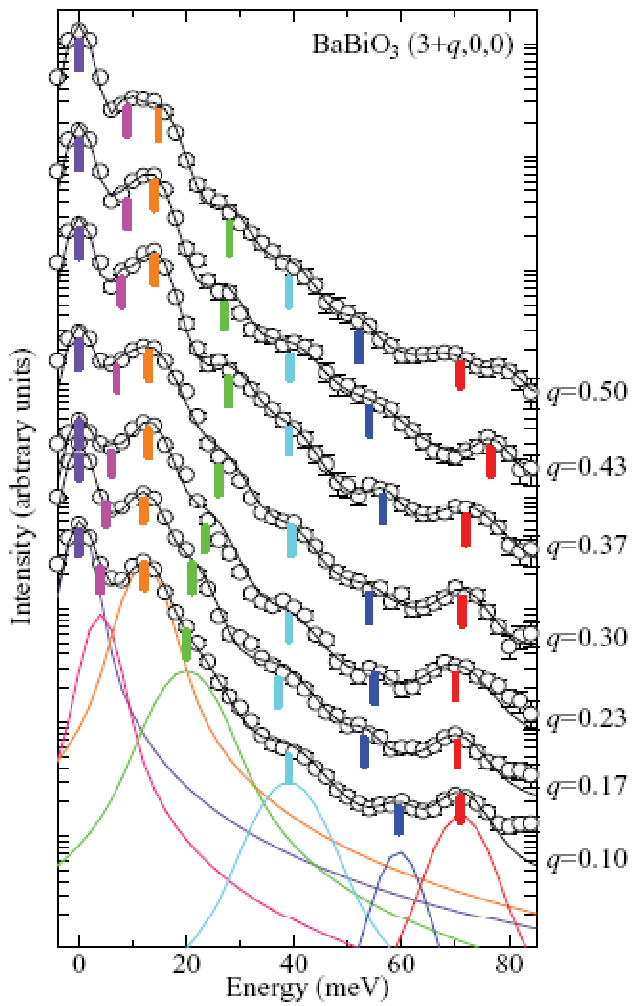


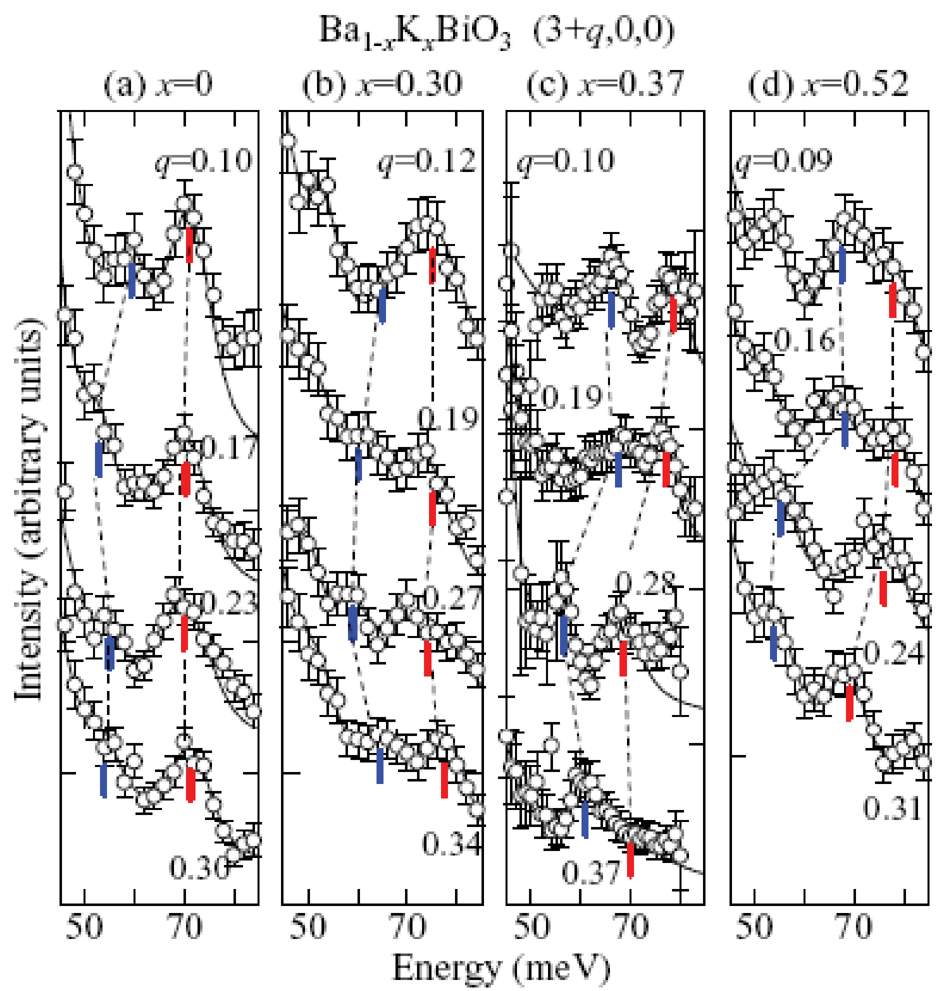
Phonon Spectrum

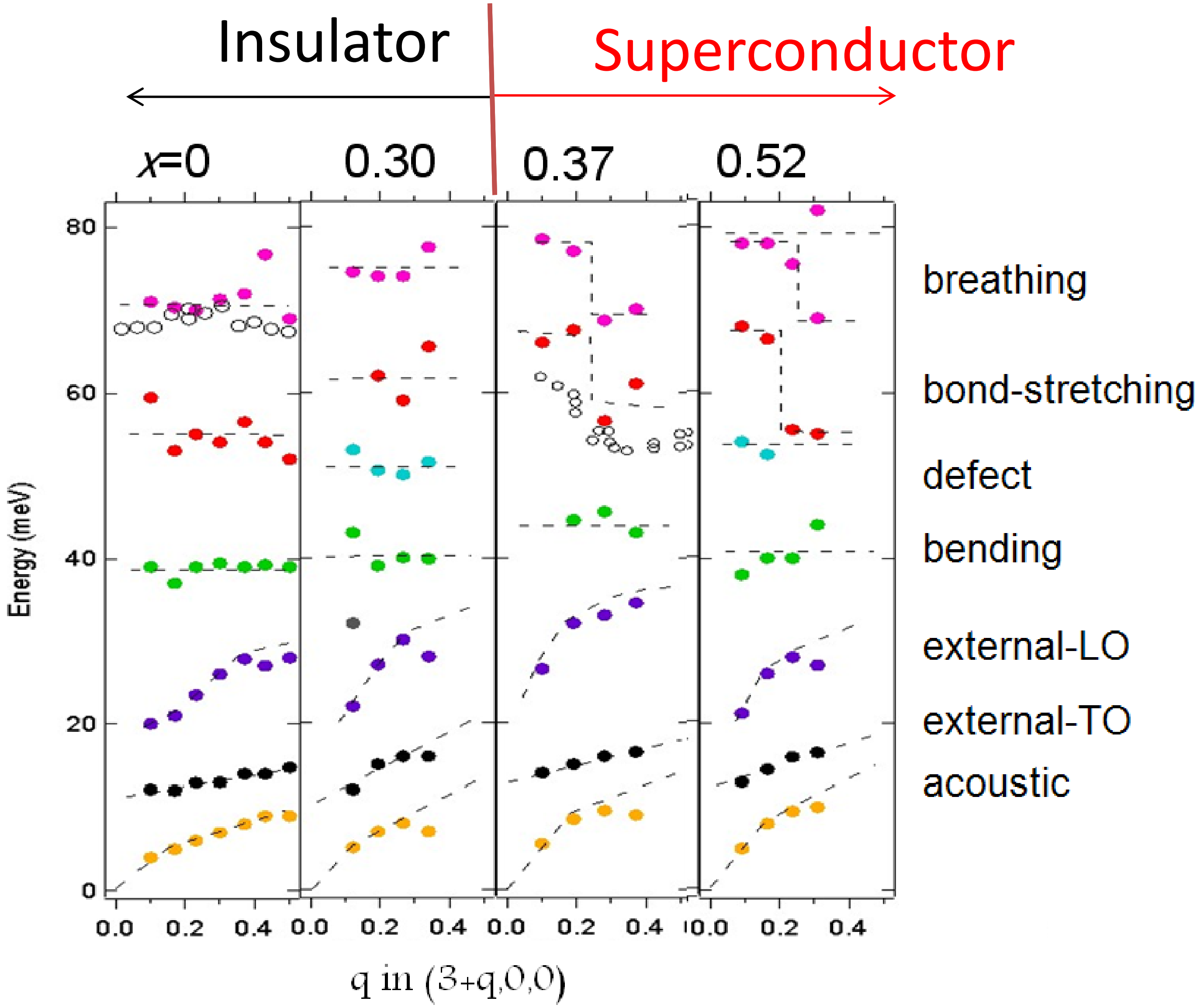


$$I(\omega) = I_0 \left\{ \frac{2\eta}{\pi} \frac{\Gamma}{\Gamma^2 + 4(\omega - \omega_0)^2} + \frac{2(1-\eta)}{\Gamma} \left(\frac{\ln 2}{\pi}\right)^{0.5} \exp\left(-4 \ln 2 \left(\frac{\omega - \omega_0}{\Gamma}\right)^2\right) \right\}$$

Momentum & Doping dependence







Insulator
Superconductor
x=0
0.30
0.37
0.52
Energy (meV)
80
60
40
20
0
0.0 0.2 0.4 0.0 0.2 0.4 0.0 0.2 0.4 0.0 0.2 0.4
q in (3+q,0,0)
breathing
bond-stretching
defect
bending
external-LO
external-TO
acoustic

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Softening of bond-stretching phonon mode in $Ba_{1-x}K_xBiO_3$ at the metal-insulator transition

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The dispersion of phonons in $Ba_{1-x}K_xBiO_3$ along the $(3+q, 0, 0)$ direction in reciprocal space was determined for $x = 0$, 0.30, 0.37, and 0.52 using high-resolution inelastic x-ray scattering. The observed phonon energies

Thank You