

The Power of Core-level Spectroscopy

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Outline of talk

- Introduction to EELS and XAS
- What you can measure
- What information you can get
- What it is used for



Electron energy loss spectroscopy in a Transmission Electron Microscopy

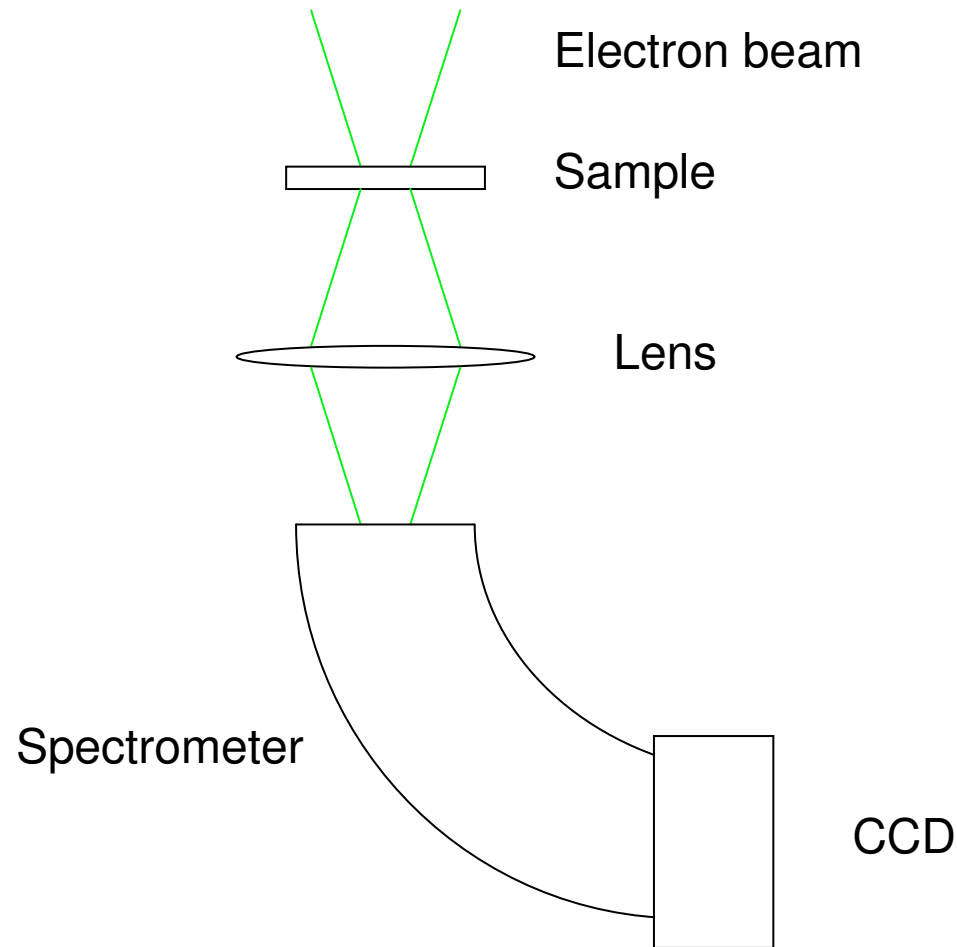
electron gun

sample
(3mm disc)

spectrometer



Electron energy loss spectroscopy in a TEM

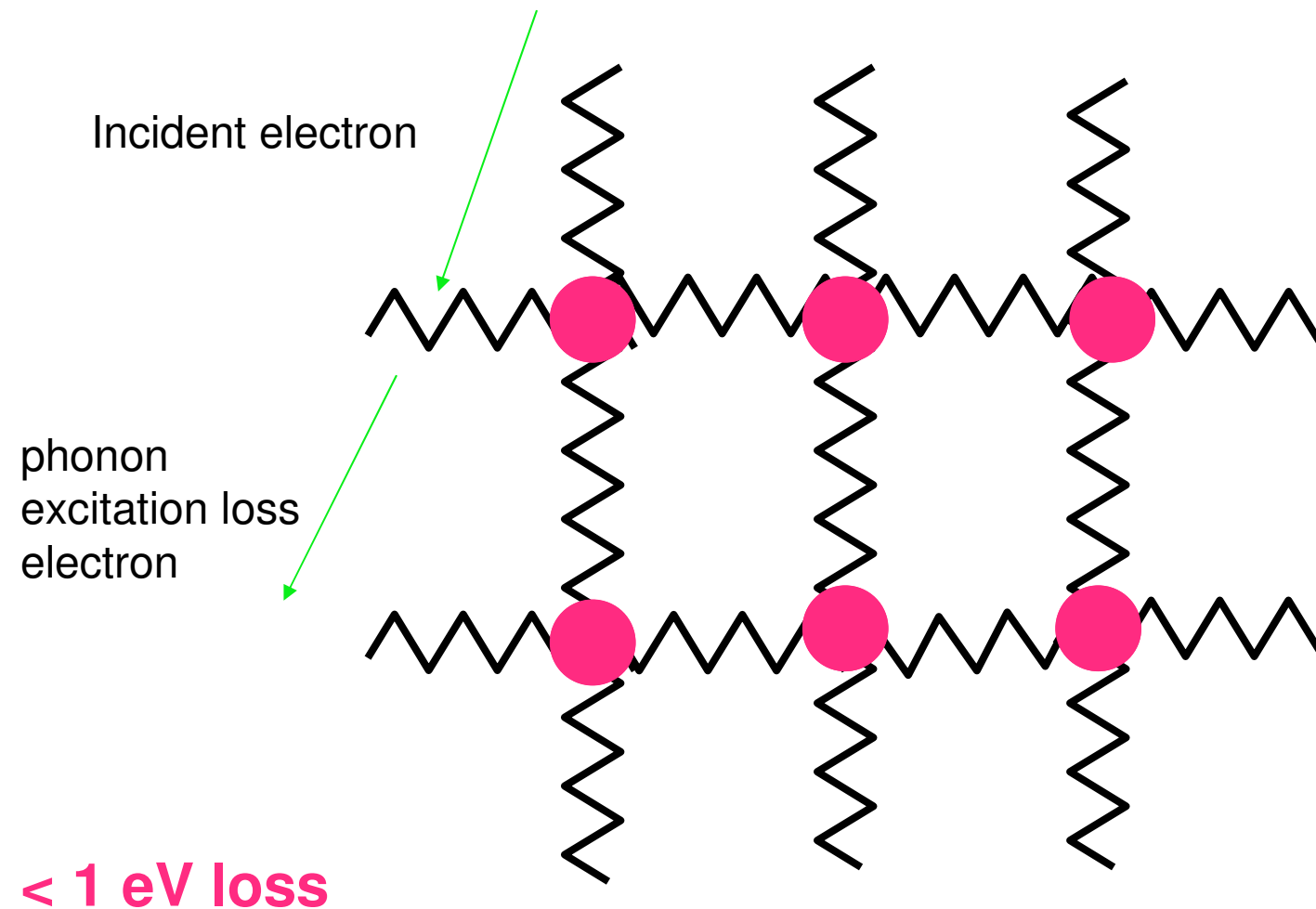


Inelastic scattering

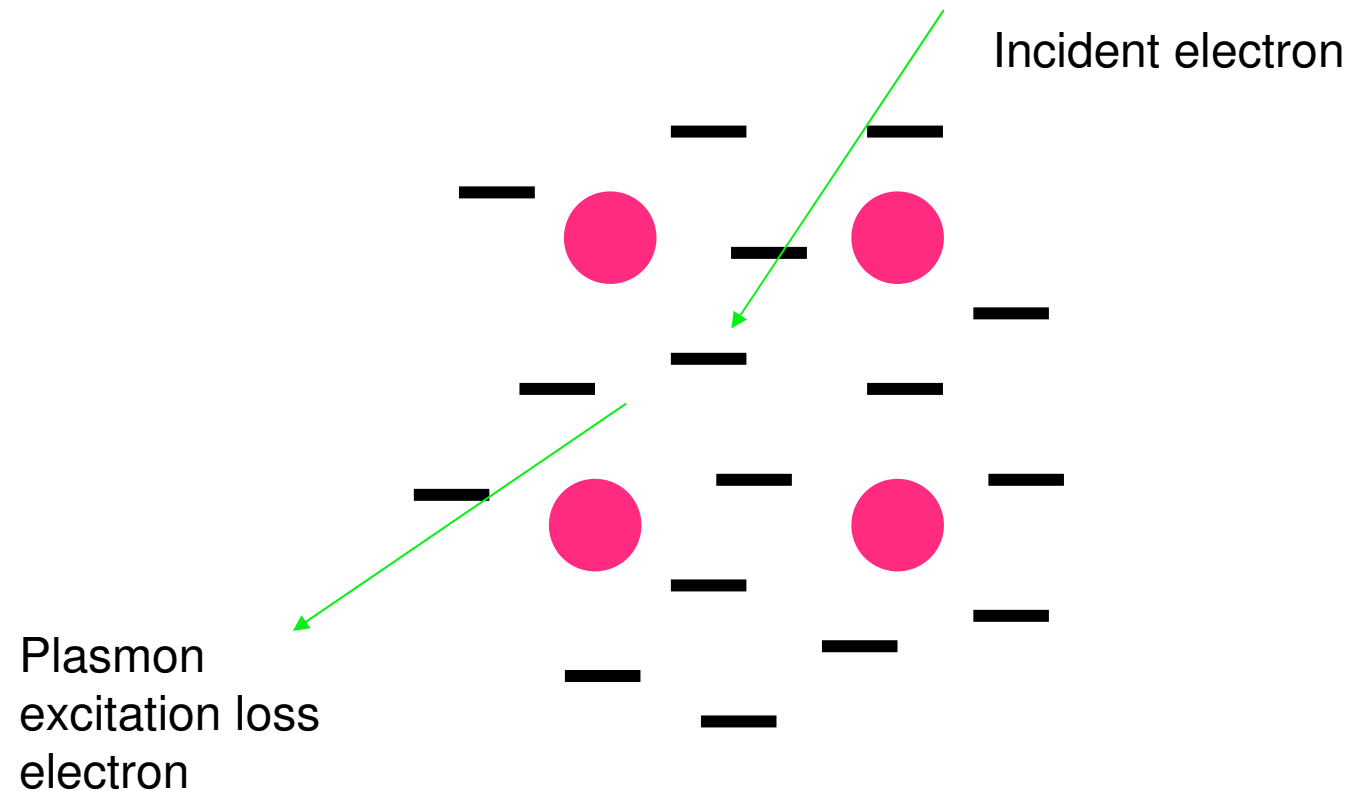
- Phonon excitation
- Plasmon excitation
- Single electron excitation
- Direct radiation losses



Phonon excitations



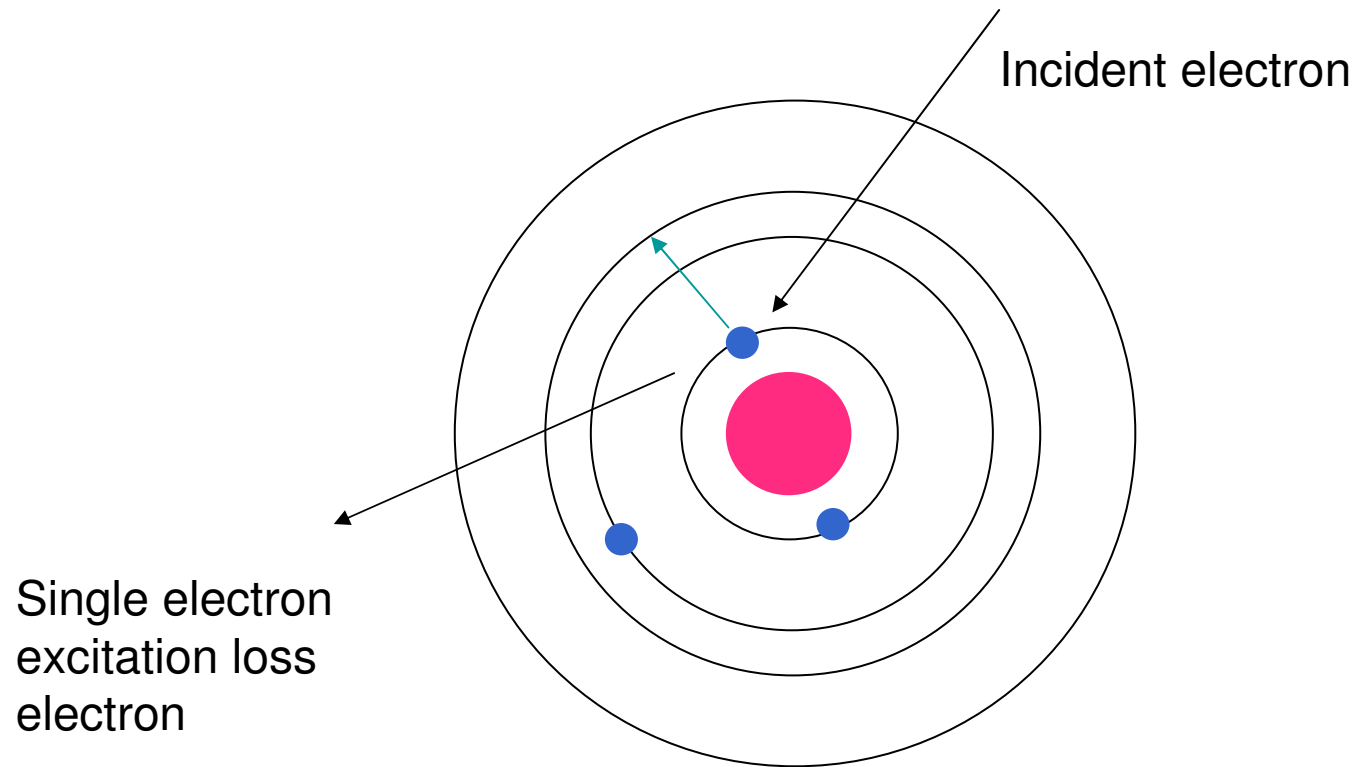
Plasmon excitations



~5-30 eV loss



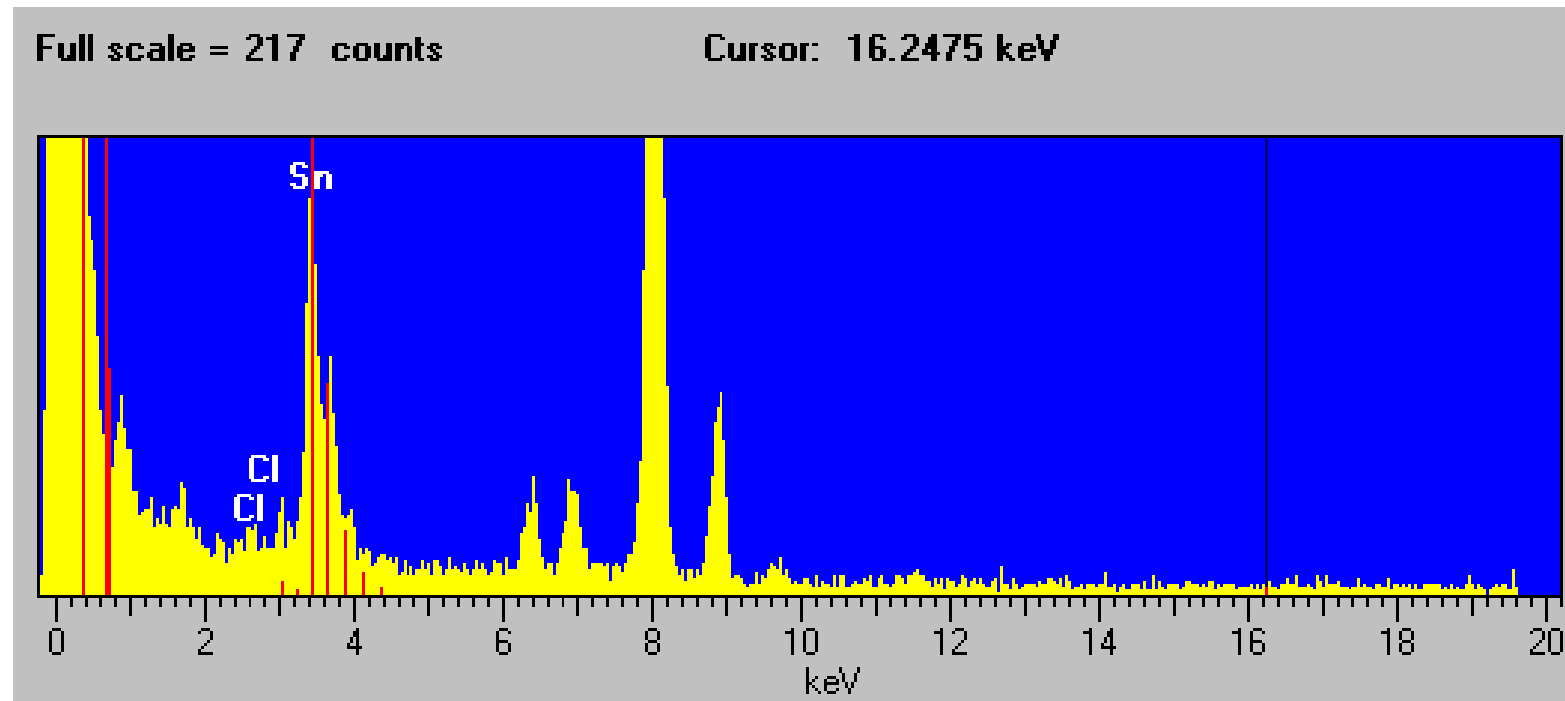
Single electron excitations



~50 - >2000 eV loss



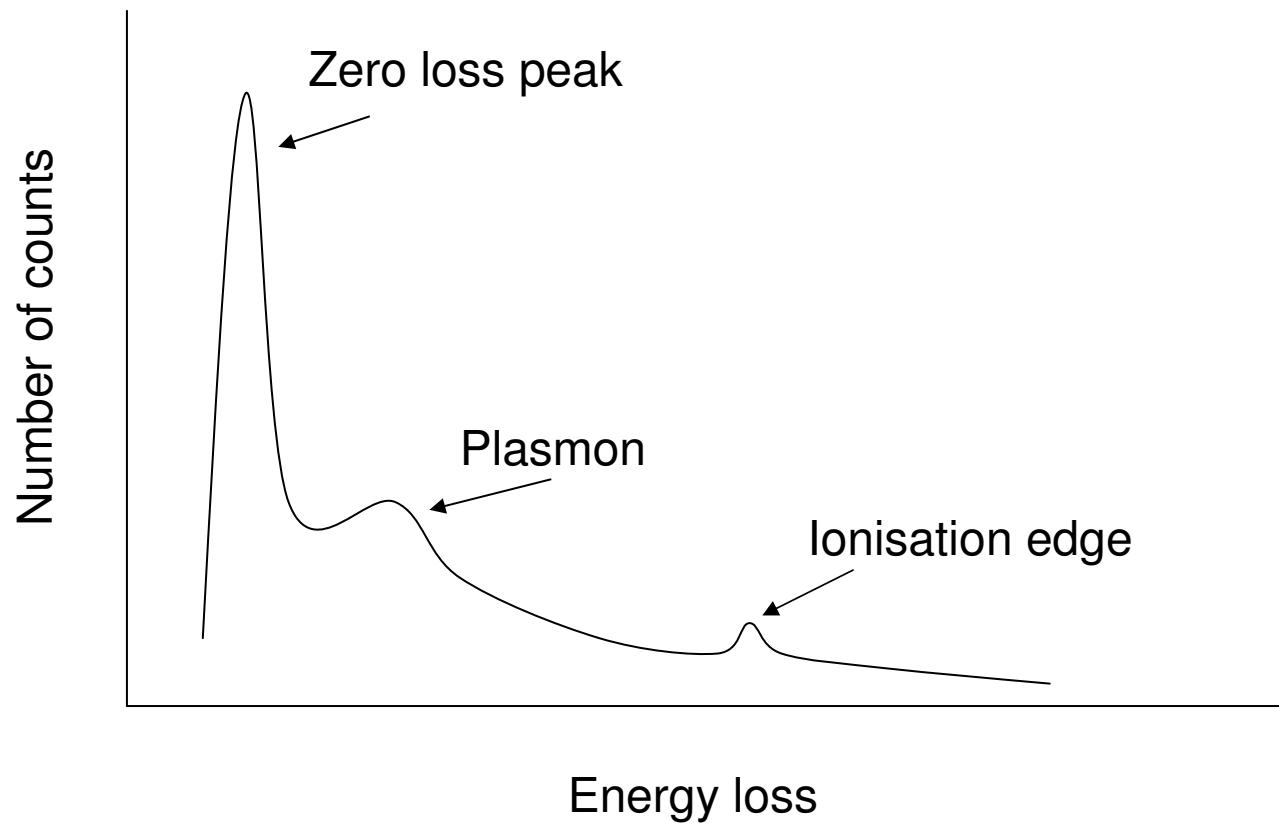
Direct radiation losses



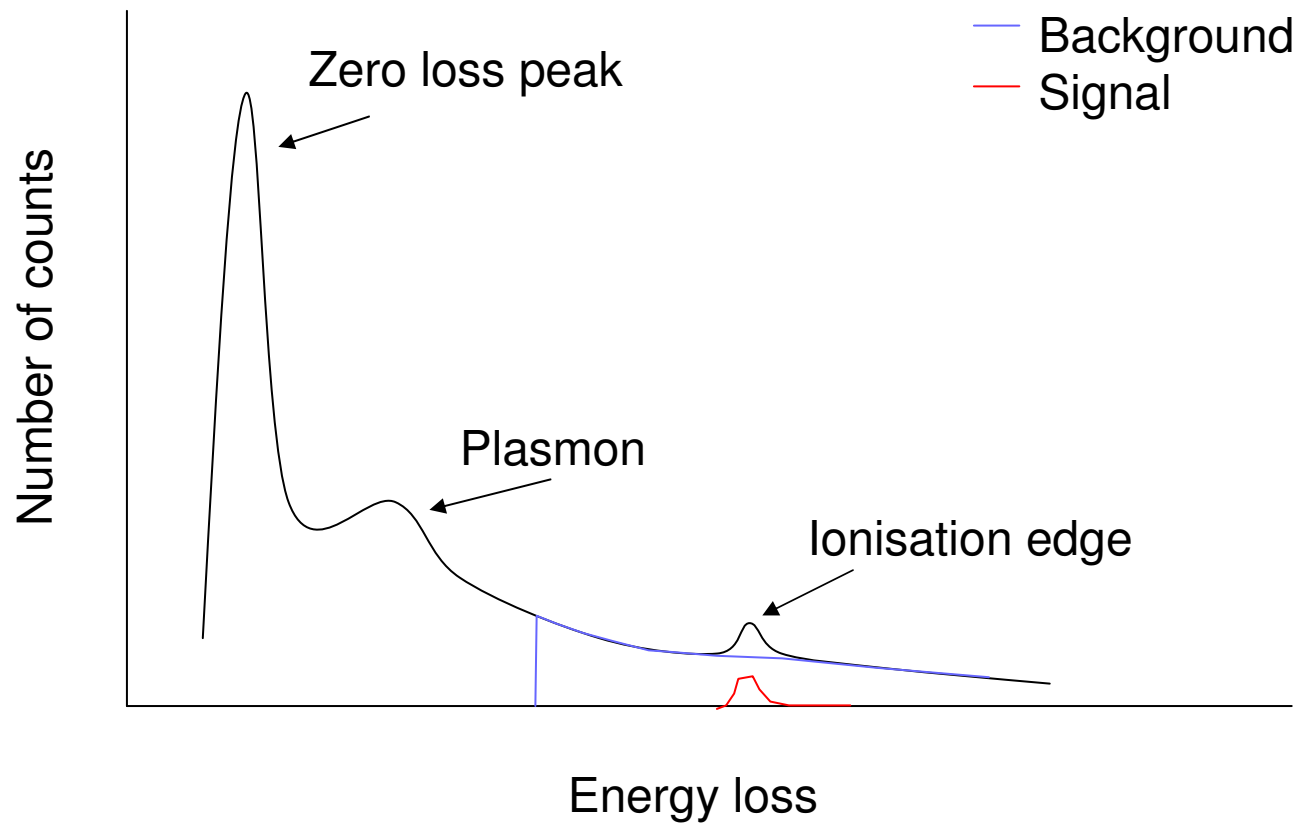
**Electron slows down, energy release
produces X-rays (Bremsstrahlung)**



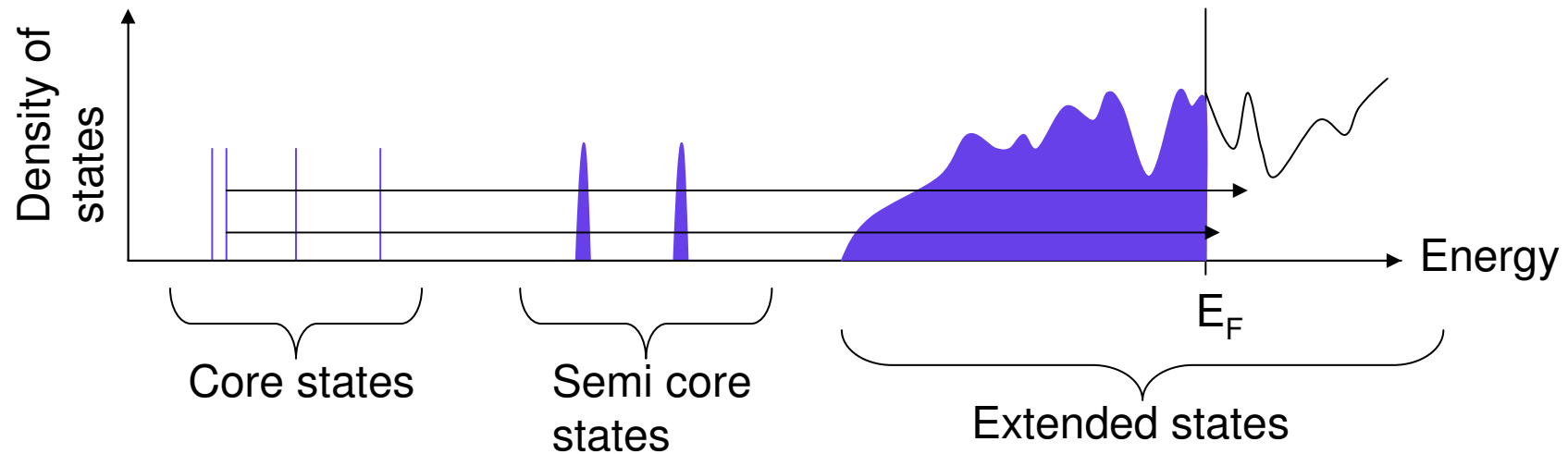
Electron energy loss spectrum



Background removal



Ionization edge



$$I(E) \propto N(E)$$



XAS

Diamond light source (<http://www.diamond.ac.uk/Home.html>)



XANES and ELNES

- XANES

High energy resolution, ~50nm spatial resolution, need a relatively large amount of sample, collect smaller energy range, less damage

- ELNES

Good spatial resolution, monochromators give good energy resolution, small amount of sample, collect large energy range



What you can measure

- EELS (TEM)

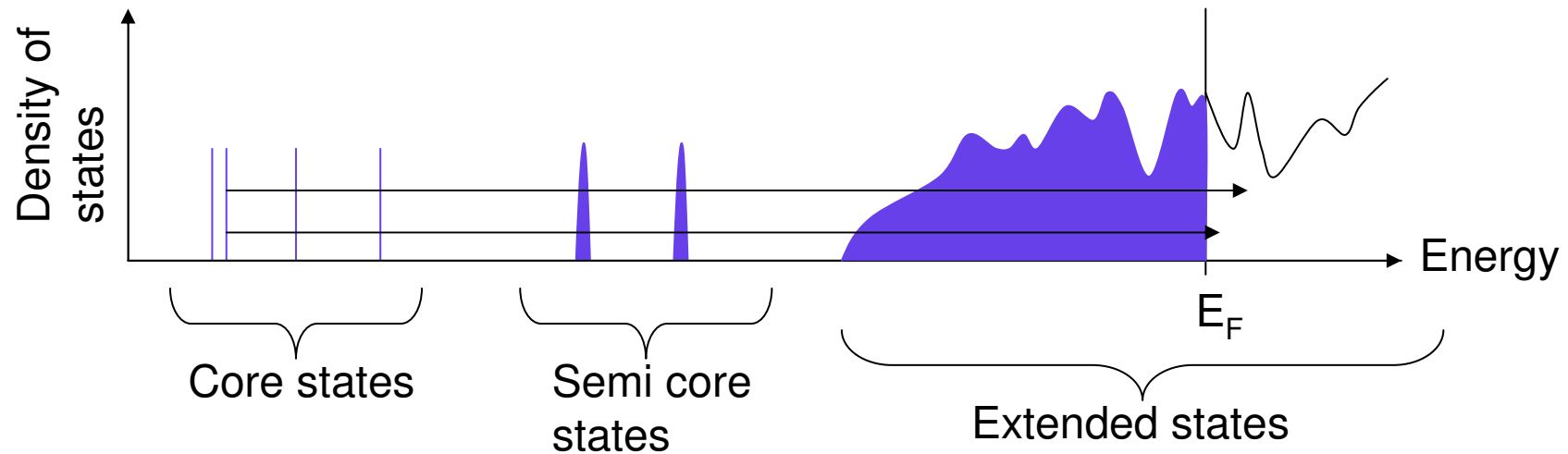
Imaging, diffraction, thickness maps, EDX, STEM, EFTEM, in situ experiments, spectrum imaging, energy range 0 – 3000eV

- XAS

Diffraction, in situ experiments (temperature and pressure), tuneable energy range



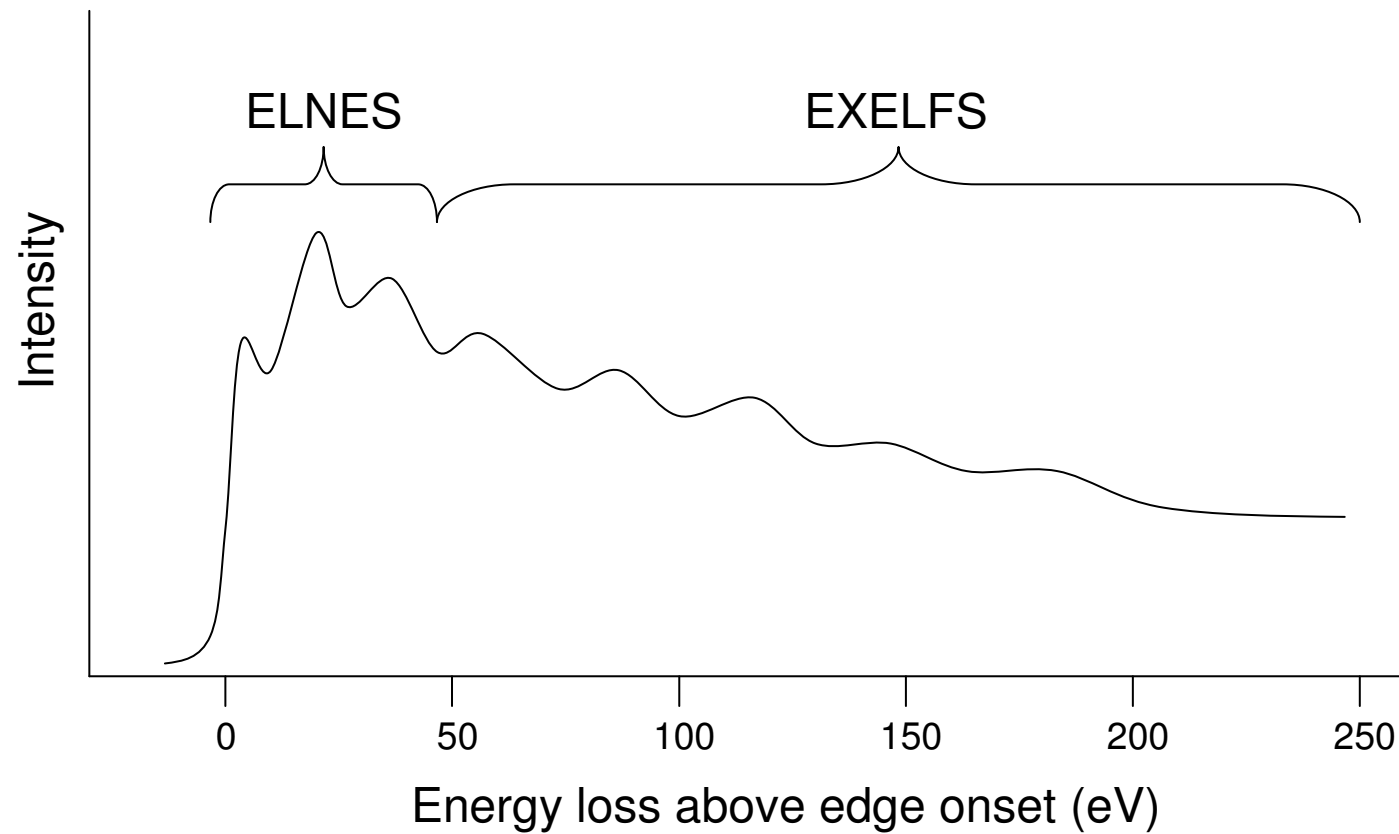
Ionization edge



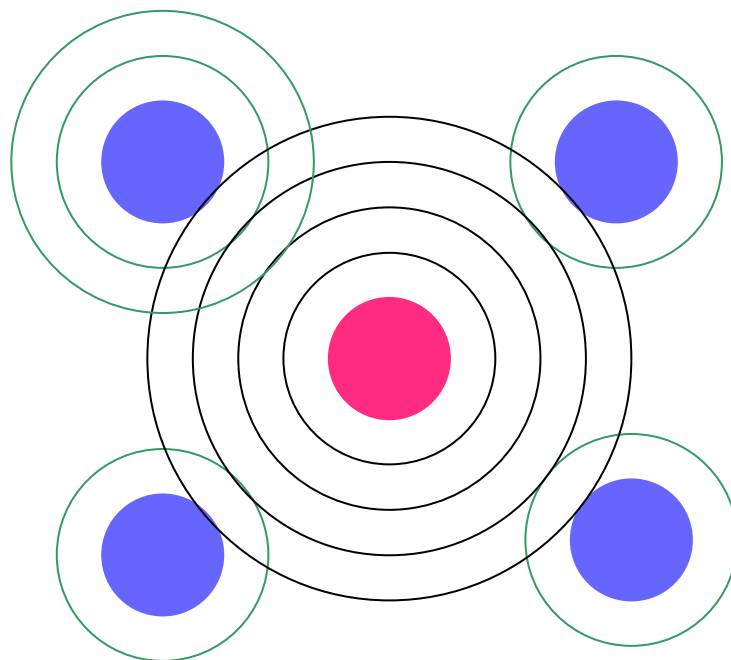
$$I(E) \propto N(E)$$



ELNES and EXELFS



Chemical information from ionization edge



As the energy of the ejected electron increases, it's lifetime decreases



Chemical information from ionization edge

- ELNES – bonding environment
valence state
- EXELFS – nearest neighbour distances



Edge notation

Core electron	Edge
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$1s^{1/2}$	K
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$2s^{1/2}$	L_1
------------	-------

$2p^{1/2}$	L_2
------------	-------

$2p^{3/2}$	L_3
------------	-------

$3s^{1/2}$	M_1
------------	-------

$3p^{1/2}$	M_2
------------	-------

$3p^{3/2}$	M_3
------------	-------

$3d^{3/2}$	M_4
------------	-------

$3d^{5/2}$	M_5
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Angular momentum state

$2p^{1/2}$

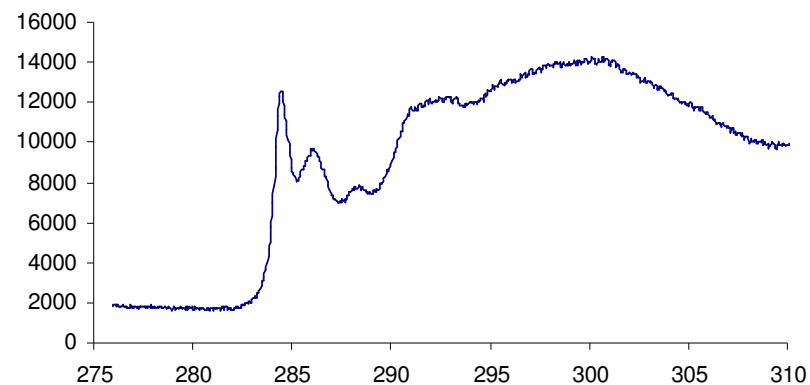
Principle quantum
number

j quantum number
(combination of
spin and angular
momentum)

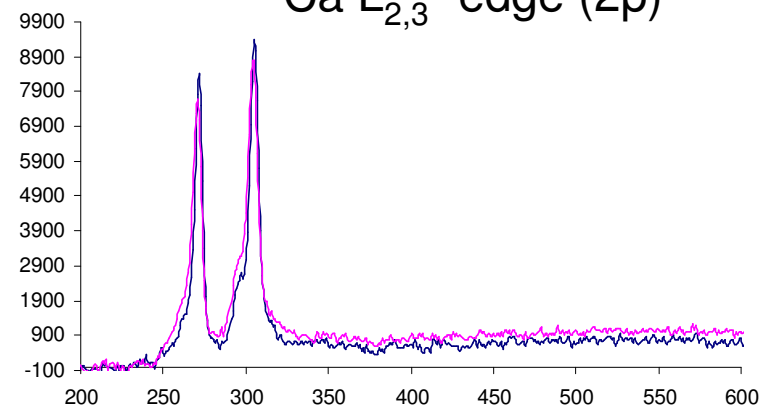


Examples of edge shapes

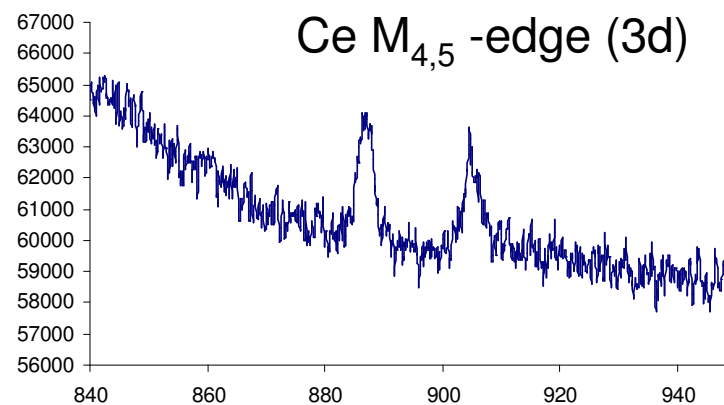
C K-edge (1s)



Ca L_{2,3}-edge (2p)



Ce M_{4,5}-edge (3d)



Periodic table

1 H																	2 He						
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne						
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar						
19 K	20 Ca	21 Sc		22 Ti												29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y		40 Zr												47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	71 Lu		72 Hf												79 Au	80 Hg	81 Ti	82 Pb	83 Bi	84 Po	85 At	86 Rn

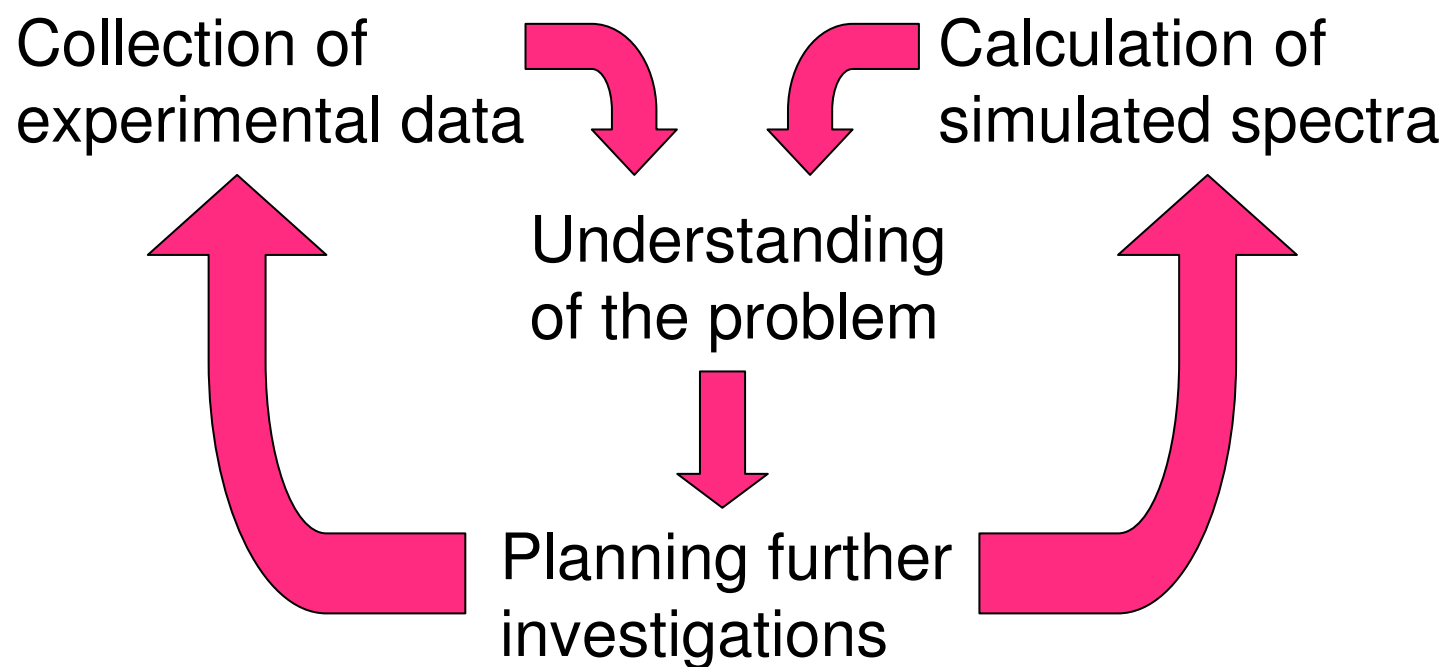


Information you can get

- Bonding environment
- Valence state
- Nearest neighbour distances
- Combine with other techniques / experiments
- Low-loss data



Combining experiment and modelling



Recommended books and useful websites

R Egerton – *Electron Energy Loss in the Electron Microscope* Plenum

R Brydson – *Electron Energy Loss Spectroscopy* RMS Microscopy Handbook

EELS database - <http://www.cemes.fr/eelsdb/>

Diamond light source - <http://www.diamond.ac.uk/Home.html>



Acknowledgements

- David Cockayne, Duc Nguyen-Manh, David Pankhurst, Seung Mi Lee
- Gianluigi Botton, Sorin Lazar
- Jonathan Yates, Chris Pickard, Shang-Peng Gao
- David McComb, David Eustace, James Perkins
- Kevin Jorissen
- Andrew Scott

