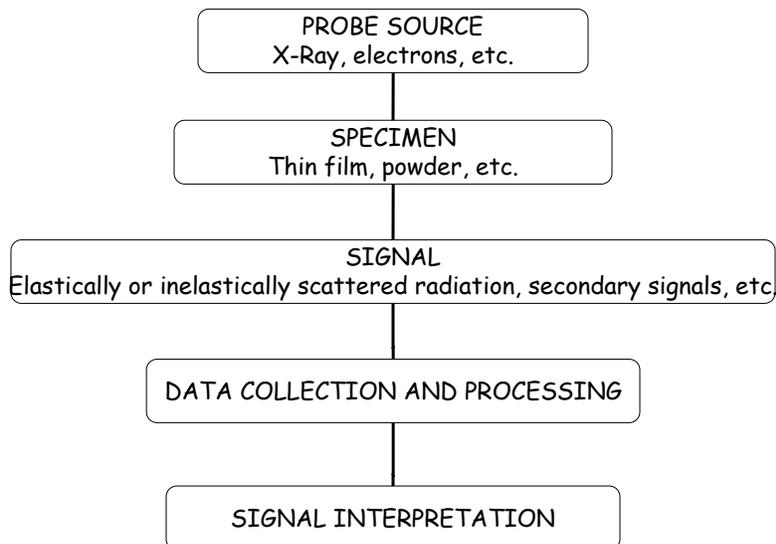


# Interaction Radiation - Matter

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## Characterization of (Nano)Materials



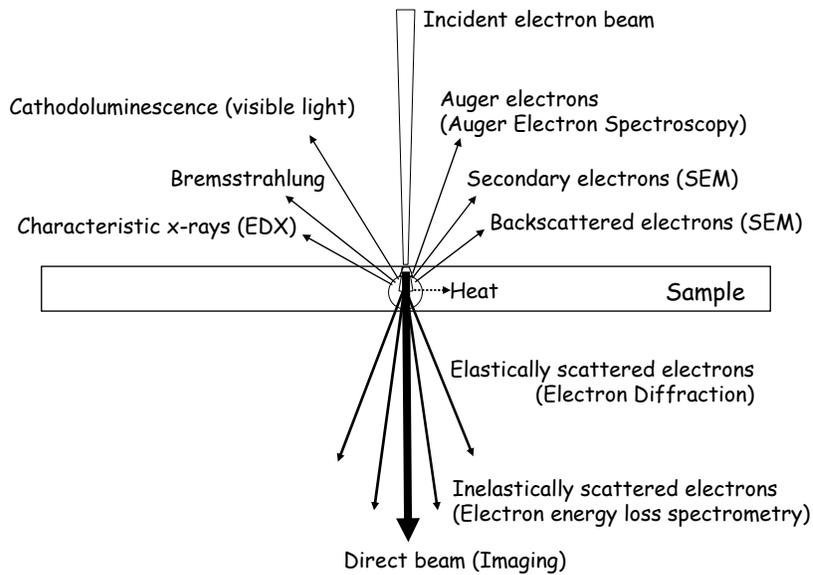
## Interaction Radiation-Matter

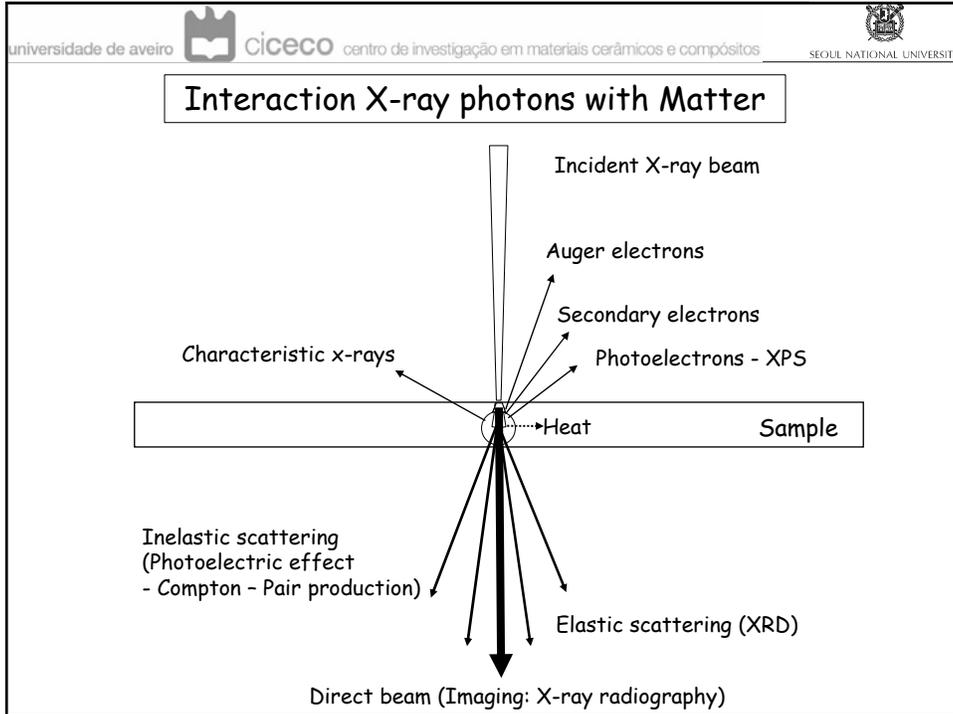
As the characterization of a nanostructure is achieved by allowing some form of probe to interact with a particular specimen. At first we should (re)learn what are the different interactions between the incident radiation (probe) with a solid (specimen).

Electrons and X-rays are two types of "ionizing radiation", which is the general term given to a radiation that is capable of removing one of the tightly bound inner-shell electrons from the attractive field of the nucleus.

One of the properties of ionizing radiation is that it gives rise to a wide range of secondary signals from the specimen. Many of these signals are used in "analytical electron microscopy" and various spectroscopies.

## Interaction of high energy electrons with Matter





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### Some Examples

#### X-ray photoelectron spectroscopy (XPS)

Upon interaction of the incident X-ray radiation with the specimen an ionization event takes place.  
i.e. an electron is emitted (photoelectric effect).

The energy of the emitted electrons (photoelectrons) is equal to the difference between incident X-ray energy, the binding energy of the level concerned and the work function.

Therefore, it is characteristic of the atom, its chemical state and environment.

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## Some Examples

Energy dispersive X-ray spectroscopy (EDX or EDS)

Interaction between incident electrons (e.g. in an electron microscope), but also X-ray and protons, and a specimen.

As in the case of XPS the incident radiation is used to promote ionization.

The relaxation process can lead to the emission of a photon of a given energy, which is characteristic of the atom.

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## Fundamental Properties of Electrons

You know that electrons show both particle and wave characteristics

$$\lambda = h/p$$

The equation relating the particle momentum  $p$  to its wavelength  $\lambda$  through the Planck's constant  $h$  based on de Broglie's hypothesis of the wave-particle duality.

The kinetic energy of the electron can be written as (non relativistic):

$$eV = \frac{m_0 v^2}{2}$$

$eV$  is the kinetic energy (acceleration voltage in the electron microscope),  $m_0$  is the mass of the electron and  $v$  is the velocity.

The momentum  $p = m_0 v$  can be written as:

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$$p = m_0 v = (2m_0 eV)^{1/2}$$

Finally we can write the relation between the electron wavelength and the kinetic energy of the electron.

$$\lambda = \frac{h}{(2m_0 eV)^{1/2}}$$

-> by increasing the kinetic energy the wavelength of the electrons decreases.

Exercise: Calculate the nonrelativistic electron wavelength and the speed for typical commercial TEM operating at 100, 200 and 300 keV.

**Table 1.1. Fundamental Constants and Definitions**

Charge ( $e$ )	(-) $1.602 \times 10^{-19}$ C
1 eV	$1.602 \times 10^{-19}$ J
Rest mass ( $m_0$ )	$9.109 \times 10^{-31}$ kg
Rest energy ( $m_0 c^2$ )	511 keV
Kinetic energy (charge $\times$ voltage)	$1.602 \times 10^{-19}$ N m (for 1 volt potential)
Planck's constant ( $h$ )	$6.626 \times 10^{-34}$ N m s
1 ampere	1 C/sec
Speed of light in vacuum ( $c$ )	$2.998 \times 10^8$ m/sec

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The classical treatment neglects relativistic effects. However, they cannot be ignored at the energies used in electron microscopy. Indeed, the velocity of the electrons becomes greater than half the speed of light.

$$\lambda = \frac{h}{\left[2m_0 eV \left(1 + \frac{eV}{2m_0 c^2}\right)\right]^{1/2}}$$

Comparison of the electron properties as a function of the kinetic energy

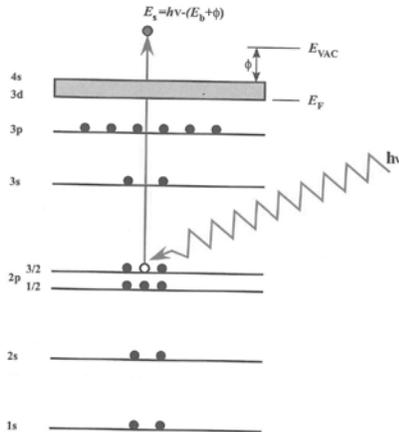
**Table 1.2. Electron Properties as a Function of Accelerating Voltage**

Accelerating voltage (kV)	Nonrelativistic wavelength (nm)	Relativistic wavelength (nm)	Mass ( $\times m_0$ )	Velocity ( $\times 10^8$ m/s)
100	0.00386	0.00370	1.196	1.644
120	0.00352	0.00335	1.235	1.759
200	0.00273	0.00251	1.391	2.086
300	0.00223	0.00197	1.587	2.330
400	0.00193	0.00164	1.783	2.484
1000	0.00122	0.00087	2.957	2.823

These numbers are important to keep in mind, especially when we consider the resolution of the electron microscope and when we need to make calculations about the interaction of the electrons with matter

## Photoelectric Effect

The energy carried by an incoming X-ray photon is absorbed by the target atom raising it to an excited state from which it relaxes by emission of a photoelectron with kinetic energy equal to the difference between the incident X-ray energy, the binding energy of the level concerned and the work function.



$\Phi$ : workfunction of the material

$E_s$ : kinetic energy

$E_b$ : binding energy

$h\nu$ : incident photon energy

A 2p photoelectron is emitted from copper as the result of the excitation by absorption of an X-ray photon

Electron are emitted from all energy levels of the target atom and, hence the electron spectrum is characteristic of the emitting atom type.

This property is used in X-ray photoelectron spectroscopy (XPS)

Photoelectron spectroscopy is a "low energy process". XPS generally uses  $Al_{K\alpha}$  and  $Mg_{K\alpha}$  X-ray sources (~1000 eV)

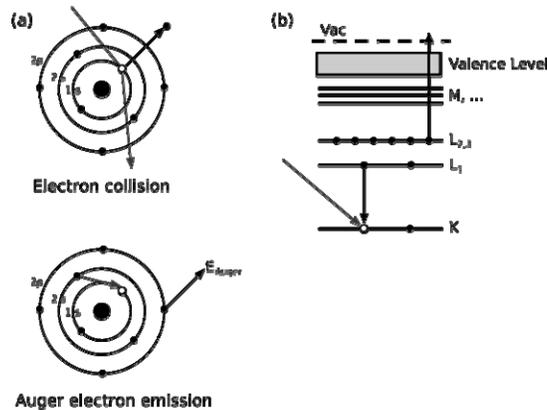
At higher energy additional processes can take place such as Compton scattering and pair production (MeV range).

## Auger Effect

The Auger effect is a phenomenon in physics in which the transition of an electron in an atom filling in an inner-shell vacancy causes the emission of another electron.

When an electron is removed from a core level of an atom, leaving a vacancy, an electron from a higher energy level may fall into the vacancy, resulting in a release of energy. Although this energy can be released in the form of an emitted photon (X-ray fluorescence), the energy can also be transferred to another electron, which is ejected from the atom. This second ejected electron is called an Auger electron.

Upon ejection the kinetic energy of the Auger electron corresponds to the difference between the energy of the initial electronic transition and the ionization energy for the electron shell from which the Auger electron was ejected. These energy levels depend on the type of atom and the chemical environment in which the atom was located. Auger electron spectroscopy involves the emission of Auger electrons by bombarding a sample with either X-rays or energetic electrons and measures the intensity of Auger electrons as a function of the Auger electron energy. The resulting spectra can be used to determine the identity of the emitting atoms and some information about their environment.



Two views of the Auger process. (a) illustrates sequentially the steps involved in Auger deexcitation. An incident electron creates a core hole in the 1s level. An electron from the 2s level fills in the 1s hole and the transition energy is imparted to a 2p electron which is emitted. The final atomic state thus has two holes, one in the 2s orbital and the other in the 2p orbital. (b) illustrates the same process using spectroscopic notation,  $KL_1L_{2,3}$ .

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## Spectroscopic and X-Ray Notations

Different ways to specify atomic ionization states as well as atomic and molecular orbitals

Spectroscopist's notation: the atomic orbitals are labeled according to the scheme  $n\ell_j$

$n$  is the principal quantum number (integers 1,2,3)

$\ell$  is the quantum number describing the orbital angular momentum of the electron (integers 0,1,2,3) but usually denoted by a letter (s,p,d,f,...)

Because of the interaction between the electron angular momentum due to its spin with its orbital angular momentum (spin orbit coupling), orbitals whose angular momentum quantum number are greater than 0 are usually split into two.

Each electron has a quantum number associated with its spin angular momentum,  $s$ . ( $s$  can be  $+1/2$  or  $-1/2$ ).  $j$  is the quantum number taking the value  $j=|l+s|$ .  
Ex: an electron from a  $p$  orbital can have a  $j$  value of  $1/2$  and  $3/2$

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## Spectroscopic and X-Ray Notations

X-ray notation: the principal quantum numbers are given letters  $K, L, M, N$ , etc.

The subscript number refer to the  $\ell$  and  $j$  values.

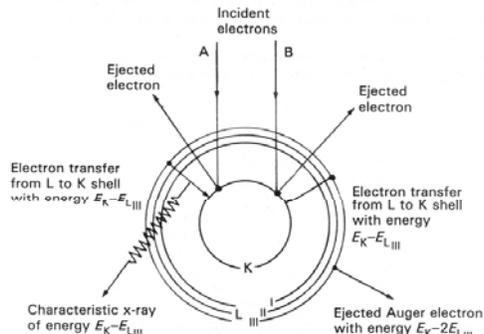
Quantum Numbers			X-ray	Spectroscopic
$n$	$\ell$	$j$		
1	0	1/2	K	1s <sub>1/2</sub>
2	0	1/2	L <sub>1</sub>	2s <sub>1/2</sub>
2	1	1/2	L <sub>2</sub>	2p <sub>1/2</sub>
2	1	3/2	L <sub>3</sub>	2p <sub>3/2</sub>
3	0	1/2	M <sub>1</sub>	3s <sub>1/2</sub>
3	1	1/2	M <sub>2</sub>	3p <sub>1/2</sub>
3	1	3/2	M <sub>3</sub>	3p <sub>3/2</sub>
3	2	3/2	M <sub>4</sub>	3d <sub>3/2</sub>
3	2	5/2	M <sub>5</sub>	3d <sub>5/2</sub>

Notations for 4f orbitals ?

## Emission of characteristic X-ray

The emission of X-ray is a competitive relaxation phenomena to the Auger effect.

Upon ionization of an atom the relaxation process can produce an Auger electron or X-ray emission. The two relaxation processes are in competition



The characteristic X-rays are used in energy dispersive spectroscopy

Fig. 2.3. Schematic diagram showing emission of characteristic x-ray by electron A and emission of Auger electron by electron B.

## Emission of X-ray: Transitions notations

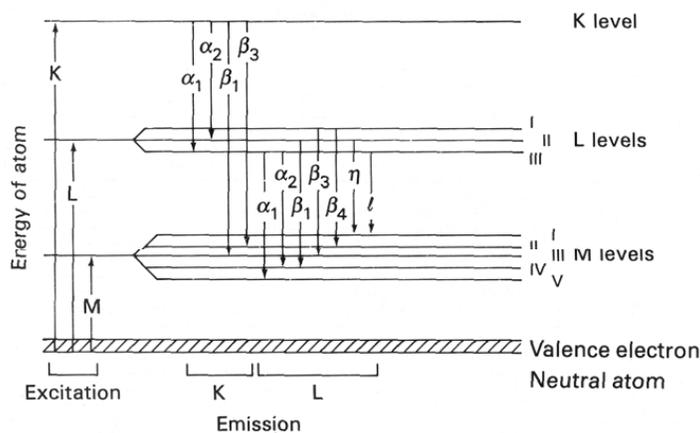
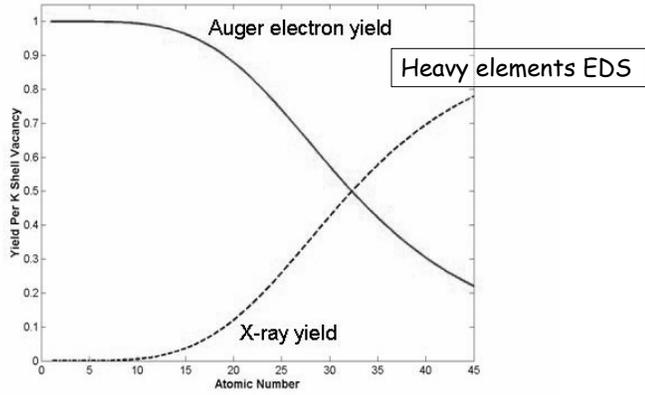


Fig. 2.2. Schematic diagram showing common x-ray emission lines with their designation for an element with atomic number ( $Z$ ), where  $29 < Z < 37$ .

These transitions obey to the electric dipolar selection rules ( $\Delta l \neq 0, \Delta j = 0, \pm 1$ )

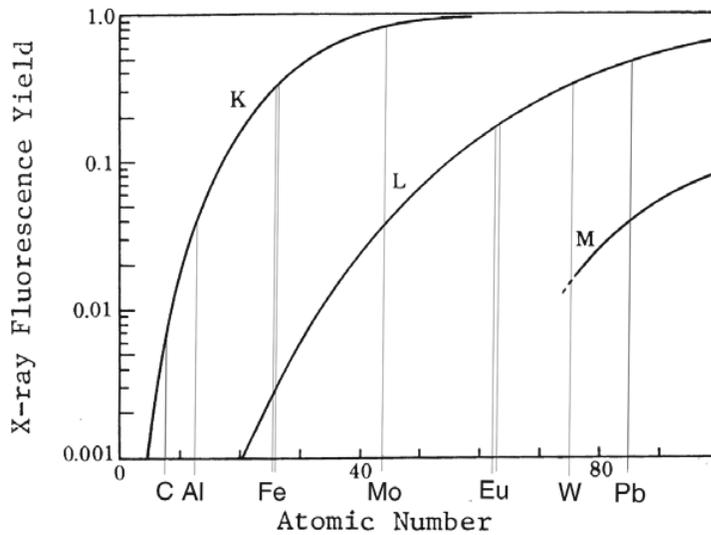
Relative efficiency of X-ray and Auger emission vs. atomic number for K lines

Light elements Auger Spectroscopy



Light element atoms return to fundamental state mainly by Auger emission. For that reason, their K-lines are weak. In addition their low energy makes them easily absorbed.

X-ray fluorescence yield for K, L and M shells



X-ray fluorescence yield for K-, L-, and M-shells, as a function of atomic number.

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### Bremsstrahlung (braking radiation)

If the incident electrons penetrate completely through the electron shells they can interact inelastically with the nucleus.

If the electron is decelerated by the Coulomb (charge) field of the nucleus, it emits an X-ray.

Since the electron can suffer any amount of deceleration depending on the strength of its interaction, then these X-rays can have any energy up to the incident electron energy.

The bremsstrahlung radiation participate to the background signal in EDS

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### Backscattered Electrons (BSE)

A fraction of the incident electron beam can be backscattered (reflected) out of the specimen by elastic (or nearly elastic) scattering interactions.

If the incident electron penetrates the electron cloud and approaches the nucleus, it will be strongly attracted and may be scattered through a large angle.

The fraction of the incident beam backscattered depends rather sensitively on the atomic number of the atoms constituting the specimen. Heavy atoms backscatter electrons more strongly than light elements.

These electrons are useful in scanning electron microscopy in order to obtain atomic contrast within a specimen. BSE electrons are used to differentiate regions with different chemical composition.

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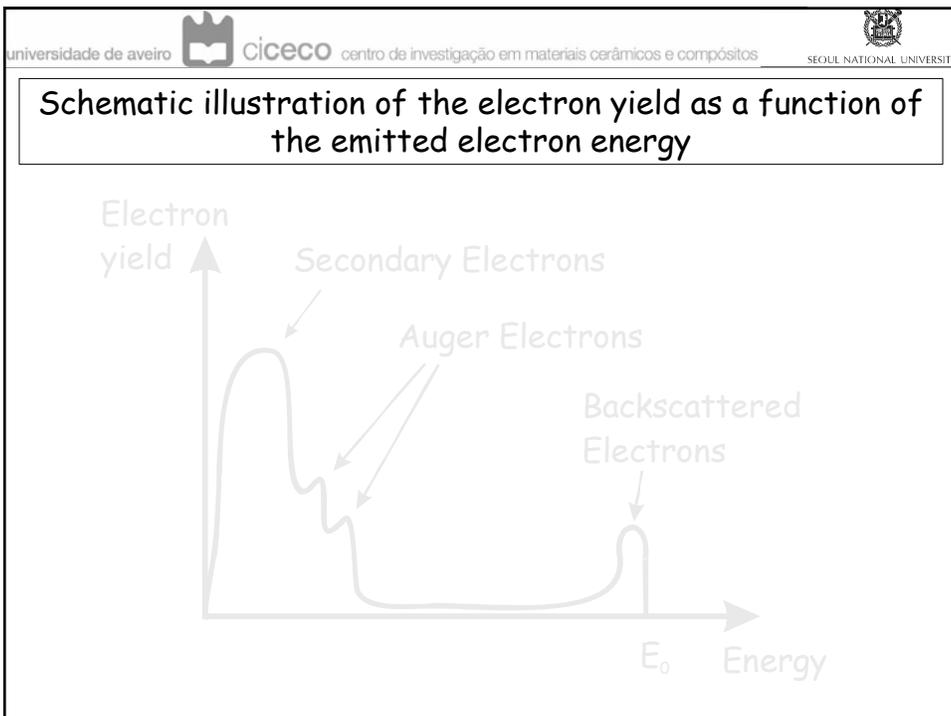
## Secondary Electrons

Is a general term defining electrons generated by ionization events caused by the incident radiation.

They are called secondary because they are generated by the incident radiation (the "primary" radiation e.g. electrons in electron microscopy).

The secondary electrons can be conveniently "divided" in 3 distinct groups

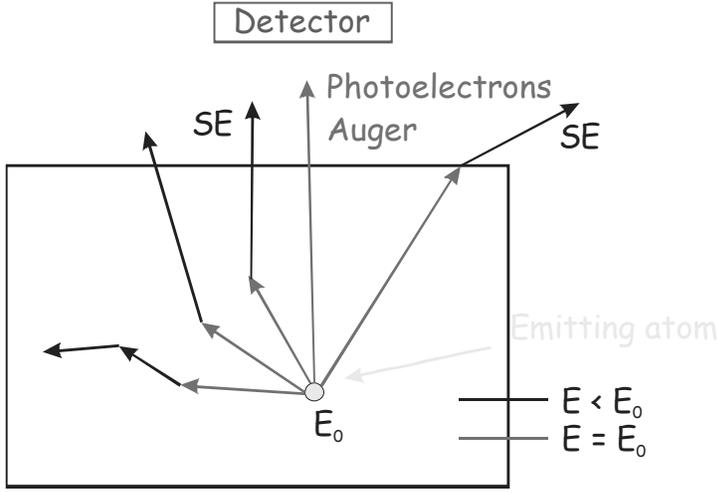
- 1) Slow secondary electrons:  
If the electrons are in the conduction or valence band then it does not take much energy to eject them. Their energy is typically below about 50 eV
- 2) Fast secondary electrons:  
If the electrons are strongly bound inner-shell electrons they are less readily ejected, but when they are thrown out of their shells they can have a significant fraction of the incident radiation energy
- 3) Auger electrons: are also secondary electrons



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### How long an electron can "travel" through the solid?

In the diagram below the different arrows represent the possible trajectories of the emitted electrons.



Detector

Photoelectrons  
Auger

SE

SE

Emitting atom

$E_0$

$E < E_0$   
 $E = E_0$

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Due to the high probability to suffer inelastic scattering only a small portion of the electrons escape from the surface.

Moreover, the number of electrons pertaining the original energy  $E_0$  is even lower.

More the electron is emitted deeper in the specimen less is the chance that it can escape.

-> These particular properties of the emitted electrons are responsible for:

- 1) The surface sensitivity of XPS and Auger spectroscopy
- 2) The high resolution achievable in SEM as the SE detected are emitted very close to the surface of the specimen

What does "very close" means? -> Inelastic mean free path (IMFP)

## How long an electron can "travel" through the solid?

Question: how to calculate the probability of an electron traveling a distance ( $x$ ) through the solid without undergoing inelastic scattering?

$\lambda$  is the inelastic mean free path IMFP: the average distance that an electron travels between scattering events.

The probability that in an element  $dx$  there will be a collision is  $dx/\lambda$  (which is independent of the position  $x$ )

The probability  $P(x)$  that no collision occurs in a path of length  $x$  can be calculated by setting up a differential equation for  $P$

The probability  $P(x+dx)$  that no collision occurs in a path of length  $(x+dx)$  is equal to the product of the probability  $P(x)$  that no collision occurs in a path of length  $x$  times the probability  $(1-dx/\lambda)$  that no collisions occurs in the additional length  $dx$ .

By using a Taylor expansion around  $x/\lambda$  one obtains:

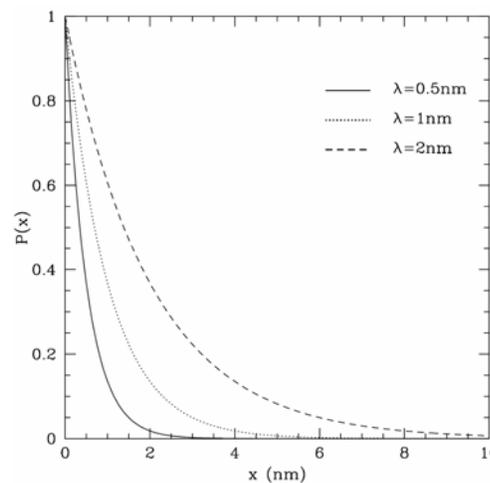
By using a Taylor expansion around  $x/\lambda$  one obtains:

$$P(x + dx) = P(x) + \frac{dP(x)}{dx}dx = P(x) \left( 1 - \frac{dx}{\lambda} \right)$$

$$\frac{dP(x)}{dx} = -\frac{1}{\lambda}P(x)$$

Integration

$$P(x) = e^{-\frac{x}{\lambda}}$$



Exercise: Calculate the probability that no collision occurs for  $x=1\lambda$ ,  $2\lambda$  and  $3\lambda$

$$P(1\lambda) = \exp(-x/\lambda) = \exp(-1) = 0.368$$

$$P(1\lambda) = \exp(-x/\lambda) = \exp(-2) = 0.135$$

$$P(1\lambda) = \exp(-x/\lambda) = \exp(-3) = 0.050$$

The large majority of the electrons that are detected (e.g. in XPS or Auger spectroscopy) come from within one "IMFP" of the surface

The IMFP depends on:

- The initial kinetic energy of the electron
- The nature of the solid

In the energy range 30-100 eV the IMFP is lower than 1 nm for metals!

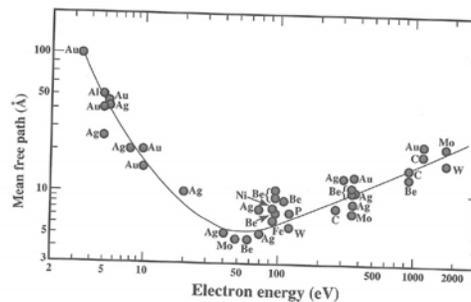


Figure 8.3 Attenuation length for electrons detected normal to the surface for a variety of different solids as a function of their energy. Note the broad minimum in the range 10–500 eV that corresponds to just a few atomic layers. (Courtesy of L.C. Feldman and J.W. Mayer, Fundamentals of Surface and Thin Film Analysis, Elsevier Science Publishing Co.).

For insulators IMFP can reach few nanometers in this energy range

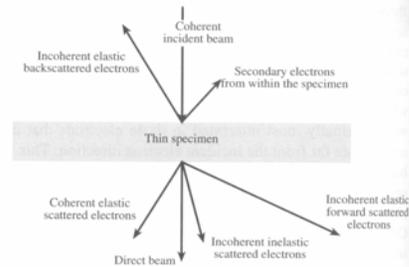
Typical values of  $\lambda$  for scattering at TEM voltages are of the order of tens of nm.

## Transmitted Radiation

Electrons that are not scattered by the specimen are used in transmission electron microscopy for imaging

-> "Mass-thickness contrast"

Since the amount of electrons that undergoes scattering increases with the thickness of the sample (number of atoms in the path of the beam) and the atomic number (density)



-> The contrast obtained depends on the specimen thickness and its density

In life science mass-thickness contrast is almost the only mode used

Elastically scattered electrons are used for electron diffraction

In the TEM for high resolution imaging, both transmitted electrons that did not undergo scattering and the elastically scattered electrons are used

-> the difference in the path length followed by the different beams will result in an interference pattern in the image plane (Phase contrast)

Electrons that are inelastically (forward) scattered in the TEM are used for chemical analysis of the specimen. Electron energy loss spectrometry (EELS)

The inelastic scattering process can promote:

- 1) The transition of an electron from an inner-shell (K,L,M) to an unoccupied energy level (i.e. above the Fermi level) or to the vacuum (ionization).
- 2) Transition of a valence electron across the energy gap (insulators and semiconductors) or excitation of a plasmon resonance (collective oscillation of free electrons)

The energy loss by the incident electrons is characteristic of the chemical properties of the specimen

In EELS we are interested in measuring the "number of electrons" that have lost a given amount of energy. -> this traduces the relative probability that a particular transition occurs

When a core electron is promoted to an unoccupied state, the density of these final states determines the relative probability of the transition

By EELS one can study the electronic structure (Density of states above the Fermi level) of a material with resolution at the nanometer scale !

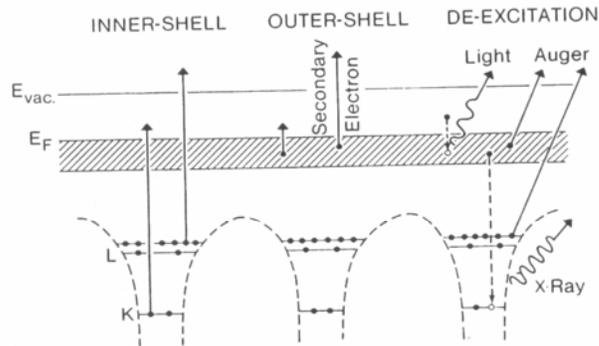


Figure 1.2. Energy-level diagram of a solid, including K- and L-shell core levels and a valence band of delocalized states (shaded);  $E_F$  is the Fermi level and  $E_{vac}$  the vacuum level. The primary processes of inner- and outer-shell excitation are shown on the left, secondary processes of photon and electron emission on the right.

## Terminology of Scattering (electrons)

We already used the most important terms: elastic and inelastic (loss of energy) scattering (in this case we tend to consider electrons as particles)

However, we can also separate scattered electrons into coherent and incoherent -> which refers to their wave nature

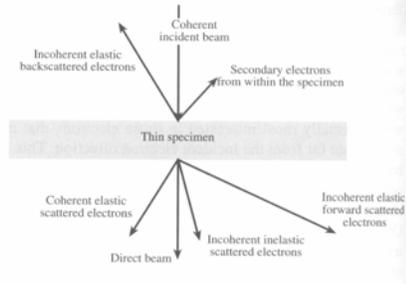
These distinctions are related, since elastically scattered electrons are usually coherent and inelastically scattered are usually incoherent

If we assume that the incident electron waves are coherent (e.g. the electrons are in phase with one another) and of a fixed wavelength. (i.e. in an electron microscope)

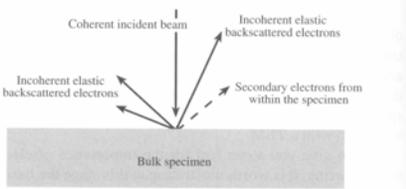
Then coherently scattered electrons are those that remain in step and incoherently scattered electrons have no phase relationship after interacting with the specimen

The nature of the scattering can result in different angular distributions.

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Thin specimen



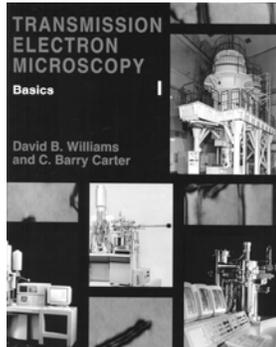
Bulk specimen

A

- Elastic scattering is usually coherent, if the specimen is thin and crystalline
- Elastic scattering usually occurs at relatively low angles ( $1-10^\circ$ ), i.e. in the forward direction
- At higher angles ( $>10^\circ$ ) elastic scattering becomes more incoherent
- Inelastic scattering is almost always incoherent and relatively low angle forward scattering
- As the specimen gets thicker, less electrons are forward scattered and more are backscattered

Figure 2.2. Different kinds of electron scattering from (A) a thin specimen and (B) a bulk specimen: a thin specimen permits electrons to be scattered in both the forward and back directions while a bulk specimen only backscatters the incident beam electrons.

TRANSMISSION ELECTRON MICROSCOPY  
Basics  
David B. Williams and C. Barry Carter



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If the specimen is very thin one can approximate all scattering within the specimen to a single scattering event

i.e. an electron either undergoes a single scattering event or it suffers no scattering

If the electron is scattered more than once we use the term plural scattering, and if it is scattered more than 20 times we say multiple scattering

Up to now we know what can happen when an electron hits a specimen

But, how to know (to quantify) what is the part of electrons that are scattered in the forward direction, elastically or inelastically, what is the scattering angle, how the thickness and the nature of the specimen influence the processes, etc.?

-> "Some" theory...

## The Interaction Cross Section

When physicists consider the theory of electron interactions with a solid, they usually consider scattering of electrons by a single, isolated atom, then progress to agglomeration of atoms first in amorphous state and then in crystalline solids

The incident radiation is scattered through an angle  $\theta$  into a solid angle  $\Omega$  measured in steradians

The characteristics of the scattering event are controlled by factors such as the electron energy and the atomic number of the scattering atom.

When we consider a specimen rather than a single atom, factors such as the thickness, the density and the crystallinity of the specimen also become important.

-> To understand these variables, we need to examine (briefly) the physics of scattering in more detail

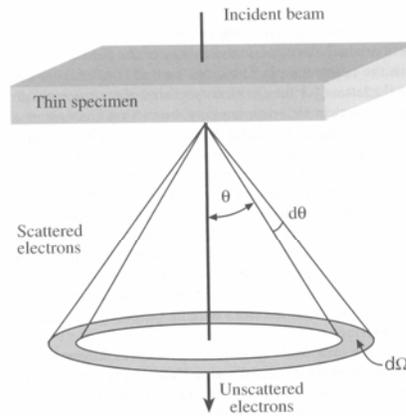


Figure 2.3. Electron scattering by a single isolated atom. The electrons are scattered through a semiangle  $\theta$  and the total solid angle of scattering is  $\Omega$ . An incremental increase in scattering angle  $d\theta$  gives an incremental increase in a solid angle  $d\Omega$ .

The chance of a particular electron undergoing any kind of interaction with an atom is determined by an interaction cross section, which is well described by the following analogy:

If I throw a ball at a glass window one square foot in area, there may be one chance in ten that the window will break and nine chances in ten that the ball will just bounce. In the physicist's language this particular window, for a ball thrown in this particular way, has a disintegration (inelastic!) cross section of 0.1 square feet and an elastic cross section of 0.9 square feet.

The cross section ( $\sigma$ ) has units of area

We can define the cross section ( $\sigma$ ) in terms of the effective radius of the scattering center,  $r$

$$\sigma = \pi r^2$$

Where  $r$  is a different value for each scattering processes

Ex elastic scattering by the nucleus:

$$r_{elastic} = \frac{Ze}{V\theta}$$

$V$  is the potential of the incoming electron,  $e$  the charge (in Statcoulomb),  $\theta$  the angle and  $Z$  the atomic number



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Because of the importance of the angle of scattering we need to introduce the concept of the differential cross section ( $d\sigma/d\Omega$ )

This term describes the angular distribution of scattering from an atom

The electrons are scattered through an angle  $\theta$  into a solid angle  $\Omega$  and there is a simple geometrical relationship between  $\theta$  and  $\Omega$

$$\Omega = 2\pi(1 - \cos\theta)$$

$$d\Omega = 2\pi \sin\theta d\theta$$

So, the differential scattering cross section can be written as:

$$\frac{d\sigma}{d\Omega} = \frac{1}{2\pi \sin\theta} \frac{d\sigma}{d\theta}$$

We can now calculate  $\sigma$  for scattering into all angles larger than  $\theta$ :

$$\sigma_{\theta} = \int_{\theta}^{\pi} d\sigma = 2\pi \int_{\theta}^{\pi} \frac{d\sigma}{d\Omega} \sin\theta d\theta$$



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This relation is important especially because it permits to determine  $\sigma$  from  $d\sigma/d\Omega$ , which is what we can (often) measure experimentally

Moreover, we can use the cross section to estimate the total scattering cross section from the whole specimen (containing  $N$  atoms/unit volume). Which will allow, for example to calculate the TEM image contrast.

$$Q_T = N\sigma_T = \frac{N_0\sigma_T\rho}{A}$$

$N_0$  is the Avogadro Number,  $A$  (g/mole) is the atomic weight of the atoms in the specimen which has density  $\rho$  (so  $N A = N_0 \rho$ )  
 -> for a sample of thickness  $t$ :

$$Q_T t = \frac{N_0\sigma_T(\rho t)}{A}$$

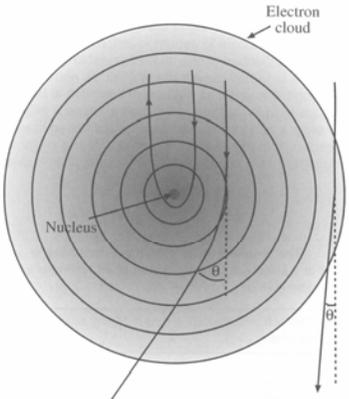
Moreover, the mean free path is directly related to the cross section

$$\lambda = \frac{1}{Q_T} = \frac{A}{N_0\sigma_T\rho}$$

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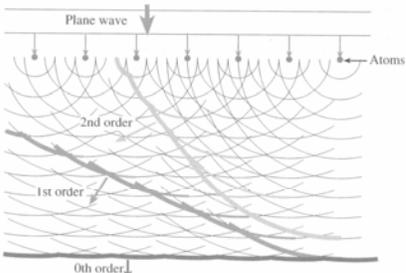
## Elastic Scattering

### Isolated Atoms



**Figure 3.1.** Two mechanisms by which a high-energy electron is scattered by an isolated atom. Coulombic interaction within the electron cloud results in low-angle ( $\theta$ ) scatter while Coulombic attraction by the nucleus causes high  $\theta$  scatter and perhaps complete backscatter. The potential within the electron cloud is always positive.

### Collective scattering from many atoms together



**Figure 3.2.** A plane coherent electron wave generates secondary wavelets from a row of scattering centers (e.g., atoms in the specimen). The secondary wavelets interfere, resulting in a strong direct (zero-order) beam and several orders of coherent beams scattered (diffracted) at specific angles.

Particle description of the electrons

Wave description of the electrons

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## Scattering from isolated atoms

The electron-electron and electron-nucleus scattering cross sections

$$\sigma_{electron} = \pi r_e^2 = \pi \left( \frac{e}{V\theta} \right)^2$$

$$\sigma_{nucleus} = \pi r_n^2 = \pi \left( \frac{Ze}{V\theta} \right)^2$$

$r_e$  and  $r_n$  are the effective radii of the scattering associated to the electron cloud and to the nucleus, respectively

At high angle the electron-nucleus interaction is analogous to the backscattering of a particles from a thin metal foil  $\rightarrow$  Rutherford experiment (1911)

$\rightarrow$  Rutherford differential cross section:

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{e^4 Z^2}{16 (E_0)^2 \sin^4 \frac{\theta}{2}}$$

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The expression assumes that the incident electron does not lose significant energy through inelastic processes ( $E_0$  is fixed)

Substitution of the known constant and integration from 0 to  $\pi \rightarrow$

$$\sigma_{nucleus} = 1.62 \times 10^{-24} \left( \frac{Z}{E_0} \right)^2 \cot^2 \frac{\theta}{2}$$

Again we see that the electron energy ( $E_0$ ), the angle of scattering ( $\theta$ ), and the atomic number ( $Z$ ) all effect the probability that an electron will be scattered by the nucleus

As before we can modify the expression in order to take into account the scattering from atoms in a TEM specimen of thickness  $t$

$$Q_{nucleus} t = \left( N_0 \frac{\rho}{A} t \right) \sigma = 1.62 \times 10^{-24} \left( N_0 \frac{\rho}{A} t \right) \left( \frac{Z}{E_0} \right)^2 \cot^2 \frac{\theta}{2}$$

The mass thickness dependence  $\rho t$  is still there. Moreover, the strong dependence on  $Z$  is now obvious

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Rutherford differential cross section neglects screening effects due to the surrounding electron cloud

$\rightarrow$  reduction of the differential cross section

The screening effect can be taken into account by modifying the Rutherford differential cross section by replacing:

$$\left[ \sin^2 \frac{\theta}{2} \right] \quad \text{by} \quad \left[ \sin^2 \frac{\theta}{2} + \left( \frac{\theta_0}{2} \right)^2 \right]$$

$\theta_0$  is the screening parameter and it is given by:

$$\theta_0 = \frac{0.117 Z^{\frac{1}{2}}}{E_0^{\frac{1}{2}}}$$

When the scattering is larger than  $\theta_0$  we can neglect electron-electron interactions and the nuclear interaction is dominant. ( $\theta_0 \sim 2^\circ$  for Cu at 100 KeV)

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We should also note that the Rutherford differential cross section is nonrelativistic. However, relativistic effects are significant for electrons with energy greater than 100 keV.

-> expression of the differential cross section using the relativistic corrected wavelength ( $\lambda_R$ ) associated to the electrons

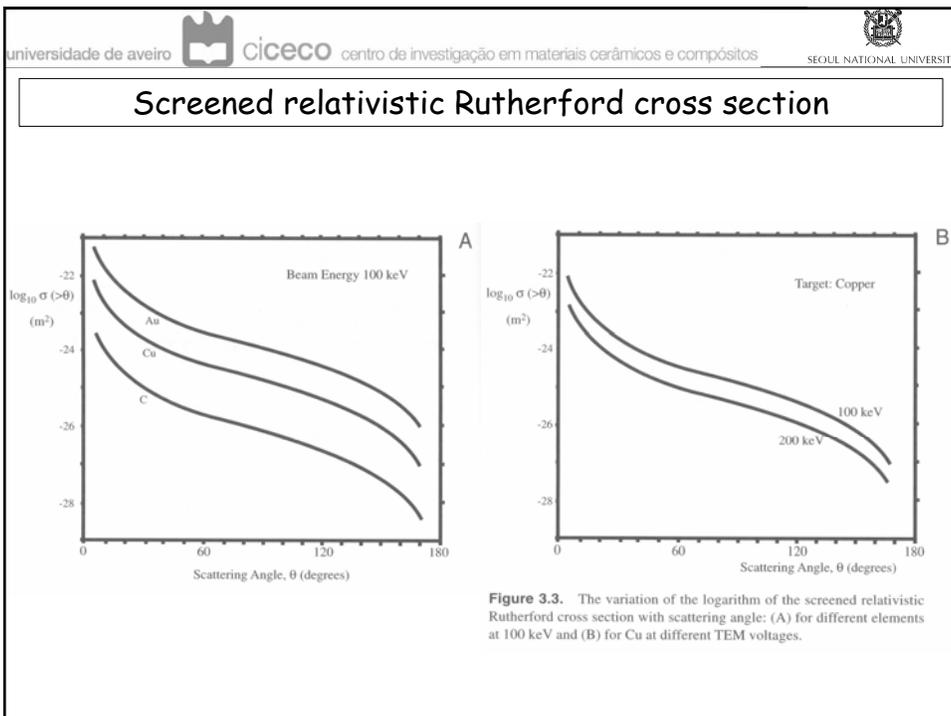
$$\frac{d\sigma(\theta)}{d\Omega} = \frac{\lambda_R^4 Z^2}{64\pi^4 (a_0) \left( \sin^2 \frac{\theta}{2} + \left( \frac{\theta}{2} \right)^2 \right)^2}$$

$\epsilon_0$  is the dielectric constant and  $a_0$  is the Bohr radius of the scattering atom  
 $a_0 = 0.0529 \text{ nm}$

$$a_0 = \frac{\hbar^2 \epsilon_0}{\pi m_0 e^2}$$

This is the screened relativistic Rutherford cross section

This is one of the most widely used cross section for TEM calculations

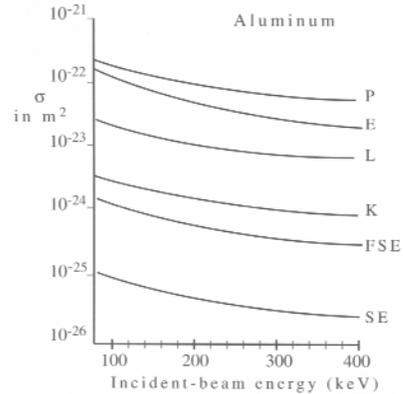


## Inelastic Scattering

We already discussed the different processes associated to inelastic scattering

What is the probability that each energy-loss process will occur?

-> Evaluation of the various cross sections



**Figure 4.1.** Cross sections for the various inelastic scattering processes in Al as a function of the incident electron energy, assuming a small angle of scatter ( $\theta = 0^\circ$ ); plasmon (P), K and L-shell ionization (K, L), fast and slow secondary electron generation (FSE, SE). For comparison purposes the elastic cross section (E) is also included. The values are relatively insensitive to the beam energy.

## Ionization cross section from electrons (Bethe theory 1930)

Total (i.e. not differential) ionization cross section

$$\sigma_{ionization} = \left( \frac{\pi e^4 b_s n_s}{E_0 E_c} \right) \log \left( \frac{c_s E_0}{E_c} \right)$$

$n_s$  is the number of electrons in the ionized subshell (2, 8, 18,...)

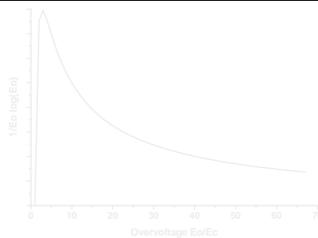
$b_s$  and  $c_s$  are constants for the shell

$E_c$  is the critical ionization energy

$E_0$  is the energy of the incident electrons

-> This cross section is not a strong function of the energy

-> Important parameter is the overvoltage  $U = E_0/E_c$



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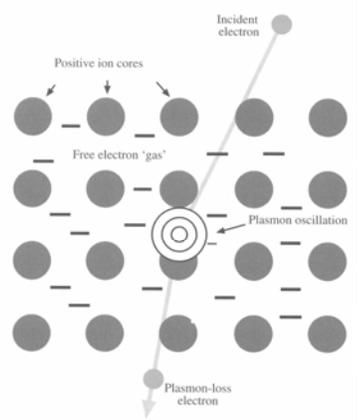
The differential form of the Bethe expression show mainly two important features:

- 1) The electron that ionized the atom is deviated only through a small angle ( $< \sim 10$  mrad)
- 2) The resultant characteristic X-ray is emitted uniformly in all the directions

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### Excitation of plasmon resonances

Plasmons are collective oscillations of free electrons that occur when the beam electron passes through the free electron "gas"



Plasmons are longitudinal oscillations which create regions of varying electron density

These oscillations are damped out in less than a femtosecond and the wave is localized to less than 10 nm

We already showed that plasmon excitation process has the largest cross section among inelastic interaction processes

Plasmons can occur in any material with weakly bound or free electrons, but they occur predominantly in metals, particularly ones like aluminium which have large Fermi surface and thus a high free-electron density

Differential cross section for plasmon excitation (Ferrel 1956)

$$\frac{d\sigma_{\theta}}{d\Omega} = \frac{1}{2\pi a_0} \left( \frac{\theta_E}{\theta^2 + \theta_E^2} \right)$$

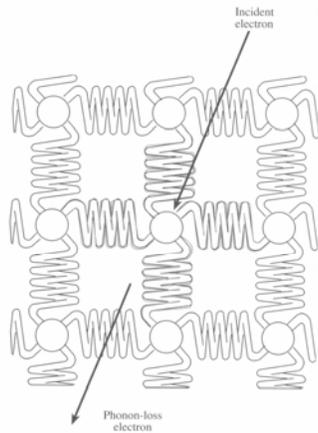
$a_0$  is the Bohr radius,  $\theta$  is the scattering angle and  $\theta_E$  is the "characteristic scattering angle" given by  $E_p/2 E_0$ ,  $E_p$  is the plasmon energy (15-25 eV)

This cross section is a strong function of  $\theta$  dropping rapidly to zero for  $\theta > 10$  mrad

Figure 4.9. Schematic diagram of a high-energy beam electron exciting a plasmon oscillation in a free electron gas that permeates the ion cores in a metal.

## Phonons

Phonons are oscillations where all the atoms in the crystal lattice vibrate collectively



**Figure 4.10.** An illustration of the crystal lattice as a group of atoms linked elastically by springs. The bonds vibrate when struck by a high-energy electron creating lattice oscillations or phonons. The lattice absorbs heat by creating phonons, so phonon excitation is equivalent to heating the specimen.

The incident electron can generate phonons in any solid sample, even in amorphous ones

Phonons can be excited also by other inelastic processes occurring with the atom (the energy of Auger or X-Ray emission or interband transitions is sometimes converted internally to lattice vibrations)

The excitation of phonons (i.e. of extra vibration of the atoms) is equivalent to heating up the specimen. In some specimens it induces damage.

Typically a phonon vibration causes a very small energy loss of < 0.1 eV but the phonon scattered electrons are scattered out to quite large angles (5-15 mrad)

These electrons accounts for the diffuse background intensity present between the Bragg spots in diffraction patterns

Phonon scattered electrons carry no useful information, nor do they carry contrast useful in electron microscopy

Phonon scattering increases with Z with a dependence on  $Z^{3/2}$