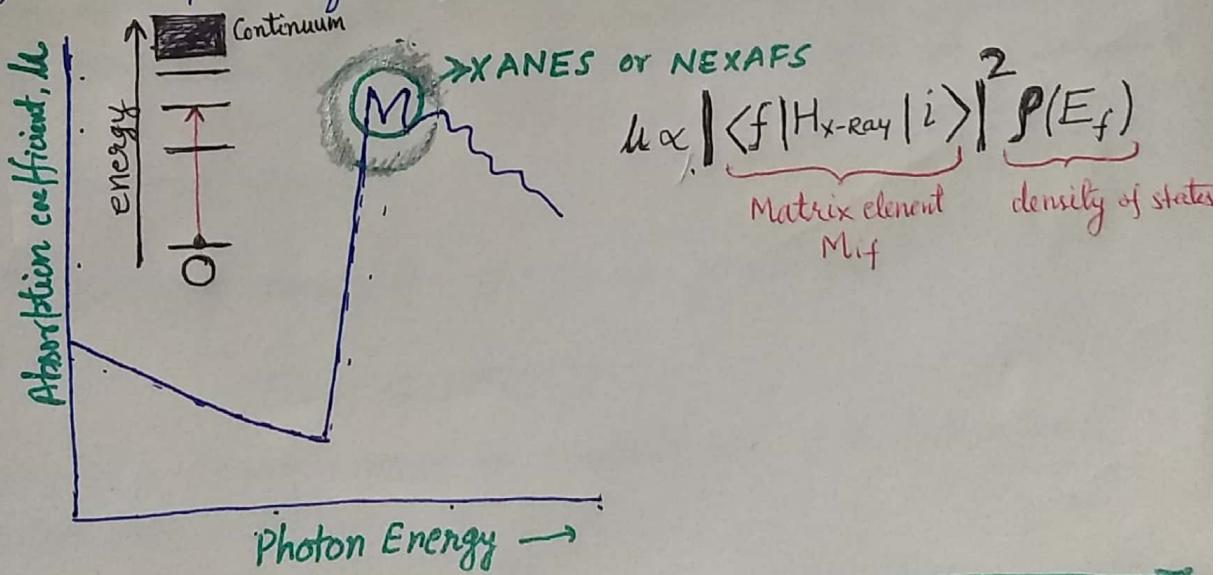


X-RAY ABSORPTION NEAR EDGE STRUCTURE (XANES) :

- * X-Rays absorption near edge refers to structure which lies close to the absorption edge.
- * Upper limit is usually set arbitrarily about 50 eV above the edge.
- * This is characterized by transition of the photo electron to unoccupied bound states.
- * XANES region is also referred to as the near edge x-rays absorption fine structure (NEXAFS).

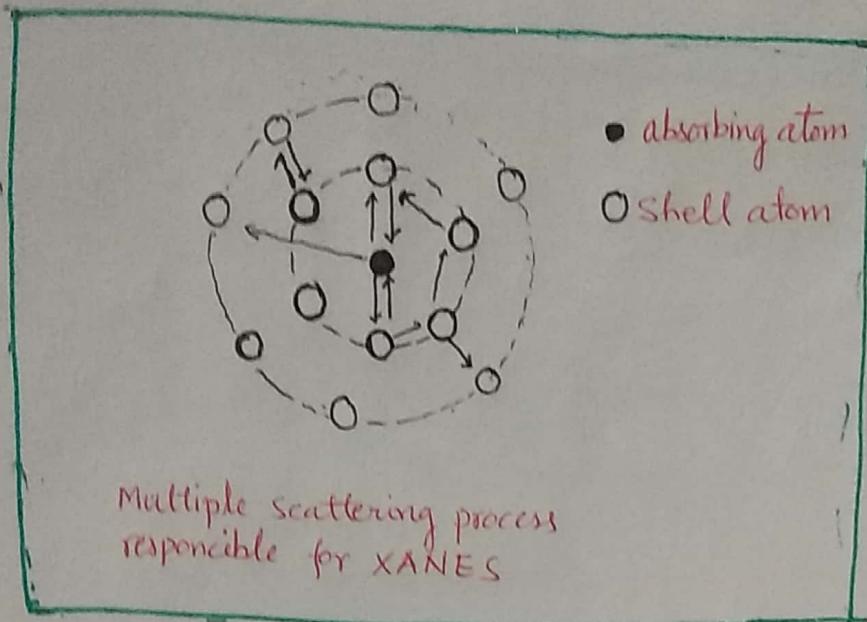


When kinetic energy of photo electron is greater than ~ 10 eV, the inelastic scattering of valence electrons contributed significantly in lowering the mean free path of the photoelectrons which falls to a few angstroms.

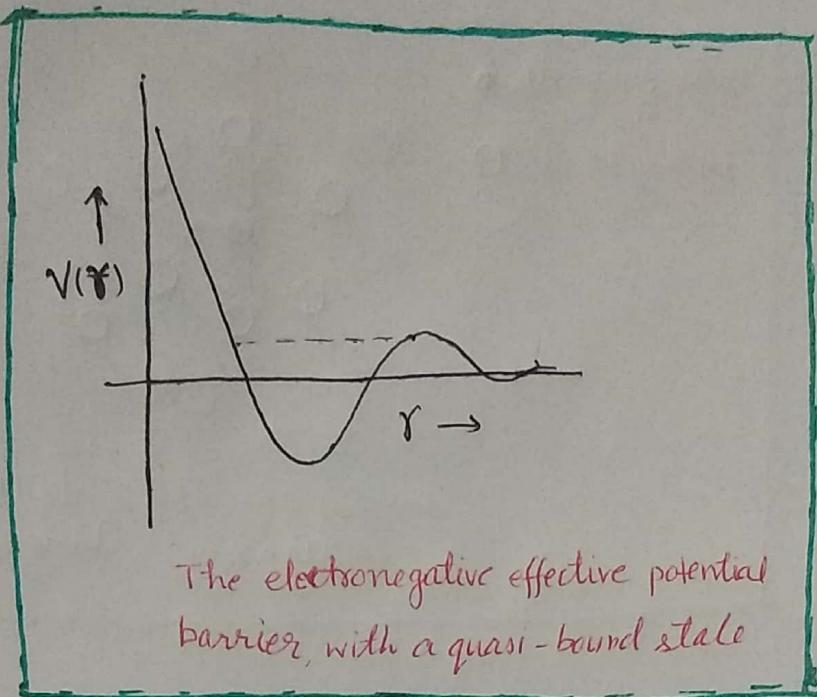
Elastic scattering is mainly due to bound electrons at greater binding energy, which generally do not participate in the chemical bonding. Hence the structure above 10 eV, due to interference effect on the photoelectron wave function, determined by the elastic scattering with neighbouring atoms, can be described by multiple scattering within a small atomic cluster.

The resulting multiple-scattering resonances of the photoelectrons in the

continuum gives rise to the XNEAS in the range $\sim 10\text{ eV}$ to 40 eV .



- * In XANES, the multiple scattering resonances in the $\sim 10\text{ eV}$ to 40 eV depend on the relative atomic positions of neighbouring atoms in several shells. Therefore it is sensitive to the ~~stereochemical co-ordination~~ (geometry of the arrangement of neighbouring atoms).
- * The energy range of XANES is given by
- $E[\text{eV}] < (151/d^2) - V \quad \dots \dots \dots \quad (\text{i})$
- where V is Fermi energy in metals and d is interatomic distance.
- * As E depends on d and V , the XANES energy range is different for the different substances
- * Nefedov and Dehm were the first to assign XANES to "inner well resonances" induced by an electronegative potential barrier on the first neighbour atoms. It forms a kind of "edge" that traps the final state wave function. A quasi-bound state is formed that decays away with a life time determined by the tunneling probability through the barrier.



- * In molecules barrier can be created by (a) a repulsive force due to the Pauli's exclusion principle; (b) a centrifugal effect.
- * The final state photoelectron wave function must be orthogonal to all occupied orbitals due to (a). One can also replace the orthogonality constraints by effective potential barriers in neighbourhood of electronegative atoms in molecules.
- * The centrifugal effect is more tangible. It provides the potential barrier of the form $\sim l(l+1)/R^2$, where R is the radius of the cluster beyond which potential is negligible. This idea is valid for diatomic molecules. For extended systems (crystal) R can not be defined.
- * Following various approaches of multiple scattering, one can reach at ~~same~~ conclusion that XANES above ~ 10 eV is mainly given by the geometry of the arrangement of neighbour atoms. Thus XANES gives information on co-ordination geometry and bonding angles not given by EXAFS.