

# ***EXTENDED X-RAY ABSORPTION FINE STRUCTURE***

***B. LENGELER***

*II. Physikalisches Institut B, RWTH, Aachen, Germany*

## ***1. INTRODUCTION***

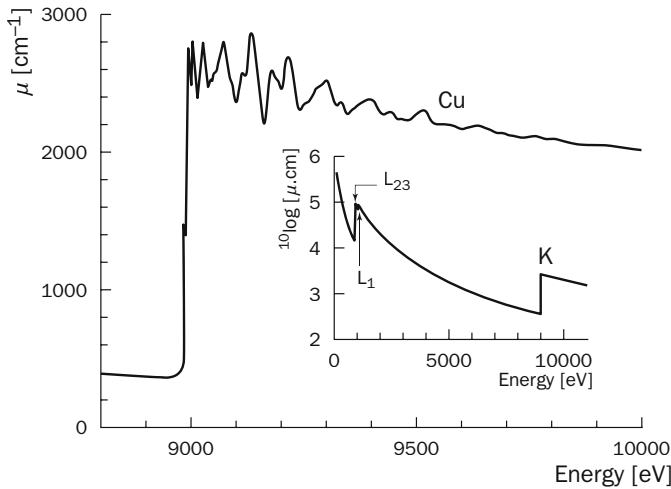
X-ray diffraction has contributed to a large extent to the understanding of the atomic arrangement in condensed matter. The structure of many thousands of inorganic and organic compounds has been determined in this way. However, for applying that technique it is necessary that the atoms are arranged in a lattice with long range order and that the sample is at least a polycrystal with crystallites of the order of 10 nm or more in size. In that case the position and the intensity of the Bragg peaks give the lattice and the position of all atoms in the unit cell. On the other hand, there are cases where the long-range order is not the relevant feature for understanding the mode of operation of a chemical or physical reaction in condensed matter. Take, for instance, the influence of an active centre in a catalyst. This is, in general, a particular atomic species that mediates a chemical reaction between 2 or more partners. This reaction happens on a length scale given by the range of chemical bonds, which is of the order of a few tenths of nanometers. For that purpose a technique which probes the local geometric and chemical structure around a given atomic species is particular useful. X-ray absorption spectroscopy (XAS) is such a technique. It is the purpose of this lecture to give a first introduction to the field of XAS. Special topics like magnetic dichroism are treated in different lectures. A few textbooks on XAS are quoted in the references [1-5].

When X-rays pass through matter they are attenuated. The intensities  $I_1(E)$  and  $I_2(E)$  in front and behind an absorber of thickness  $d$  are related by the Lambert-Beer law

$$I_2(E) = I_1(E)e^{-\mu(E)d} \quad \{1\}$$

The linear absorption coefficient  $\mu(E)$  depends on the photon energy  $E = \hbar\omega$  and on the absorbing material. Figure 1 shows the absorption coefficient of X-rays for atomic copper and for metallic copper. The basic photoabsorption process is an atomic process, characterized by absorption edges and a strong increase of absorption at the edges. Energy can only be removed from the incoming beam by absorption of quanta  $\hbar\omega$ . This is done by exciting an electron from an occupied core level to an unoccupied state, as required by the Pauli exclusion principle. The excited states are discrete states or free states above the ionization level. At an absorption edge, photons become able to excite strongly bound electrons into the continuum. A new absorption channel is opened and  $\mu$  increases drastically with photon energy. At a  $K$  edge  $1s$  electrons are excited and at  $L_I$   $L_{II}$  and  $L_{III}$  edges  $2s$ ,  $2p_{1/2}$  and  $2p_{3/2}$  electrons are removed from the atom.

In condensed matter, as e.g. in metallic copper, there is an additional fine structure at and above the edges, as shown in figure 1. This fine structure is due to backscattering of the photoelectron by other atoms which surround the absorbing atom. It contains the structural and electronic information we are interested in. Before we will discuss this point we will consider in somewhat more detail the basic absorption effect observed in isolated atoms.



**Figure 1** - Absorption coefficient  $\mu$  in the vicinity of the  $K$ -absorption edge in metallic Cu and in atomic Cu (insert).