Phenomenological approach to XANES spectroscopy

Carlo Meneghini Dip. di Fisica E. Amaldi, Università di Roma TRE, via della Vasca Navale, 84, 00146 Roma Italy. meneghini@fis.uniroma3.it

Traditionally the x-ray absorption fine structure signal (XAFS) is divided into near edge (XANES) and extended (EXAFS) regions. In the EXAFS region the data analysis is generally easier as the theory provides a simple formula, that can be used for accurate data fitting and structural refinement. Unfortunately the approximation valid in the extended region progressively fails approaching the edge region, here the theory becomes more complex and, lacking a simple formula, the ab-initio modelling and interpretation of XANES features may result in a hardly difficult task.

Even if ab-initio XANES modelling is often reserved to *specialists*, several valuable and accurate information can be derived by comparison with data of model compounds and/or following the evolution of near edge features as a function of environmental parameters such as pressure, temperature, chemical environment. In fact the XANES region contains definitively relevant information not directly accessible from the EXAFS data analysis, such as the the photoabsorber valence state, its coordination chemistry, the density of electronic states near to the Fermi level. Moreover the near edge features are generally stronger than in the extended region, so that data collection may result simpler and faster than in the extended region allowing special applications as studying materials in extreme conditions (high temperature and/or pressure), high and ultra-high diluted phases, time resolved investigations well below the millisecond scale, chemical species mapping with submicrometer resolution and so on. Moreover the magnetic effects are stronger near the edge, where the XMCD can provide detailed information on the magnetic nature of the photoabsorber.

As a matter of fact the number of researches taking advantages from XANES spectroscopy is progressively growing in different fields such as material science, catalysis, biology, environmental science and so on. Practical application of XANES based techniques, examples and special achievements are presented here