Interpretations of X-ray core electron spectroscopies in the framework of Multiple Scattering Theory

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Abstract

X-ray spectroscopies using synchrotron radiation have been widely used in recent years, especially in Japan many industries utilize them. Among X-ray spectroscopic techniques, those based on the excitation of inner-shell electrons reflect local structures and electronic states around X-ray absorbing atoms in their spectra and provide information that cannot be supplied by other spectroscopic techniques. They are particularly powerful in systems without periodic long-range order.

The recent emergence of X-ray free electron lasers (XFELs), with their extremely high brightness and femtosecond order pulse widths, has enabled previously unseen short time dynamics to be seen. In particular, femtosecond XFEL pulses are well suited for the study of atomic vibrations and molecular dynamics, where the dynamics occur in the femtosecond to sub-picosecond range, depending on the type of atom.

Thus, X-ray core-level excitation spectra are becoming more and more important, and accordingly, developments in their interpretation are required. For this reason, theories and theoretical analyses of these spectroscopic methods are advancing. However, in actual theoretical analysis, different approximations have been introduced for each theoretical method, and researchers must choose the most appropriate method for the phenomenon to be interpreted.

X-ray absorption spectra (XAS or XAFS) can be divided into peaks for transitions to bound states near edge region and transitions to continuum states above the vacuum level. According to a general optical theorem, at each energy, the number of photoelectrons emitted corresponds to the X-ray absorption cross section. This is the so-called total electron yield. This shows that it is necessary to take into account the fact that the final state is a continuum state except sharp bound state peaks very near edge in the analysis of the X-ray absorption cross section.

In this presentation, I will discuss the multiple scattering theory and its interpretation, which is suitable for the treatment of continuum final states.