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NEXAFS, XANES

Glass systems are often multi-component and the constituent species can span the range of low Z elements such as oxygen and phosphorus to the high Z elements such as Pb. Due to the tunability of synchrotron X-rays, atom-species-specific information can be obtained using X-ray Absorption Spectroscopy (XAS) from nearly every known constituent element of every known inorganic glass forming system. In principle, using chemical and structural information from each of the constituent elements, the local structure of any inorganic glass system can be solved. This presentation elucidates how chemical information one can be obtained from XAS. Chemical information is contained within the first 50 eV of the absorption edge in an XAS spectrum. Depending on whether the technique is used in the hard X-ray or the soft X-ray regime, the analysis of this near-edge region of XAS is referred to as X-ray Near-edge Fine Structure (XANES) or Near-edge X-ray Absorption Fine Structure (NEXAFS), respectively. We will look specifically at the use of various objective ways of analyzing large data sets in order to identify the number and type of various chemical species during chemical transformations. In particular, we will look at the use of isosbestic points in the data, the use of principal component analysis and the use of linear combination analysis. Finally, we will demonstrate the use of the nearly linearly polarized synchrotron beam to probe the electronic structure along different molecular orbitals in organized structures such as self-assembled surface adsorbates on the surface. This type of analysis could be useful in studying devitrification of glasses, for example