Science at High Pressure: the emerging role of X-ray absorption spectroscopies

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The last decades have witnessed an unprecedented surge in the study of matter and materials at high pressure The fundamental importance of this research stems from the fact that such extreme conditions can deeply modify chemical bonds and induce myriad changes in materials. Many breakthroughs have been achieved in fields ranging from Earth and planetary sciences to fundamental physics, chemistry and materials research. Many of the physical and chemical consequences of extreme pressure on matter, such as changes in local structure, melting, modifications of the valence state, breaking or formation of chemical bonds, are optimally observed through X-Ray Absorption Spectroscopy (XAS).

XAS has been applied in high pressure research for decades. The unique properties of XAS, namely, chemical selectivity and sensitivity to local, electronic and magnetic structure, not only make this method very complementary to the more commonly used diffraction techniques, but also provide information on compressed matter that cannot be obtained by other methods. However, it has not seen the same level of activity or exposure of diffraction techniques. Experimentally, strong anvil absorption at low resonant energies and Bragg peak contamination from single crystalline anvils have been important limiting factors. Intrinsic limitations in energy resolution due to core-hole lifetime broadening have obscured the amount of detail with which electronic structure can be resolved. Limited brilliance of synchrotron radiation sources have imposed constraints on the time scale over which dynamical response could be measured. Interpretation of XAS data has relied on the accuracy of state of the art theoretical calculations, an additional challenge.

In this lecture I will give a few recent examples that illustrate how this landscape is rapidly changing due to the combined effect of advances in high pressure and X-ray science technology and in theoretical calculations. The recent availability of nano-polycrystalline diamond has been a breakthrough for the application of extended X-ray absorption fine structure (EXAFS) spectroscopy to high pressure science. Crystal analyzers, that allow selection of X-ray emission or inelastically scattered photons with high energy resolution, have seen improvements leading to studies of electronic structure and excitations with unprecedented resolution. XAS-based techniques, such as resonant inelastic X-ray scattering and X-ray Raman Spectroscopy are now being applied also to high pressure science thanks to development of larger area analyzer crystals coupled to brilliant hard X-ray sources. X-ray detectors have evolved to a point that a single 100 ps X-ray pulse can be efficiently captured and used to probe ns-lived states of dynamically compressed matter. Finally, first principle calculations are starting to play a key role in the interpretation of x- ray absorption near edge structure and x-ray magnetic circular dichroism spectra for a better understanding of emergent phenomena in condensed matter physics at high applied pressure.

Examples will cover studies on Earth minerals, noble gases, metals, and highly correlated electron materials.