Lattice Dynamics at Ultra-high Pressures: Quantification of Phonon Energies Using High-resolution Inelastic X-ray Scattering

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Traditionally, experimental determination of phonon energies away from the zone center was solely the domain of inelastic neutron scattering. While our understanding of many physical properties was greatly enhanced by the large body of neutron studies performed from the 1960's to the present, the restrictions on sample size imposed by the technique relegated the achievable information to low or at most moderate pressures (~10 GPa). However, with the advent of third generation synchrotron sources and the construction of beamlines dedicated for inelastic x-ray scattering experiments (IXS), these limitations have to a great degree been overcome.

Over the past few years our group has focused a large experimental and theoretical effort on quantifying the vibrational energies in transitional metals at high-pressures and high-temperatures. Our interest in the high-pressure properties of these elements is motivated by the rich variety of intriguing phenomena displayed by their lattice dynamics at room pressure as well as the lack of detailed understanding of the underlying physics that control their physical properties at pressure and their importance as constituents in the cores of many planetary bodies and. IXS has addressed a number of phenomenological problems of great importance, such as the nature of the acoustic anisotropy of the Earth's inner core, by direct measurements on the high-pressure hcp-phase of iron, as well as by proxy experiments on cobalt. We have also pursued more general studies of condensed matter at high-pressure important for the understanding of many fundamental physical properties in systems as varied as Mo, Ce, and even Pu. Indeed, with the application of pressures approaching 100 GPa, we are able to perturb the energy of condensed systems on the order of ~1 eV. Thus, performing lattice dynamics measurements under these conditions allows us to probe systems that have undergone fundamental changes the energetics of the chemical bonds. Such experiments have now begun to shed light on important magneto-elastic interactions, electron-phonon coupling and have the singular potential to provide critical data on the newly observed elastic perturbations across pressure induced spin-transitions.

Finally, we note that the state of the art with respect to synchrotron beamlines has come so far over the past few years, that in most cases we are no longer limited by the IXS beamlines. In fact, from the high-pressure experimental side, IXS experiments at high-pressure routinely require state of the art experimental capabilities from the standpoint of sample preparation and sample environment. In the case of transition metals, the development of the techniques for the production of small (~30 μm x 20 μm), high-quality, single-crystal disks as well as novel new diamond anvil cells accommodating either large angular apertures or stable high temperatures have been at the core of our ability to make lattice dynamics measurements at extreme conditions.