[MS32- 02] High Pressure Behavior of Single-Crystal and Nanocrystalline ZnO studied with XRD and BS.

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-Single-crystal x-ray diffraction (XRD) and Brillouin spectroscopy (BS) are the most powerful technique for studies elastic and structural properties of materials at ambient conditions. At high-pressure, however, the single-crystal technique is restricted by limited angular access to the sample in the high pressure vessel and by the requirement of having a high-quality thin crystal sustained in the desired pressure-temperature range [1]. As a result, in a number of cases at extremely high pressure and high temperature conditions, polycrystalline samples with various grain sizes are still the most routinely used for structure solution and physical property measurements. While effect of crystal size on structural and elastic properties of solid is well known at ambient condition the high pressure data is very limited [2]. In this work, we present a new approach in high pressure research employing the combination of BS with synchrotron XRD for characterization of ZnO in three crystalline forms: single-crystal, polycrystalline and nano-sized. The main reasons for using nano-structural materials in adition to single crystal and polycrystalline forms are to (1) reduce the anisotropy of samples probed with BS/XRD and (2) avoid significant effects on the Brillouin spectra due to the high sensitivity of acoustic velocities to crystallographic direction. The ability to perform simultaneous measurements of velocities and bulk modulus Ks (by BS), and the volume/density (by XRD) independent of any pressure standard in the same pressure-temperature environment provides essential information to resolve discrepancies between experimental data and theoretical calculations. First order phase transition from hexagonal (wurtzite, B4) to cubic (rock salt, B1) was observed with XRD technique in pressure range of 8-12 GPa for all samples associated with significant jump in density. At the same time the sound velocities show a slight softening of shear acoustic mode and quick raise after B4-B1 phase transition while longitudinal mode shows rather smooth behavior across the transition region. We were able to collect shear and longitudinal modes of ZnO up to 176 GPa, which is currently the highest known pressure where both Vs and Vp were measured simultaneously for known material structure and density. Important physical properties such as aggregate acoustic velocities, isothermal and adiabatic bulk and shear moduli, thermal expansion, structure, density, and other thermodynamic constants essential for understanding the nature of phase transition and compression mechanisms could be derived from combined studies single crystal and nano-sized materials with BS and x-ray synchrotron techniques [3].

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