Structural progressions in Nano-Materials under the influence of varying Pressure and Temperature

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Abstract
Materials, especially nano-materials, have strategic applicability only when they are stable under externally varied conditions such as pressure or temperature. The stability manifests in various forms such as structural transformations, metal-insulator transitions, enhancement or collapse of magnetic ordering and amorphization, etc. under variations in externally applied pressure or temperature. Under externally applied pressure, the bonding patterns for the systems change dramatically, causing profound effects on numerous physical and chemical properties often leading to formation of new classes of materials. On the other hand, the temperature dependence of the materials can be attributed to the anharmonic terms in the vibrational potential energy. Size effects in nano-crystals are also expected to modify the anharmonicity and the phonon decay times as compared to their bulk/polycrystalline counterparts. The estimation of these anharmonic parameters requires the mode Gruneisen parameter, which is obtained from the pressure dependent frequency variation of the phonon modes.

Raman scattering is one of the most powerful techniques to investigate the phonon modes, electron phonon coupling, structural phase transitions, and anharmonic behavior of the optical modes. Investigations of such effects using Raman investigations have a very high sensitivity, since Raman spectroscopy permits finger-printing analysis of composition and state of a material. With change in temperature, most materials typically show both the line center and the line-width variation in their Raman spectra with development of new phonon modes in case of structural phase transition. We at NPL have investigated strategic materials to unravel these effects which may impact the potential applications of these materials. Among these we have primarily investigated the nano-crystalline rare earth sesquioxides, carbon nanotubes, magnetic materials and thermoelectric materials Cu_3SbSe_3, Bi_2Se_3 etc. Major results obtained and the trends observed would be discussed.

Brief CV-Nita Dilawar Sharma

Dr (Ms.) Nita Dilawar Sharma is presently working as a Senior Principal Scientist at National Physical Laboratory, New Delhi. She has an M.Tech. and Ph.D. from IIT Delhi. Her research activities include standardization of National pneumatic pressure standards which involves primary as well as secondary pressure standards, simulations on piston-cylinder behavior under the application of pressure using ANSYS (Finite element) and Monte-Carlo simulations, investigation of high pressure and low temperature structural changes in advanced materials studied mainly through in-situ Raman spectroscopy etc. Dr Nita Dilawar has been a recipient of several awards and honor, to name a few Asia Pacific Metrology Programs (APMP) Iizuka award for young scientists from Japan in 2004, Council of Scientific and Industrial Research's (CSIR) Young Scientist award in 2001, Young research award for best oral presentation at IUMRS-International Conference in Asia, 1998, I.I.Sc. Bangalore. She has about 78 published papers, four book chapters and more than 100 conference presentations to her credit.