Structural stability, elastic properties and dynamics of some elemental solids at high pressures

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Recent developments and the availability of accurate electronic codes have greatly enriched the understanding of the properties and phase transformation mechanisms of solids at high pressure. In this presentation, results of recent investigations on the dynamic and elastic properties of several high pressure solids will be reported. A generalization of the stress-strain method to the calculation of the elastic constants of any crystal symmetry will be illustrated. We will present experimental vibrational density of states of krypton determined from 83Kr nuclear inelastic scattering experiments. In comparison with theoretical calculations, we note that even in this simple system, subtle discrepancies between theory and experiment remains. Dynamical calculations were also employed to study the stability and superconductivty of the Si-V and Si-VI phases. It is found that the Si-VI, though energetically more stable than the Si-V and Si-V phases, it is found to be dynamically unstable and therefore maybe entropically stabilized at high temperature. Quantum mechanical dynamical and transport calculations were used to characterize the electron topological transitions and superconductivity in high pressure Nb. We found that a similar transition may explain the anomaly observed in the equation of state for Os.