SHOCK13-2013-020080

Abstract for an Invited Paper
for the SHOCK13 Meeting of
the American Physical Society

Band Gap of Materials from Refractive Indices at High Pressure

JOHN TSE[1], University of Saskatchewan

The band gap of a material is one of the most fundamental properties. One approach to obtain energy gap information at high pressure is to measure the reflectivity of the material in a diamond anvil cell and analyzed with the effective oscillator model (EOM). In this study, the assumptions underlying the EOM are examined through comparison with theoretical dielectric response functions obtained from solving the Bethe-Salpeter equation (BSE) and band gap energy calculated from the GW method. The validity the EOM method in the estimation of the band gap energies from refractive index data in high pressure ice VII and solid hydrogen is evaluated. The research was performed in collaboration with Y. Liang, H. Shi, W. Yim, C.S. Zha and R.J. Hemley.

[1]In collaboration with Yong Xue, University of Saskatchewan.