Ab-initio calculations of high pressure equation of state and ideal strength of MgO D. MUKHERJEE, K.D. JOSHI, S.C. GUPTA, Bhabha Atomic Research Centre, Mumbai, India - 400085 — Isotherm at 0 K of fcc MgO is determined from ab-initio calculations and used to derive the 300 K isotherm, isentrope and Hugoniot of MgO. The shock parameters C and s obtained from theoretical Hugoniot are 6.74 km/s and 1.23 as compared to the experimental values of 6.87 km/s and 1.24, respectively. Further, we have determined ideal compressive strength and tensile strength of MgO single crystal subjected to uniaxial compressive and tensile loading along [001] direction under two deformation conditions, namely uniaxial strain condition and uniaxial stress condition. Examination of elastic stability conditions suggests that for [001] compressive loading, the MgO fails mechanically due to shear instability, whereas for expansion it fails due to vanishing of tensile modulus. The ideal compressive strength under uniaxial strain condition and uniaxial stress condition is determined to be 293 GPa and 123 GPa, respectively. However, ideal tensile strength is evaluated to be -20 GPa and -11 GPa, respectively, for two loading conditions. Our results suggest that MgO single crystal offers higher resistance against failure for compression as well as expansion under uniaxial strain condition than that for the uniaxial stress condition.

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