PHASE TRANSITION AND THERMODYNAMIC PROPERTIES STUDY OF ZIRCONIA USING FIRST PRINCIPLES METHOD

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Zirconium dioxide (ZrO2) ceramics are of highly scientific and industrial interest. Since zirconia performs high melting temperature and small thermal conductivity, this material is well developed and commonly used for thermal barrier coating material in industry. This study investigates zirconium dioxide properties based on first principles calculation. Structural properties, including band structure, density of state, lattice parameter, as well as elastic constant for both monoclinic and tetragonal zirconia were computed. Pressure based phase transition of tetragonal zirconia (t-ZrO2) was calculated using DFT method CASTEP code. This work is based on band structure and tetragonal distortion change under compression pressure. The results predict a transition from monoclinic structure to a fluorite-type cubic structure at pressure of 37 GPa. Monoclinic phased zirconia (m-ZrO2) thermodynamic property calculations were also carried out using the Vienna ab initio Simulation Package VASP coupled with PHONOPY. The temperature dependence of specific heat capacity, entropy, free energy, Debye temperature of monoclinic zirconia, from 0 to 1000K, were computed and compared well with those reported from other relevant work.