Structural, elastic, electronic, optical and thermal properties of c-SiGe2N4

We have investigated the structural, elastic, electronic, optical and thermal properties of c-$SiGe_2N_4$ by using the ultrasoft pseudopotential density functional method within the generalized gradient approximation. The calculated structural parameters, including the lattice constant, the internal free parameter, the bulk modulus and its pressure derivative are in agreement with the available data. The independent elastic constants and their pressure dependence, calculated using the static finite strain technique, satisfy the requirement of mechanical stability, indicating that c-$SiGe_2N_4$ compound could be stable. We derive the shear modulus, Young's modulus, Poisson's ratio and Lamé's coefficients for ideal polycrystalline c-$SiGe_2N_4$ aggregate in the framework of the Voigt-Reuss-Hill approximation. We estimate the Debye temperature of this compound from the average sound velocity. Band structure, density of states, Mulliken charge populations and pressure coefficients of energy band gaps are investigated. Furthermore, in order to understand the optical properties of c-$SiGe_2N_4$, the dielectric function, refractive index, extinction coefficient, optical reflectivity and electron energy loss are calculated for radiation up to 40 eV. Thermal effects on some macroscopic properties of c-$SiGe_2N_4$ are predicted using the quasi-harmonic Debye model in which the lattice vibrations are taken into account. We have obtained successfully the variations of the primitive cell volume, volume expansion coefficient, heat capacities and Debye temperature with pressure and temperature in the ranges of 0-40 GPa and 0-2000 K. For the first time, the numerical estimates of the elastic constants and related parameters, and the thermal properties are performed for c-$SiGe_2N_4$.