Pressure-induced structural transition in amorphous GeO2: a molecular dynamics simulation

Peralta, Joaquín

Gutiérrez, Gonzalo

We studied the structural and dynamical properties of amorphous germanium dioxide(GeO2) from lowto high pressure by means of the classical molecular dynamics technique. The simulationswere done in the micro-canonical ensemble, with systems at densities ranged from 3.16 to6.79 g/cm3, using apairwise potential. The network topology of the systems is analyzed at atomic levelthrough partial pair correlations, coordination number and angular distributions. Thedynamic properties were characterized by means of the vibrational density of states.According the density increases, a structural transformation from a short-range order,defined by a building block composed by a basic (GeO4) tetrahedron, to a basic(GeO6) octahedronis observed. The vibrational density of states also presents important changes when thedensity increases, with a low frequency band lessened, and a high density band wider andflatter.