Mechanical and thermodynamic properties of 3C structure of silicon carbide using molecular dynamics and density functional theory methods

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Abstract

Silicon carbide (SiC) is an attractive ceramic for most industries due to its unique mechanical, physical, thermodynamical and chemical properties. In this research, the mechanical, and thermodynamical properties of 3C silicon carbide were estimated by molecular dynamics and density functional theory in high temperature and pressure. The results were compared and validated by valid theoretical and experimental results. The molecular dynamics calculations were carried out by Tersoff, and Vashishta interatomic potentials. The results indicated that both potentials have high capability in optimizing SiC structure. The estimated mechanical properties of 3C silicon carbide including elastics constants, Bulk, Young, and Shear moduli and Poisson ratio in high temperature and pressure (50 GPa and 1000 K, respectively) which were calculated by Tersoff potential were in good agreement with experimental results. The thermodynamic properties including melting point, Debye temperature, specific heat capacities at constant volume and pressure, linear thermal expansion coefficient, and thermal conductivity in ambient and high pressure were calculated by molecular dynamic and functional theory.

Keywords: Silicon carbide, Molecular dynamics, density functional theory, high temperature and pressure, mechanical and thermo dynamical properties

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