MOLECULAR DYNAMIC SIMULATION OF ISOTHERMAL AND SHOCK-INDUCED COMPRESSION OF METHANE

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Keywords: A molecular dynamic (MD) simulation of isothermal compression of liquid methane ($T = 110$ K) using LAMMPS code and ReaxFF potential is performed. The influence of Nosé–Hoover thermostat and barostat on thermodynamic properties is analyzed. Isothermal curves for $T = 110$ K and $P = 50$–1800 atm were simulated. Hugoniostat simulation was conducted for pressures $P = 1000$–$44\,000$ atm. For the same interval of pressures, a simulation using Exp-6 potential was carried out. A Hugoniot curve for liquid methane and a dependence of shock wave velocity on the particle velocity were obtained. The MD simulation provides very good estimates for the thermodynamic properties of methane when applied to the isothermal and shock-induced compression.

Keywords: molecular dynamic simulation; isothermal compression; shock Hugoniot, methane

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