MOLECULAR DYNAMICS SIMULATION OF SHOCK COMPRESSION OF RDX SINGLE CRYSTAL USING A MODIFIED REACTIVE FORCE FIELD ReaxFF-lg

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Abstract: The characteristics of isothermal compression of RDX single crystal were analyzed by molecular dynamics simulation. A pressure–compression ratio curve for a single RDX crystal was obtained at constant temperature $T = 300$ K in the pressure range $P = 0.05$–40 GPa. The simulation results showed that the modified reactive force field ReaxFF-lg accurately predicts the equations of state and are consistent with the experimental isotherm for a single RDX crystal. Molecular dynamics simulations of the RDX single-crystal isotropic shock compression were conducted by the Hugoniot method. The pressure–compression ratio and temperature–pressure Hugoniot curves were calculated in the wide pressure range $P = 1$–40 GPa. The calculated shock curves for a single RDX crystal are in good agreement with experimental data.

Keywords: molecular dynamics; reactive force field ReaxFF-lg; Hugoniot method; shock curve

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