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The molecular dynamics simulation of the isothermal and elastic properties of HMX FENGLEI HUANG, WEI YAO, beijing Institute of technology — The isotherms and elastic properties of β-HMX crystals were calculated through molecular simulations in NPT ensemble using COMPASS force field. The pressure-induced changes of the lattice parameters showed the anisotropic compression of β-HMX. The isotherm of β-HMX was simulated and the bulk modulus K_0 and its pressure derivative $K_0^{'}$ were obtained by fitting the isotherms to different equations of state. However, the values of K_0 and $K_0^{'}$ obtained from the isotherm are sensitive to the fitting form of equation of state. The elastic constants and modulus were calculated by statistic analysis mode at different pressures in the range of 0$\sim$27GPa. Cauchy pressure $C_{12} - C_{44}$ and G/K ratios were also calculated which indicated that β-HMX would become harder as the pressure increased, and as well the β-HMX elastic property transformed from brittleness to ductibility.

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