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QMD and classical MD simulation of alpha boron and boron-carbide behavior under pressure ALEXEY YANILKIN, PAVEL KOROTAEV, ALEXEY KUKSIN, PAVEL POKATASHKIN, All-Russia Research Institute of Automatics — Boron and some boron-rich compounds are super-hard and light-weighted material with a wide range of different applications. Nevertheless, the question of its behavior under pressure is still open. In the present work we study the equation of state (EOS), stability and deformation of α-B and B4C under high pressure within quantum and classical molecular dynamics (QMD and MD). Based on QMD results the finite temperature EOSs are revealed. CBC chain bending, amorphization and recrystallization of B4C are investigated under hydrostatic, uniform and uniaxial compression. The influence of nonhydrostatic loading is discussed. Angular dependent interatomic potentials are derived by force-matching method. The properties of α-B and B4C, obtained by classical potential, are verified. Structure, bulk modulus, pressure-volume relation, Gruneisen and thermal expansion coefficients are in good agreement with both ab initio and experimental data. These potentials are used to study shock wave propagation in a single crystal of α-B and B4C. Two mechanisms of shear deformation are observed: stacking fault formation and local amorphization. The crystallographic orientations of defects are in a good agreement with experiments.

Vasily Zhakhovsky
All-Russia Research Institute of Automatics

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