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Equation of State of Al Based on Quantum Molecular Dynamics Calculations[1] DMITRY V. MINAKOV, PAVEL R. LEVASHOV, KONSTANTIN V. KHISHCHENKO, JIHT RAS, Moscow, Russia — In this work, we present quantum molecular dynamics calculations of the shock Hugoniots of solid and porous samples as well as release isentropes and values of isentropic sound velocity behind the shock front for aluminum. We use the VASP code with an ultrasoft pseudopotential and GGA exchange-correlation functional. Up to 108 particles have been used in calculations. For the Hugoniots of Al we solve the Hugoniot equation numerically. To calculate release isentropes, we use Zel'dovich's approach and integrate an ordinary differential equation for the temperature thus restoring all thermodynamic parameters. Isentropic sound velocity is calculated by differentiation along isentropes. The results of our calculations are in good agreement with experimental data. Thus, quantum molecular dynamics results can be effectively used for verification or calibration of semiempirical equations of state under conditions of lack of experimental information at high energy densities.

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