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First-principle Calculations of Equation of State for Metals at High Energy Density DMITRY MINAKOV, PAVEL LEVASHOV, KONSTANTIN KHISHCHENKO, Joint Institute for High Temperatures RAS — In this work, we present quantum molecular dynamics calculations of the shock Hugoniots of solid and porous samples as well as release isentropes and isentropic sound velocity behind the shock front for aluminum. Also we perform similar calculations for nickel and iron. We use the VASP code with ultrasoft and PAW pseudopotentials and GGA exchange-correlation functional. Up to 512 particles have been used in calculations. To calculate Hugoniots we solve the Hugoniot equation numerically. To obtain 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 of pressure along isentropes. The results of our calculations are in good agreement with experimental data at densities both higher and lower than the normal one. 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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