

Abstract Submitted  
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**Equation of state and stability of metal crystals at high pressure by DFT calculations<sup>1</sup>** DMITRY MINAKOV, PAVEL LEVASHOV, Joint Institute for High Temperatures of the Russian Academy of Sciences — In this work we present *ab initio* equation-of-state calculations for crystals of some metals. Density functional theory at finite temperature (VASP code) is used to obtain the properties of electrons; lattice is simulated in quasi-harmonic approximation at non-zero temperature of electrons. Anharmonic effects are taken into account by the thermal expansion of a crystal. All calculations were performed for aluminum, copper and gold. We compare our results with available shock-wave data in crystal phase, including isentropic expansion. The melting curves are calculated by different criteria; the effect of different temperatures of electrons and ions is taken into account. Also we determine thermodynamic and kinetic boundaries of stability of crystals. Our calculations demonstrate that *ab initio* approaches can be used to theoretically reconstruct thermodynamically complete EOS of metallic crystals.

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