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Ab initio study of mechanic, thermodynamic and transport properties of gold after electronic excitation SERGEY STARIKOV, VLADIMIR STEGAILOV, GENRI NORMAN, OLEG SERGEEV, PETR ZHILYAEV, Joint Institute for High Temperatures of Russian Academy of Sciences — The electronic excitation after the femtosecond laser irradiation drastically changes mechanical and electronic properties of metals. In this work we calculate, on the example of gold, the effective interatomic potential in the EAM form that parametrically depends on the electron temperature. This potential is created by the force matching procedure based on the ab initio data calculated with the VASP package for the representative sets of atomic structures. The potential is verified by the recent experimental data. The electronic heat capacity, electronic conductivity and electron-phonon coupling constant are calculated at the DFT level using plane-wave pseudopotential approach. The dependence of these properties on the electron temperature and their deployment together with the new EAM potential in the two-temperature atomistic model of ablation are discussed.

Sergey Starikov
Joint Institute for High Temperatures of Russian Academy of Sciences

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