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Essential parameters in comprehensive hybrid modeling of metals irradiated by femtosecond laser WEIRONG YUAN, TATYANA SIZYUK, Center for Materials under Extreme Environment (CMUXE), School of Nuclear Engineering, Purdue University — Study of femtosecond laser interaction with metals using two temperature model requires accurate calculation of several major optical and thermodynamic parameters including laser photon reflectivity and penetration depth, electron thermal conductivity, heat capacity, and electron-lattice coupling factor. All these parameters are still not well determined through the theoretical studies or experiments and have great effects on the physical processes. In this work, the comprehensive hybrid, two temperature and molecular dynamics, model was developed. The effect of nonequilibrium electrons was considered, and major parameters were calculated as functions of electron and lattice temperatures and lattice density. The effect of each individual parameter and the synergistic effects will be discussed. By tuning these parameters, we benchmarked our results with recent experimental data and other simulation results. The benchmarking includes electron and lattice temperature, surface displacement, and phase transition. Verified parameters were then used for further studies such as damage threshold, laser ablation rate, and nanoparticle production.

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