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Molecular Dynamics Simulation of Electron-Ion Temperature Relaxation in Dense Hydrogen: Electronic Quantum Effects. QIAN MA, JIAYU DAI, ZENGXIU ZHAO, National University of Defense Technology — The electron-ion temperature relaxation is an important non-equilibrium process in the generation of dense plasmas, particularly in Inertial Confinement Fusion. Classical molecular dynamics considers electrons as point charges, ignoring important quantum processes. We use an Electron Force Field (EFF) method to study the temperature relaxation processes, considering the nuclei as semi-classical point charges and assume electrons as Gaussian wave packets which includes the influences of the size and the radial motion of electrons. At the same time, a Pauli potential is used to describe the electronic exchange effect. At this stage, quantum effects such as exchange, tunneling can be included in this model. We compare the results from EFF and classical molecular dynamics, and find that the relaxation time is much longer with including quantum effects, which can be explained directly by the deference of collision cross sections between quantum particles and classical particles. Further, the final thermal temperature of electron and ion is different compared with classical results that the electron quantum effects cannot be neglected..

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