Coupling MD Simulations of Laser Ablation with PIC-DSMC Simulations of Plasma Plume Expansions and subsequent Laser-Plasma Interactions

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Plasmas created by laser light interacting with metals are of great interest regarding numerous fields, e.g., medical laser applications, spacecraft propulsion or material processing. The process of laser-solid interaction is examined by atomistic Molecular Dynamics (MD) simulations for a detailed description of the creation of lattice ions and their removal from the target surface[1]. In order to investigate the expansion of the plasma plume for larger spatial and temporal dimensions, the MD results are used as initial conditions for Particle-In-Cell (PIC) simulations, where particle collisions are incorporated using the Direct Simulation Monte Carlo (DSMC) method, which considers chemical reactions, e.g., impact ionization and recombination processes. These combined methods[2] offer an elaborate simulation of the expansion characteristics, which are crucial for subsequent laser pulses interacting with the expanding plasma plume. The simulations are performed using PICLas[3], a parallel high-order three-dimensional PIC-DSMC solver developed cooperatively by the Institute of Space Systems and Institute of Aerodynamics and Gas Dynamics at the University of Stuttgart.

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