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Atomistic simulations of laser ablation of metals in liquid environment CHENG-YU SHIH, CHENGPING WU, MAXIM SHUGAEV, LEONID ZHIGILEI, University of Virginia — Laser ablation of metal target in liquid environment is actively used for generation of clean colloidal nanoparticles with unique shapes and functionalities. The fundamental mechanisms responsible for the nanoparticle formation are not fully understood. In this presentation, we report the results of the first atomistic simulations of laser ablation of metal targets in liquid environment. A model combining a coarse-grained representation of liquid, a fully atomistic description of laser interactions with metal targets, and acoustic impedance matching boundary conditions is developed. In contrast to nanoparticle generation in vacuum, the phase decomposition in the liquid environment is partially suppressed and the hot mixture of metal vapor and clusters ejected from the irradiated target is localized in a low-density mixing region where the liquid is brought to the supercritical state. The main nanoparticle formation mechanism is found to be the condensation of clusters from the metal vapor, followed by coalescence and coarsening within the supercritical water region. The results of the simulations support the notion of the important role of the cavitation bubble in the process of nanoparticle formation. The simulations also predict that larger nanoparticles can be generated at sufficiently high laser fluences via Rayleigh-Taylor instability of the plume – supercritical liquid interface, leading to the formation of a bimodal nanoparticle size distribution commonly observed in experiments.

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