

# Molecular Dynamics Study of Cluster Emission, Condensation, and Impact at a Liquid Copper Surface under Conditions of Laser-Induced Vaporization

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Understanding the fundamental mechanisms of laser-induced evaporation is important for advancing high-temperature material processing technologies, including laser ablation, thin-film deposition, and selective laser melting. In conventional hydrodynamic and kinetic models of vaporization, it is assumed that only monomers evaporate from the surface of a liquid metal in the regime of surface (normal) evaporation, while cluster formation occurs through nucleation and aggregation in the vapor phase. In the present work, equilibrium and non-equilibrium molecular dynamics simulations are used to investigate the fundamental mechanisms governing cluster emission, condensation, and impact at the liquid copper surface. Using an embedded atom method potential and a special algorithm to distinguish stable clusters from unstable activated atomic complexes with short lifetimes, we study the distributions of clusters directly emitted from the surface under liquid-vapor equilibrium conditions. The simulations indicate that the total molar fraction of clusters of various sizes can be as high as 40% (Fig. 1(a)). The clusters emitted directly from the surface can serve as centers of further condensation, e.g., in the laser-induced vapor plumes. In this case, an artificially large number of triple collisions leading to the formation of dimers, which are usually assumed in theoretical models, is not required for the onset of vapor condensation. The velocity distributions of emitted clusters are found to be close to Maxwellian but at relaxation temperatures lower than the surface temperature. The equilibrium evaporation and non-equilibrium condensation coefficients are found to be close to each other. Both of them are significantly smaller than 1 at temperatures exceeding 3000 K. Furthermore, non-equilibrium impact simulations of small atomic clusters (Fig. 1(b)) show that the number of spattered atoms strongly depends on the angle of incidence. These results are used to refine the material removal models in kinetic simulations of laser vaporization of metals.

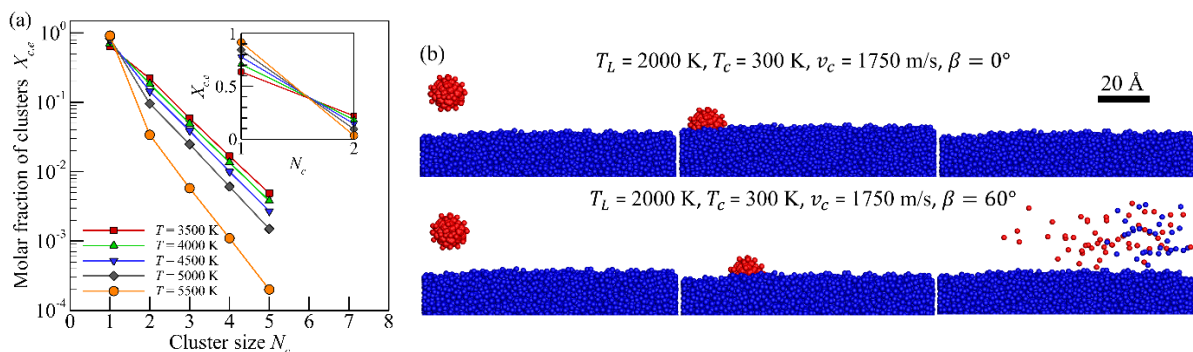


Fig. 1. (a) Equilibrium molar fractions of clusters directly evaporated from the liquid copper surface at various temperatures  $T$  ( $N_c$  is the number of atoms in a cluster); (b) Snapshots of impact of solid Cu cluster with a diameter of 2 nm and impact speed of 1750 m/s on the liquid copper surface with a temperature of 2000 K at the angle of incidence  $0^\circ$  (top row) and  $60^\circ$  (bottom row).

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