Dynamics of Laser-Induced Phase Explosion in Ag Films: Insights from Atomistic Simulations and Optical Imaging

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This study employs molecular dynamics simulations to delve into the interaction between ultrashort laser pulses and thin metal films – a phenomenon of high practical importance for applications ranging from nanoparticle synthesis to high-precision micro/nanomanufacturing in microelectronics. The simulations of femtosecond laser interactions with silver thin films provide microscopic insights into the complex mechanisms governing thin film removal (ablation) from optically transparent substrates. The density fluctuations precipitating phase separation during laser ablation are examined and related to the predictions of the classical nucleation theory. The transition from superheated liquid to a mixture of vapor and liquid droplets is monitored, with a particular focus on processes that define the droplet size distribution. To facilitate experimental validation of the computational predictions, the variation of scattering and reflectivity of the ablation plume is calculated for atomic configurations predicted in the simulations and related to the results of pump-probe optical imaging [1] of the ablation plume.

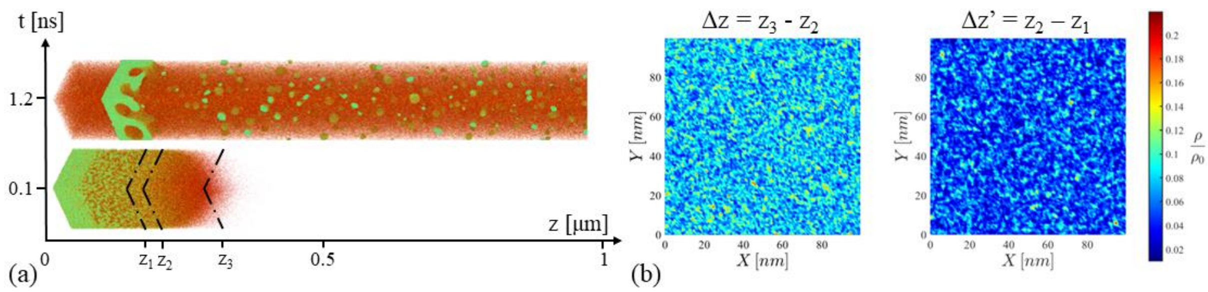

Figure 1. (a) Atomic configurations, colored by potential energy, obtained in a simulation of a 50 nm Ag film irradiated by a 200 fs laser pulse at an absorbed fluence of 800 J/m^2 (phase explosion regime) in vacuum. (b) Lateral density distributions in two slices of the ablation plume calculated at the initial stage of the plume expansion. The density is normalized by the initial density of the solid Ag film prior to the laser irradiation, ρ_0.

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References:

[1] M. Park, J. Jeun, G. Han, and C. P. Grigoropoulos, *Appl. Phys. Lett.* **116**, 234105 (2020).