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ATOMIC-SCALE PHOTOMECHANICAL DEFORMATION ON GOLD FILM SURFACE IRRADIATED BY FEMTOSECOND LASER

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Introduction. The study of femtosecond laser direct writing into gold thin films is of great significance in fields such as nanophotonics, micro fabrication, and functional surface preparation[1,2]. This work, combining two temperature modeling (TTM) and molecular dynamics (MD) multi-scale simulations[3,4], systematically reveals the non-equilibrium dynamics mechanism and microstructure evolution of the interaction between femtosecond lasers and gold thin films[5,6] at the atomic scale. By establishing a reasonable thermodynamic model, this work analyzes the photomechanical deformation of the gold film surface under femtosecond laser ablation at the picosecond timescale, resulting in jet and needle formation, and the corresponding spatiotemporal stress distribution. The results provide a theoretical basis for optimizing the process of femtosecond laser fabrication of metal thin films and expand its application potential in nanosensors and photothermal conversion.

Main part. Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) was used to construct model simulations of femtosecond laser ablation on gold film. The gold atomic configuration was initialized as a face-centered cubic (FCC) crystal and consisted as the simulation box of $90\times60\times9$ nm^3 in x, y and z directions, irradiated by a gaussian laser beam. To comprehensively investigate how rear boundary constraints affect stress propagation and jet evolution, two representative modeling approaches were adopted for the rear side of the gold film. In the first approach, non-reflecting boundary conditions combined with a Langevin thermostat were implemented to emulate thermal exchange and mechanical damping between the film and the substrate. In the second approach, the substrate was simplified as a rigid atomic layer interacting with the film through Lennard–Jones (LJ) potentials, thereby preserving only mechanical contact while neglecting explicit energy dissipation. By examining the dynamic responses obtained under these two limiting boundary scenarios, it becomes possible to distinguish the respective influences of substrate confinement, stress wave reflection, and dissipative effects on the development of jets and needle structures.

Conclusion. This work demonstrates that the formation of protrusions, jets, and needle structures during laser ablation of gold thin films is a non-equilibrium thermodynamic and mechanical process regulated by electron thermal diffusion, energy absorption characteristics, and rear side boundary conditions. Spatiotemporal analysis of stress and stress rate indicates that under transversely confined laser excitation, material separation is initially triggered by the rapid localization of near surface non-equilibrium tensile stress. The mechanical confinement on the rear side determines the stability and continuous evolution of the jets or clusters after formation, thus providing clear initial mechanical conditions for subsequent morphological rearrangement dominated by surface tension.

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