European XFEL Theory Seminar

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Campus Schenefeld, main building (XHQ) room E1.096

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Large-scale atomistic simulations of nanoparticle generation and material modification by short laser pulses in vacuum and liquid environment

Atomistic and coarse grained molecular dynamics (MD) simulations of laser-materials interactions are playing an increasingly important role in investigation of complex and highly nonequilibrium processes involved in short pulse laser processing of materials and surface modification. This role is defined by the ability of MD simulations to reveal the microscopic mechanisms of structural and phase transformations induced by the laser excitation and, at the same time, to provide clear visual representations, or “atomic movies,” of laser-induced dynamic processes. In this presentation, an overview of recent results of large-scale MD simulations of the direct laser-induced modification of surface morphology and microstructure, laser ablation, and generation of nanoparticles will be provided. The effect of the liquid environment on the laser-induced surface nanocrystallization and generation of nanoparticles will also be discussed based on computational predictions and related to experimental observations.

In the case of direct laser modification of metal targets in vacuum, the processes responsible for the formation of a sub-surface porous region covered by a nanocrystalline surface layer with random crystallographic orientation of nanograins and a high density of stacking faults, twins, and nanoscale twinned structural elements with five-fold symmetry will be discussed and related to the experimental observations of surface swelling, growth twinning, and incubation effect in multi-pulse laser ablation [1-3].

For laser interactions with metals in liquid environment, the nanoparticle generation through the nucleation and growth of small (mostly ≤ 10 nm) nanoparticles in the metal-water mixing region and the formation of larger (tens of nm) nanoparticles attributed to the Rayleigh-Taylor instability of the interface between the ablation plume and liquid environment will be discussed [4]. Computational predictions on the effect of the liquid environment on surface nanocrystallization in the regime of melting and resolidification, below the thresholds for laser spallation and ablation, will also be presented [5].

[1] C. Wu, M. S. Christensen, J.-M. Savolainen, P. Balling, and L. V. Zhigilei, Generation of sub-surface voids and a nanocrystalline surface layer in femtosecond laser irradiation of a single crystal Ag target, *Phys. Rev. B* **91**, 035413, 2015.

[2] C. Wu and L. V. Zhigilei, Nanocrystalline and polyicosahedral structure of a nanospike generated on metal surface irradiated by a single femtosecond laser pulse, *J. Phys. Chem. C* **120**, 4438-4447, 2016.

[3] X. Sedao, M. V. Shugaev, C. Wu, T. Douillard, C. Esnouf, C. Maurice, S. Reynaud, F. Pigeon, F. Garrelie, L. V. Zhigilei, and J.-P. Colombier, Growth twinning and generation of high-frequency surface nanostructures in ultrafast laser-induced transient melting and resolidification, *ACS Nano* **10**, 6995-7007, 2016.

[4] C.-Y. Shih, C. Wu, M.V. Shugaev, and L.V. Zhigilei, Atomistic modeling of nanoparticle generation in short pulse laser ablation of thin metal films in water, *J. Colloid Interface Sci.* **489**, 3-17, 2017.

[5] M. V. Shugaev, C.-Y. Shih, E. T. Karim, C. Wu, and L. V. Zhigilei, Generation of nanocrystalline surface layer in short pulse laser processing of metal targets under conditions of spatial confinement by solid or liquid overlayer, *Appl. Surf. Sci.*, in press, 2017.

Host: Evgeny Gorelov