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Large-scale atomistic simulations of surface nanostructuring by short pulse laser irradiation[1] CHENGPING WU, MAXIM SHUGAEV, LEONID ZHIGILEI, University of Virginia — The availability of petascale supercomputing resources has expanded the range of research questions that can be addressed in the simulations and, in particular, enabled large-scale atomistic simulations of short pulse laser nanostructuring of metal surfaces. A series of simulations performed for systems consisting of 10^8 – 10^9 atoms is used in this study to investigate the mechanisms responsible for the generation of complex multiscale surface morphology and microstructure. At low laser fluence, just below the spallation threshold, a concurrent occurrence of fast laser melting, dynamic relaxation of laser-induced stresses, and rapid cooling and resolidification of the transiently melted surface region is found to produce a sub-surface porous region covered by a nanocrystalline layer. At higher laser fluences, in the spallation and phase explosion regimes, the material disintegration and ejection driven by the relaxation of laser-induced stresses and/or explosive release of vapor leads to the formation of complex surface morphology that can only be studied in billion-atom simulations. The first result from a billion atom simulation of surface nanostructuring performed on Titan will be discussed in the presentation.

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Chengping Wu
University of Virginia

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