Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Large-scale massively parallel atomistic simulations of short pulse laser interaction with metals[1] CHENGPING WU, LEONID ZHIGILEI, Department of Materials Science and Engineering, University of Virginia, COMPUTATIONAL MATERIALS GROUP TEAM — Taking advantage of petascale supercomputing architectures, large-scale massively parallel atomistic simulations (10^8-10^9 atoms) are performed to study the microscopic mechanisms of short pulse laser interaction with metals. The results of the simulations reveal a complex picture of highly non-equilibrium processes responsible for material modification and/or ejection. At low laser fluences below the ablation threshold, fast melting and resolidification occur under conditions of extreme heating and cooling rates resulting in surface microstructure modification. At higher laser fluences in the spallation regime, the material is ejected by the relaxation of laser-induced stresses and proceeds through the nucleation, growth and percolation of multiple voids in the sub-surface region of the irradiated target. At a fluence of ~ 2.5 times the spallation threshold, the top part of the target reaches the conditions for an explosive decomposition into vapor and small droplets, marking the transition to the phase explosion regime of laser ablation. The dynamics of plume formation and the characteristics of the ablation plume are obtained from the simulations and compared with the results of time-resolved plume imaging experiments.

[1]Financial support for this work was provided by NSF (DMR-0907247 and CMMI-1301298) and AFOSR (FA9550-10-1-0541). Computational support was provided by the OLCF (MAT048) and XSEDE (TG-DMR110090).

Chengping Wu
Department of Materials Science and Engineering, University of Virginia

Date submitted: 15 Nov 2013 Electronic form version 1.4