

Generation of defect-rich nanoparticles by short pulse laser ablation and processing in liquid

Chaobo Chen, Ozcan Seslikaya, Mikhail I. Arefev, and Leonid V. Zhigilei*

University of Virginia, Charlottesville, USA
 *Corresponding author email: lz2n@virginia.edu

The catalytic activity of metal nanoparticles can be strongly enhanced by the presence of crystal defects, making defect-rich nanoparticles desirable for catalytic applications [1]. Pulsed laser ablation in liquid (PLAL) is a nonequilibrium synthesis technique that holds a high promise for mass-producing defect-rich nanoparticles. In contrast to chemical synthesis, the conditions in the laser-enabled synthesis are far from the equilibrium and are characterized by ultrafast quench rates and nanoparticle growth under extreme supersaturation. As a result, the nanoparticles can exhibit metastable phases and high densities of crystal defects. Moreover, laser processing of colloidal nanoparticles generated by PLAL can further modify their structure, opening an opportunity for tuning the defect types and densities to the needs of applications [2]. In this presentation, the mechanisms responsible for the generation of crystal defects in nanoparticles produced by laser ablation [3,4] and fragmentation in liquid [5] are discussed based on the results of large-scale atomistic simulations. The relationships between the defect structures produced in nanoparticles and the synthesis conditions realized during their formation and growth are established. The computational predictions are related to the results of time-resolved optical and X-ray probing of laser-induced processes [6], as well as *ex-situ* characterization of nanoparticle structure.

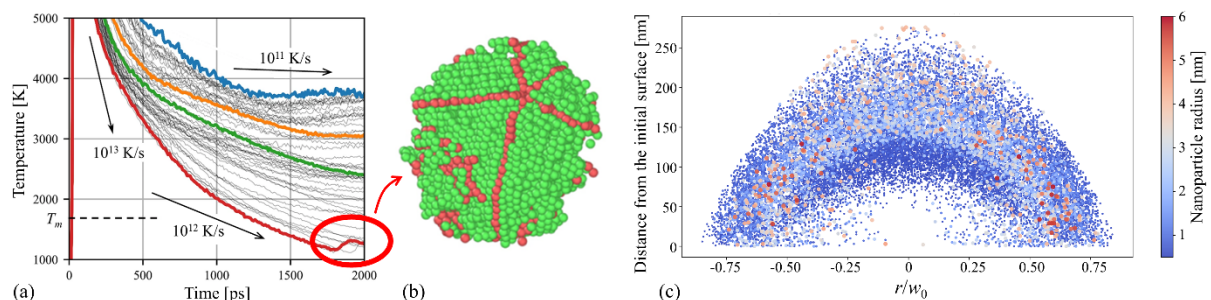


Figure: Time dependence of the temperature of 50 largest nanoparticles generated in a simulation of PLAL of a FeNi target irradiated by a 10 ps laser pulse at an absorbed laser fluence of 3000 J/m^2 (a), a snapshot of one of the particles solidified by the end of the simulation (b), and the distribution of nanoparticle sizes in a cavitation bubble generated based on the results of atomistic simulations performed at different local fluences (c) [4]. In (b), the atoms with local fcc and hcp surroundings are colored green and red, respectively, and all other atoms are blanked. With this coloring scheme, the planes of red atoms correspond to coherent twin boundaries in the fcc structure.

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