Atomistic modeling of generation of defect-rich nanoparticles by short pulse laser ablation and processing in liquid

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The synthesis of nanoparticles by pulsed laser ablation and processing in liquids is a well-established approach capable of producing large quantities of nanoparticles at a cost competitive with chemical synthesis [1]. 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. Indeed, atomistic simulations of laser ablation [2,3] and nanoparticle fragmentation [4.5] in liquid reveal that the nanoparticles exhibit high densities of twin boundaries and stacking faults. The experimental studies confirm the presence of planar defects and demonstrate a strong impact the defects make on the catalytic activity of the nanoparticles [6,7].

In this presentation, the mechanisms responsible for the generation of crystal defects in nanoparticles produced by laser ablation and fragmentation in liquid are discussed based on the results of large-scale atomistic simulations performed for FeNi, Ag, Au, and Cu targets and nanoparticles. 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, as well as *ex-situ* characterization of nanoparticle structure.

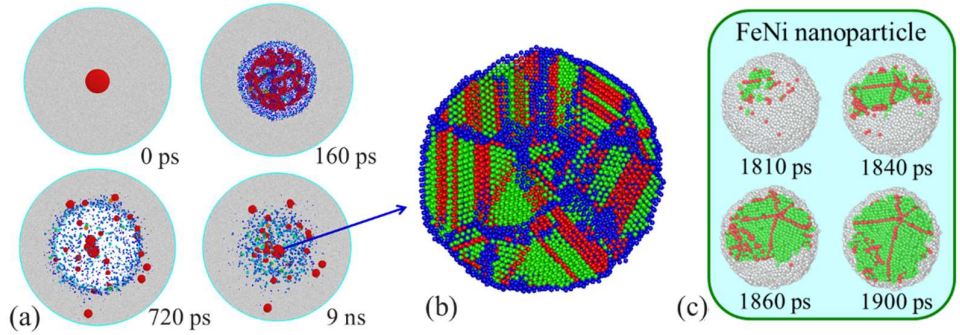

Figure: Snapshots from a simulation of laser fragmentation of Au nanoparticle in water (a), a cross-section of the largest fragment revealing the defect structure (b) [5], and the generation of twins (red atomic planes separating fcc crystallites colored green) during the crystallization in a nanoparticle generated in pulsed laser ablation of FeNi target in a liquid environment [3] (c).

References:

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