

# Modeling of laser-induced modifications of nano-objects and nanocomposite materials

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Nano-objects and nanocomposite materials have extremely interesting optical properties and hence have found numerous applications in various fields ranging from optics and photonics to medical applications [1]. In many experiments, various lasers ranging from continuous wave (CW) to femtosecond (fs) ones have been used both for their formation and for the following modifications. Efficient control of these processes remains, however, challenging and often requires numerical simulations because of a complex interplay of many physical and chemical processes involved.

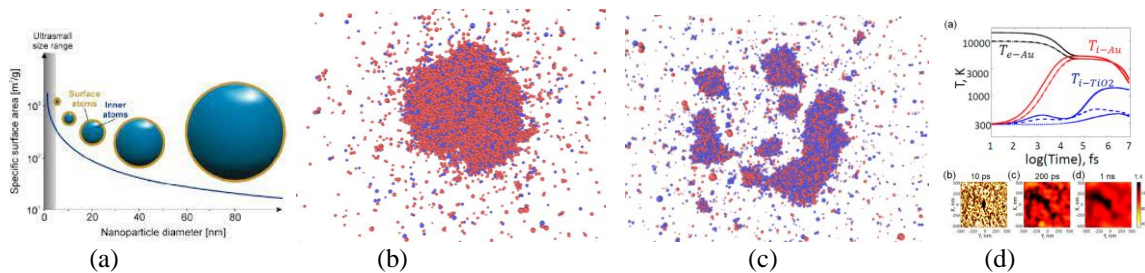


Figure 1. (a) Illustration of the role of surface energy vs nanoparticle size [2]. (b) -(c) Molecular dynamics simulation of fs laser interactions with different metallic alloy nanoparticles (different size, initial composition for AuN and AuCo). (d) Simulation of laser interactions with nanocomposite material containing bimodal-sized nanoparticles [4].

In this talk, attention will be focused on a series of atomistic modeling of laser-induced nanoparticle modifications with a particular emphasis on the essential mechanisms involved in such laser interactions. Firstly, laser interactions with single nanoparticles will be considered depending on the nanoparticle size, material, laser parameters, and ambient environment. Then, nanoparticle evaporation, fragmentation, sintering, coalescence, and aggregation will be discussed and particular attention will be given to the resulting changes in their optical properties. It should be noted that such effects result in important transient variations of the system in the case of multi-pulse laser interactions. The role of laser fluence, wavelength, and pulse duration will be shown. Finally, with the help of a combined model considering electron emission and ambient media ionization, laser interactions with nanoparticle ensembles will be examined. The effects of particle size distributions, morphology, and composition, and their roles will be analyzed and compared to the results of several available experiments [3-5].

We hope that the performed simulations can be useful not only for a better understanding of laser interactions with samples containing nanoparticles but also for the optimization of the experimental conditions.

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