

Numerical Simulation of Laser Interactions with Surfaces and Nanoparticles

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Laser interactions with surfaces and nanoparticles are widely used in numerous fields such as material analysis, nanoparticle formation, 3D laser manufacturing, surface and cancer treatment, etc. Lasers are also promising for tailoring the properties of nano-objects and, in particular, for the synthesis of alloys, core shells, or more complex multi-material nano-objects. Short and ultrashort pulsed laser interactions involve, furthermore, a set of non-linear electronic and ionic processes, phase transitions, mechanical effects, chemical reactions, etc. In addition, when nanoparticles are considered, aggregation, coalescence, or fragmentation play a role thus strongly affecting the optical properties of the resulting materials. In this talk, attention will be focused on multi-scale simulations relying on an interplay between many involved effects. Particularly, combined models were developed to account for laser propagation, energy absorption, local field enhancement, photo-induced free carrier generation, heat transfer, shock wave propagation, and phase transitions. Additionally, recent results of all-atomistic molecular dynamics simulations will be presented. The role of laser parameters and target materials are analyzed. Finally, the main conclusions and perspectives will be presented.