Modeling of nanoparticles formation process due to pulsed laser ablation in liquids

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Pulsed laser ablation in liquids (PLAL) has proven to be a powerful and efficient method of nanoparticles (NPs) generation for industrial and biomedical applications. However, due to a number of interrelated processes involved into the laser ablation phenomenon, the final characteristics of the resulting particles are difficult to control. Thus, one of the most important properties of the produced NPs such as their mean size and size distribution, depending on the irradiation parameters, frequently have a broad and multimodal distribution. In this work, we investigate the mechanism of NPs generation in liquids as a function of the pulse duration, the indecent fluence, and the irradiation regime (single-multi-pulse). For that purpose we applied the combined atomistic-continuum model to simulate ultrashort laser pulse interaction with gold sample under water layer confinement. The model described non-equilibrium laser-induced phase transitions at atomic level and accounts for the effect of free carriers in continuum. The simulation results are directly compared with the experimental data. The preformed study suggests the methodology for generation of NPs due to PLAL with predesigned morphology, size, and size distribution demanded in biomedical applications.Research carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation (project No. 075-15-2021-1347).