Theoretical Investigation of Nanostructuring Processes on Metals due to Short Laser Pulses in Liquid Media

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The physical mechanisms of materials surface restructuring in air/vacuum and liquids involves a lot of fast, non-equilibrium, and interrelated processes while the solid is in a transient state. Although the experimental investigation of the material restructuring mechanism can be limited to post-priory observations, the theoretical methods, on the other hand, working within a single computational approach with corresponding spatial and temporal scales, cannot address all physical aspects of the nanostructuring process. In this work we propose and utilize the combined atomistic-continuum approach suitable for the investigation of metallic materials restructuring mechanism due to a short laser pulse on the experimental scale. The combined model is applied to investigate the periodic UV nanopatterning process under conditions of vacuum ambient and in the regime of spatial confinement due to a thick water layer above the target. The obtained results, generated on the same temporal and spatial scales as they are in the experiment, allowed to extract the main mechanisms of nanostructuring process and the reasons for a higher quality of structures generated under water. The applied approach is extended for investigation of LIPPS structures formation and nanoparticles generation in liquids.