Theoretical Modeling of High Power Electromagnetic Waves Interacting with Plasmonic Materials and Nanostructures

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We demonstrate accurate and efficient multiphysics theoretical modeling of high power electromagnetic waves generated by ultrafast laser pulses interacting with metallic materials and nanostructures exhibiting plasmonic responses in the visible and infrared frequencies. The presented full wave simulations are performed in time domain by using a finite element method multiphysics approach. More specifically, we combine electromagnetic and heat transfer simulations to accurately compute the induced heat in nanoscale and macroscale regions of metallic (plasmonic) surfaces and nanostructures. We also investigate complicated fluid dynamic phenomena involved in the light-matter interactions occurring during the laser interaction process along the plasmonic interfaces. These include clarification of the material phase changes, as well as the role of recoil pressure and Marangoni effect to further elucidate the topology variation of metallic surfaces when illuminated by high power lasers. Furthermore, we accurately compute the electron and lattice temperature dynamics, which are key factors in understanding the short time decay and overall steady-state heat performance in plasmonic devices illuminated by ultrafast high power lasers. We fully describe the temperature dynamics of energetic ‘hot’ electrons and their transition into thermal carriers over their evolution from femtosecond to nanosecond time scales.

We apply our theoretical modeling calculations to two emerging plasmonic technologies: i) femtosecond laser surface processing (FLSP) of metals, and ii) gap-plasmon optical metamaterials. On one hand, the FLSP of metals has recently attracted increased scientific attention as an efficient, repeatable, economic, and fast fabrication of scalable omnidirectional ultrabroadband optical absorbers and hydrophobic surfaces. However, the thorough understanding of the complex formation dynamics of FLSP functionalized surfaces remains elusive and is performed based on our modeling efforts. On the other hand, gap-plasmon metamaterials are found to be one of the most efficient nanophotonic devices to generate energetic charge carriers, called ‘hot’ electrons and holes, owing to their ability to squeeze electromagnetic fields in extremely confined nanoscale regions. Nevertheless, the comprehension of the charge carrier dynamics in plasmonic devices is an arduous task due to their ultrafast time decay and tumultuous nonlinear behavior. Our theoretical model elucidates the generation mechanism of energetic charge carriers in these systems, which will be crucial for the design of new plasmonic devices used in photocatalysis and energy harvesting applications.