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Modeling of Laser Material Interactions

BARBARA GARRISON, Penn State University

Irradiation of a substrate by laser light initiates the complex chemical and physical process of ablation where large amounts of material are removed. Ablation has been successfully used in techniques such as nanolithography and LASIK surgery, however a fundamental understanding of the process is necessary in order to further optimize and develop applications. To accurately describe the ablation phenomenon, a model must take into account the multitude of events which occur when a laser irradiates a target including electronic excitation, bond cleavage, desorption of small molecules, ongoing chemical reactions, propagation of stress waves, and bulk ejection of material. A coarse grained molecular dynamics (MD) protocol with an embedded Monte Carlo (MC) scheme has been developed which effectively addresses each of these events during the simulation. Using the simulation technique, thermal and chemical excitation channels are separately studied with a model polymethyl methacrylate system. The effects of the irradiation parameters and reaction pathways on the process dynamics are investigated. The mechanism of ablation for thermal processes is governed by a critical number of bond breaks following the deposition of energy. For the case where an absorbed photon directly causes a bond scission, ablation occurs following the rapid chemical decomposition of material. The study provides insight into the influence of thermal and chemical processes in polymethyl methacrylate and facilitates greater understanding of the complex nature of polymer ablation.