Multiscale modeling of laser ablation: applications to nanotechnology

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Abstract

Computational modeling has a potential of making an important contribution to the advancement of laser-driven methods in nanotechnology. In this presentation a multiscale model for simulation of laser ablation and cluster deposition of nanostructured materials is discussed. A hierarchy of computational methods used to simulate different processes involved in laser ablation and film growth by cluster deposition is schematically illustrated in Figure 1. In the multiscale model the initial stage of laser ablation is reproduced by the classical molecular dynamics (MD) method. Two computational schemes have been developed for simulation of laser coupling to organic materials and metals. For organic materials, the breathing sphere model is used to simulate the primary laser excitations and the vibrational relaxation of excited molecules. For metals, the two temperature model coupled to the atomistic MD model provides an adequate description of the laser energy absorption into the electronic system and fast electron heat conduction. A combined MD - finite element method or the dynamic boundary condition is used to avoid reflection of the laser-induced pressure wave from the boundary of the MD computational cell. The direct simulation Monte Carlo method is used for simulation of the long term ablation plume expansion, and the MD method is used to simulate film growth by cluster deposition from the ablation plume. The proposed multiscale approach is applied to investigate the mechanisms of cluster formation in laser ablation, Figure 2, and to analyze the distributions of clusters of different sizes in the ejected plume. MD simulations of cluster deposition are performed for different impact velocities and a strong dependence of the structure of the growing films on the parameters of the deposited clusters is revealed. A new technique for controlled implantation of functional organic molecules into sub-micron regions of a polymer substrate is investigated in molecular-level simulations, Figure 3, and different regimes of molecular transfer are discussed.

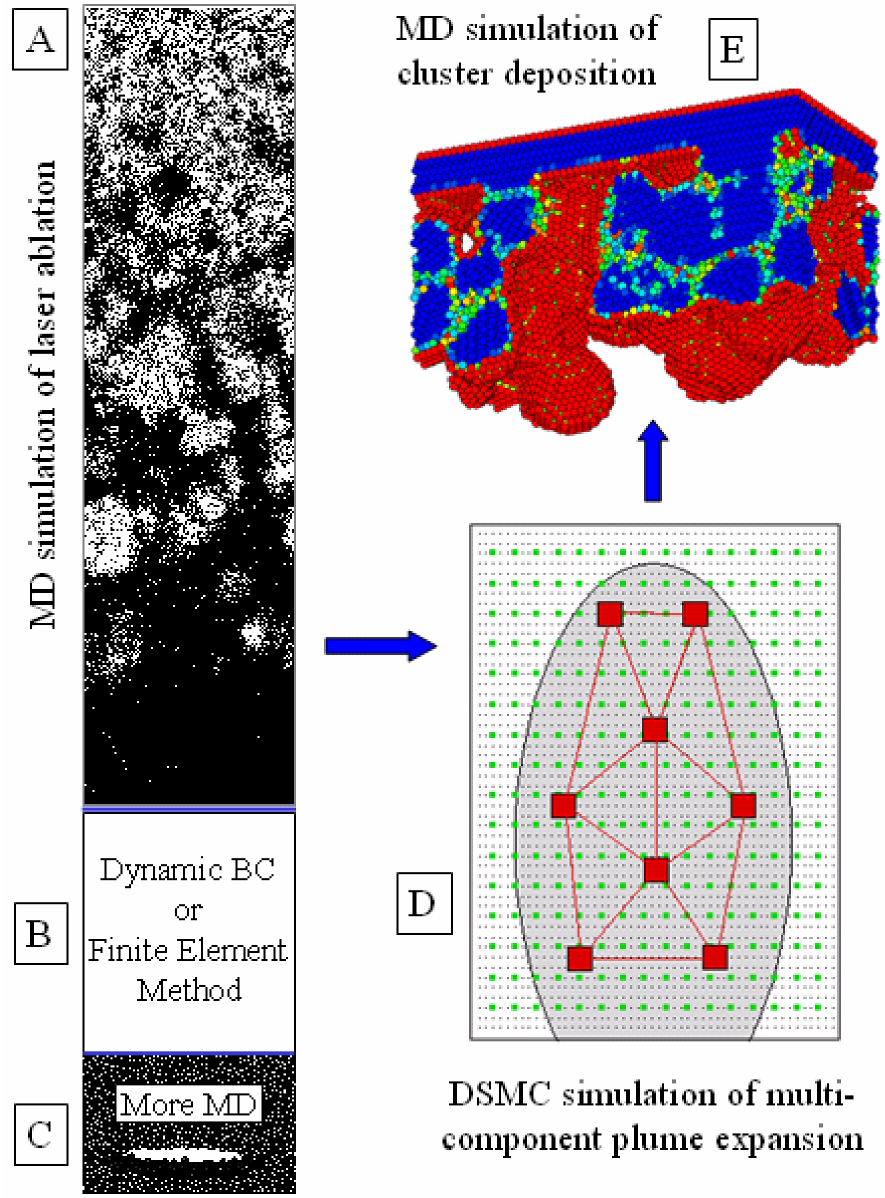

Figure 1. Schematic representation of the hierarchy of computational methods that can be used to study formation of clusters in laser ablation and film growth by cluster deposition.

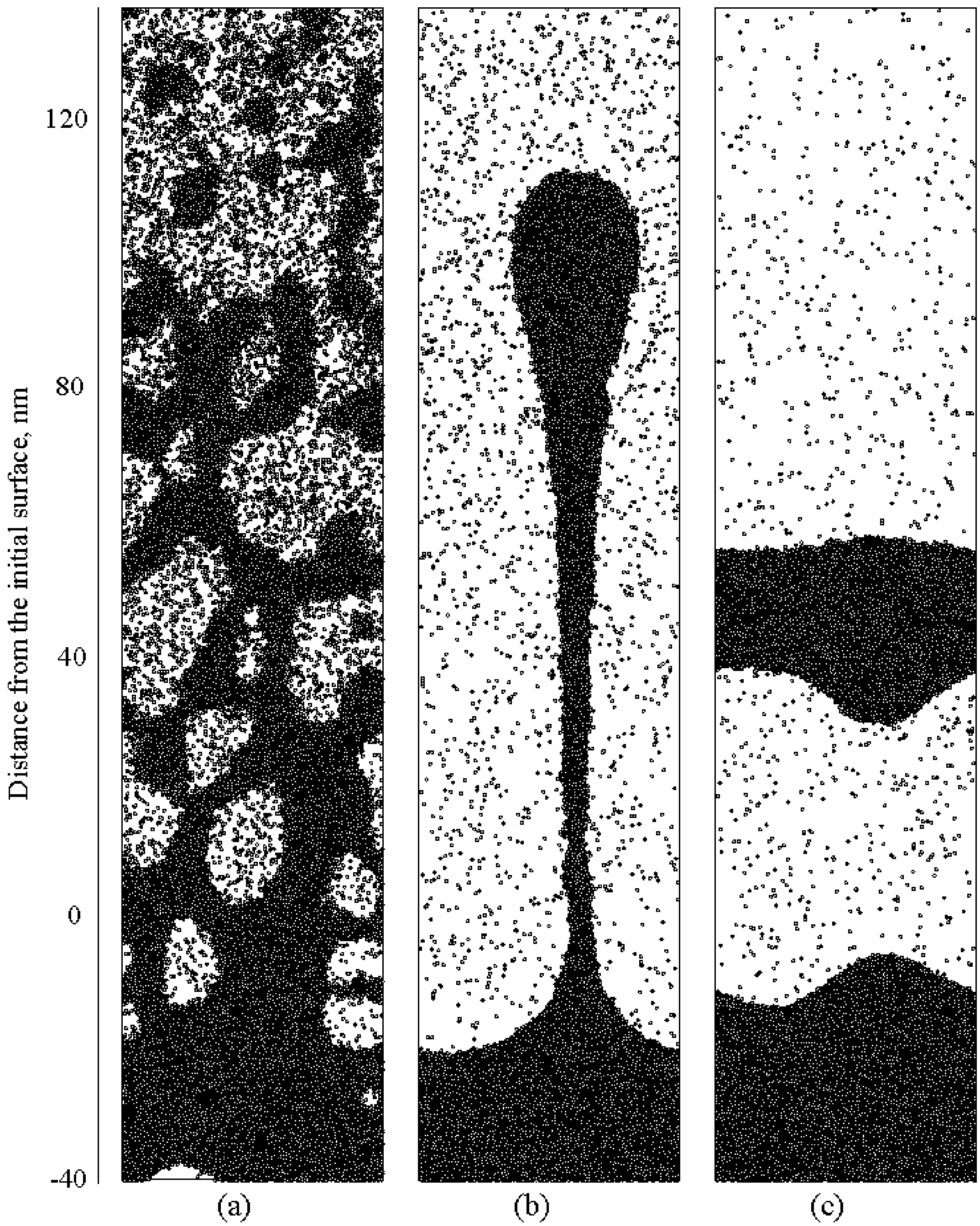

Figure 2. Generation of nanoparticles in laser ablation. Snapshots from MD simulations of laser ablation of a molecular solid illustrating different mechanisms of cluster ejection are shown: (a) phase explosion of the overheated material; (b) hydrodynamic sputtering due to a transient melting and motion of the liquid in the surface region; (c) photomechanical spallation of the surface layer caused by the relaxation of laser-induced thermoelastic stresses.

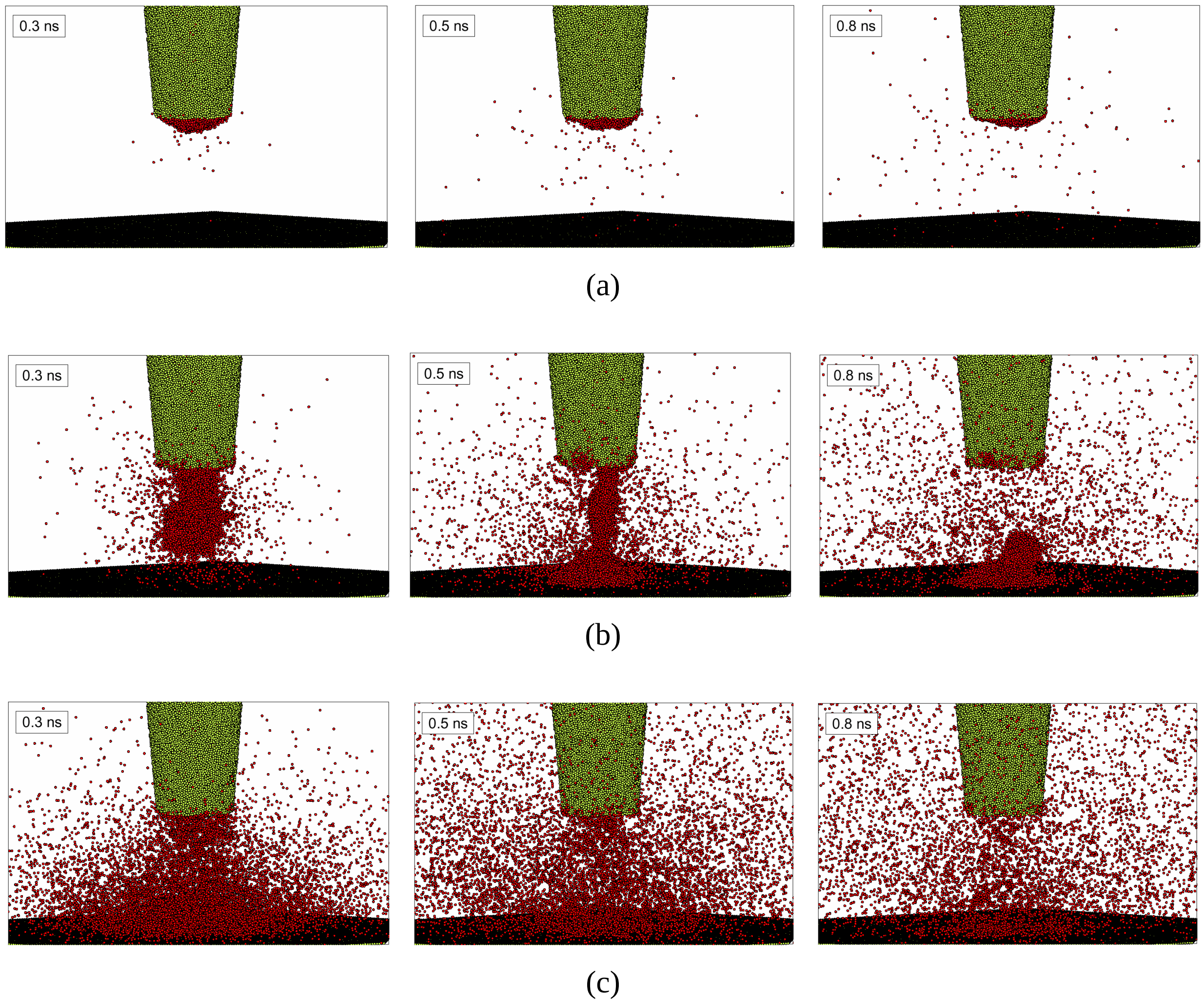

Figure 3. Molecular implantation/deposition by nano-jet ejection from a micropipette. Snapshots from MD simulations of molecular ejection from an irradiated pipette tip are shown. The laser pulse duration is 100 ps, the energy density deposited by the laser pulse are (a) 0.2 eV/molecule, (b) 0.4 eV/molecule, (c) 0.8 eV/molecule.

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