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Microscopic simulation of laser ablation and damage of organic and bio-organic materials

(as an example of multiscale computational approach to modeling of complex systems)

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General description of the multiscale computational approach

The behavior of biological systems is defined by a complex interplay of processes occurring at different time and length scales. The main obstacle for an efficient application of computational methods to biological systems is the lack of connections between the different levels of description. There is a gap between the two well-established computational methods, molecular dynamics (MD) simulation technique that provides information at microscopic/atomic level and continuum finite element method (FEM) approach that gives a macroscopic description.

A combined MD-FEM approach can be a solution in cases where a detailed atomic-level analysis is necessary in localized spatially separated regions whereas continuum mechanics and thermodynamics is sufficient in the remainder of the system.

The main computational challenge, however, is presented by the processes that occur at different length scales, but are inherently coupled and should be considered simultaneously. In these cases an innovative development of original computational models for dynamic simulation at mesoscopic length and time scales is necessary. Mesoscopic models should provide a coarse-grained description of the dynamics, but at the same time should incorporate the essential physics from the finer (atomic) level. Development of the coarse-grained mesoscopic description of the material dynamics and properties would include

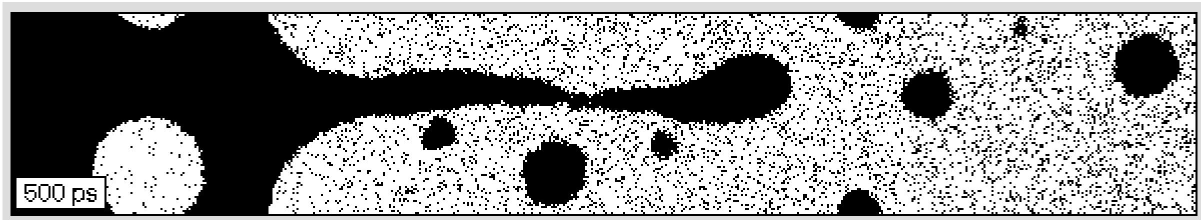
1. identifying the relevant collective degrees of freedom for the phenomenon under study,
2. deriving the set of rules governing the mesoscopic dynamics of the collective degrees of freedom from the simulations at the atomic level,

Mesoscopic simulations can serve as a bridge between the atomistic and continuum descriptions, can provide interpretation of the micro- and mesoscopic-level mechanisms and processes in terms of macroscopic material behavior and can lead to the development of the analytical description of the phenomenon.

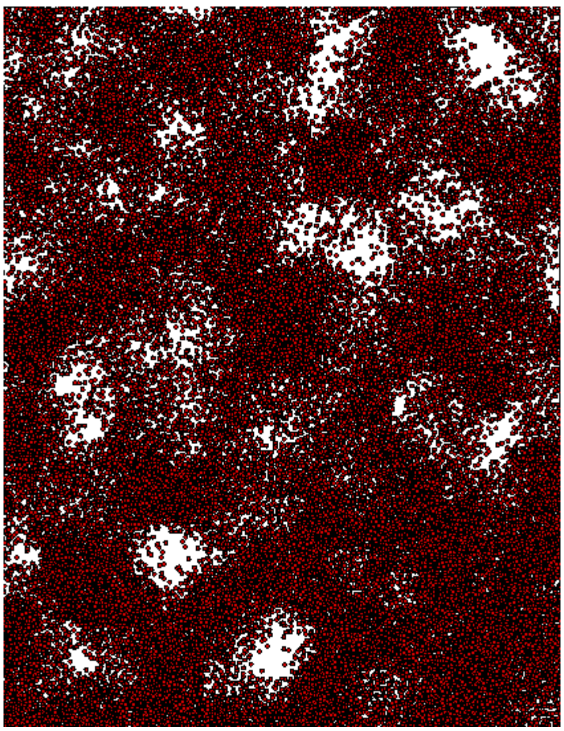
Examples of mesoscopic models include dislocation dynamics for simulation of early stages of plastic deformation, dissipative particle dynamics for hydrodynamics of complex fluids, Potts model for microstructure development in polycrystalline materials, and the breathing sphere model for simulation of laser-induced processes in organic materials that is discussed below.

Mesoscopic breathing sphere model for laser ablation of organic materials

The interaction of laser pulses with organic matter leading to massive material removal (ablation) from a target is a subject of scientific as well as applied interest. Important practical applications include laser surgery, matrix-assisted laser desorption/ionization (MALDI) of biomolecules for mass - spectrometric investigations and surface microfabrication of polymer thin films.

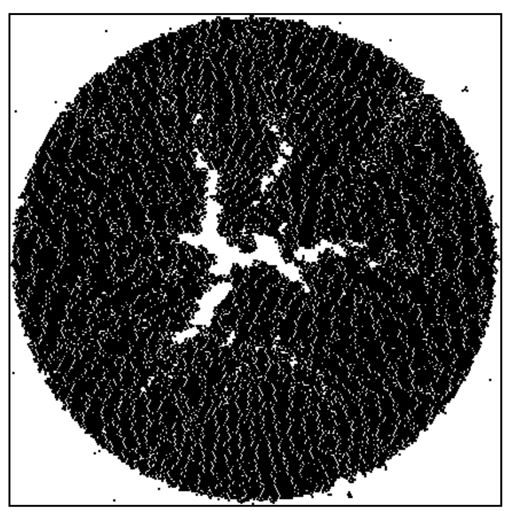


Laser ablation of organic solids is a complex collective phenomenon that includes processes occurring at different length and time scales. The complex character of the involved intertwined processes hinders an adequate analytical formulation for a continuum description of the phenomenon whereas a collective character of the laser ablation occurring at the mesoscopic rather than molecular scale does not permit a direct application of the atomistic simulation approach.



An alternative mesoscopic model has been developed recently for molecular dynamics simulation of laser ablation and damage of organic solids. The model has advantage of both addressing the effects of laser irradiation at a submicron resolution and yet incorporating a realistic description of energy relaxation of individual molecules internally excited by photon absorption.

A series of large-scale simulations are performed to study the laser fluence dependence of the ablation mechanisms. The controversy associated with the threshold behavior is addressed. The dependence of the mechanisms of laser ablation and parameters of the ejection process on irradiation conditions is discussed and related to existing theoretical models for laser desorption/ablation and experimental data. In particular, the yield of monomers and velocity distributions of ejected molecules is related to mass spectrometry experimental data, the profiles of the acoustic waves to piezoelectric measurements, and the cluster ejection to trapping plate experiments.



Mechanisms of laser damage in the case of spatially localized absorbers embedded into a transparent medium are studied and related to the experimental observations for pigmented tissues where the laser energy is absorbed within submicron granules of the biological pigment melanin. We find that mechanical intragranular fracturing due to the focusing of the tensile stresses in the central part of the absorbing granules is responsible for low energy threshold for laser damage observed for sub-nanosecond pulses.

More information on the project can be found at http://www.people.virginia.edu/~lz2n/Ablation.html.