MM 5: Nanostructured Materials II

Time: Monday 12:00–13:00 Location: H 0107

MM 5.1 Mon 12:00 H 0107

Laser-induced nanotube-nanotube interactions — •Jessica Walkenhorst[1], Martin E. Garcia[1], and Harald O. Jeschke[2] — [1]Theoretische Physik, Fachbereich Naturwissenschaften, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel — [2]Institut für theoretische Physik, Universität Frankfurt, Robert-Mayer-Str. 8-10, 60054 Frankfurt, Germany

We have investigated the possibility of achieving welding of two single wall nanotubes by making use of topological defects and femtosecond laser excitation. Based on molecular dynamics simulations performed on time-dependent potential energy surfaces, and considering explicitly the shape, energy and duration of the laser pulse, we describe the ultrafast dynamics of two defective nanotubes in contact to each other immediately after femtosecond excitation. We discuss the role of different defects and their respective behaviour under laser heating.

MM 5.2 Mon 12:15 H 0107

Breaking transition of carbon nanotubes and graphene under stress — •Juergen Dietel and Hagen Kleinert — Institut fuer Theoretische Physik, Freie Universitaet Berlin

We calculate the breaking transition of carbon nanotubes and graphene under homogeneous external stress as a function of temperature.

MM 5.3 Mon 12:30 H 0107

Modeling of Surface Modification and Nanostructuring on Metals due to a Femtosecond Laser Pulse — •Dmitriy Ivanov[1], Baerbel Rethfeld[1], Gerard O'Connor[2], Thomas Glynn[2], Zhibin Lin[3], and Leonid Zhigilei[3] — [1]Physics Department, Technical University of Kaiserslautern, Kaiserslautern, Germany — [2]National Centre for Laser Applications, National University of Ireland Galway, Galway, Ireland — [3]Materials Science Department, Univeristy of Virginia, Charlottesville, USA

The atomistic-continuum approach to study nanostructuring processes on metals due to fast laser energy deposition is presented. The intense, short-pulsed laser interactions are involving mechanical, thermal, and phase perturbations. Many of those non-equilibrium processes are impossible to study experimentally and difficult to model at all levels: abinitio, atomistic, and continuum. We address this challenge combining the advantages of different approaches. Namely, the kinetics of fast non equilibrium phase transformations is treated at atomic level; and free carrier dynamics (fast electron heat conduction and laser-induced electron-phonon nonequilibrium)is accounted for in continuum part.

The combined model was applied to study the formation of nanojets on thin Ni films in femtosecond laser pulse experiments. The calculations show that surface nanostructuring is due to the interplay of three processes: establishment of temperature gradient in radial directions causes the elasto-plastic deformations; relaxation of laser-induced pressure leads to the ejection of melted material; fast electron heat conduction in 3D effectively cools down and freezes the ejected matter.

MM 5.4 Mon 12:45 H 0107

Molecular Dynamics Simulations of Nanoglasses — •Daniel Sopu[1], Karsten Albe[1], and Herberg Gleiter[2] — [1]Institut f. Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt — [2]Inst. f. Nanotechnologie, FZ Karlsruhe, D-76021 Karlsruhe

We present molecular dynamics simulations on the structure and stability of nanoglasses that can be generated by consolidating nanometer-sized glassy spheres at high pressures (several GPa). Our results suggest that nanoglasses consist in the as prepared state of glassy regions resulting from the consolidated spheres and interfaces between these glassy regions. In these glass/glass interfaces, the free volume is enhanced and the nearest neighbor co-ordinations deviate from the ones in the glassy regions. If these nanoglasses are annealed, the enhanced free volume in the glass/glass interfaces delocalize and, thus, modifies the atomic structure of the entire material. In conclusion, nanoglasses may pave the way to tune the free volume (density) of glasses at constant chemical composition.