Simulations of irradiation-induced effects in carbon nanostructures

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The irradiation of solids with energetic particles such as electrons or ions is associated with disorder, normally an undesirable phenomenon. However, recent experiments on bombardment of carbon nanostructures with energetic particles demonstrate that irradiation can have beneficial effects and that electron or ion beams may serve as tools to change the morphology and tailor mechanical, electronic and even magnetic properties of nanostructured carbon systems, and first of all, carbon nanotubes.

We systematically study irradiation effects [1] in carbon nanotubes and other forms of nano-structured carbon. By employing various atomistic models ranging from empirical potentials to time-dependent density functional theory [2] we simulate collisions of energetic particles with carbon nanostructures, and calculate the properties of the irradiated systems.

In my presentation, I briefly review the recent progress in our understanding of ion-irradiation-induced phenomena in nano-structured carbon and compare the simulation results to the experimental data. I dwell on the application of density functional theory to simulations of production of defects under irradiation, their properties and the "beneficial" role of defects and impurities in carbon nanotubes and related systems. I will also point out the issues which still lack complete comprehension and further outline the simulation challenges in the field.

Finally, I will present the results of simulations of irradiation-induced pressure build-up inside nanotubes encapsulated with metals [3]. Electron irradiation of such composite systems in the transmission electron microscope gives rise to contraction of nanotube shells and thus to pressure in the encapsulate.As recently shown [3], irradiation-stimulated pressure can be as high as pressure up to 40 GPa, which makes it possible to study phase transformations at the nanoscale with high spatial resolution.

[1] See our publications listed at http://www.acclab.helsinki.fi/~akrashen/publist.html

[2] A.V Krasheninnikov, Y. Miyamoto, and D. Tomanek, Phys. Rev. Lett., 99 (2007) in press.

[3] L. Sun, F. Banhart, A.V Krasheninnikov, J.A. Rodriguez-Manzo, M. Terrones, and P.M. Ajayan, Science 312 (2006) 1199.