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Irradiation-induced phenomena in carbon nanomaterials

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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 [for an overview, see A.V Krasheninnikov, F. Banhart, Nature Materials, 6 (2007) 723] 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. We systematically study irradiation effects in carbon nanotubes and other forms of nano-structured carbon experimentally and theoretically by employing various atomistic models ranging from empirical potentials to time-dependent density functional theory. In my presentation, I will briefly review the recent progress in our understanding of ion-irradiation-induced phenomena in nano-structured carbon and present our recent theoretical [A.V Krasheninnikov, et al., Phys. Rev. Lett., 99 (2007) 016104, A. Tolvanen et al, Appl. Phys. Lett. 91 (2007) 173109.] and experimental [O. Lehtinen et al., to be published] results. I dwell on the "beneficial" role of defects and impurities in nanotubes and related systems. Finally, I will present the results of simulations of irradiation-induced pressure build-up inside nanotubes encapsulated with metals [L. Sun, et al., Science 312 (2006) 1199]. Electron irradiation of such composite systems in the transmission electron microscope gives rise to contraction of nanotube shells and thus to high pressure. The irradiation-stimulated pressure can be as high as 40 GPa, which makes it possible to study phase transformations at the nanoscale with high spatial resolution. I will also address the mechanisms of plastic deformation of small metal particles inside carbon shells at high temperatures, which may be important for understanding catalytic growth of carbon nanotubes.