

Invited talk - Saturday, June 20

Simulations of irradiation-induced effects in carbon nanomaterials

Arkady V. Krasheninnikov

Helsinki University of Technology

Contact e-mail: *akrashen@acclab.helsinki.fi*

The irradiation of solids with energetic particles such as electrons or ions is associated with disorder, normally an undesirable phenomenon. However, recent experiments [1] 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. Irradiation also gives rise to many interesting phenomena such as irradiation-induced pressure build-up inside carbon nanotubes [3] and onions [4] encapsulated with metals.

We systematically study irradiation effects 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 we simulate collisions of energetic particles with carbon nanostructures, and calculate the properties of the irradiated systems.

In this presentation, our latest results on the defect-mediated engineering of the electronic structure of carbon nanotubes [4] will be presented. I will also address the interaction of transition metal atoms with pristine and defected graphene sheets [5]. I will discuss the electronic structure of defected graphene sheets with adsorbed transition metal atoms and identify possible avenues for tailoring the electronic and magnetic structure of graphene by irradiation-induced defects and metal atoms. Finally I will touch upon the response to irradiation of mechanically strained carbon nanotubes and some other low-dimensional systems.

[1] For an overview, see A.V Krasheninnikov, F. Banhart, *Nature Materials*, 6 (2007) 723.

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

[3] L. Sun, A.V. Krasheninnikov, T. Ahlgren, K. Nordlund, and F. Banhart, *Phys. Rev. Lett.*, 101 (2008) 156101.

[4] A. Tolvanen, G. Buchs, P. Ruffieux, P. Groning, O. Groning, and A.V. Krasheninnikov, *Phys. Rev. B* 79 (2009) 125430.

[5] A. V. Krasheninnikov, P.O. Lehtinen, A.S. Foster, P. Pyykko, and R. M. Nieminen, Phys. Rev. Lett. 102 (2009) 126807.