V ABILO

Vljudno vabljeni na predavanje:

Prof. Baidurya Bhattacharya
Indian Institute of Technology Kharagpur

ATOMISTIC MODELING OF FRACTURE

Povzetek:

While classical fracture mechanics is based on continuum assumptions, atomistic simulations provide a first-principles based description of fracture that accounts for the discrete nature of matter. The idea of atomistic simulation was first applied to fracture during the early 1970’s; brittle fracture was studied first using simple potential models and equilibrium conditions. Advances in materials science and computational power have led to significant progress in AS of fracture. Since the early 1990’s, complex phenomena such as ductile fracture, fracture of non-homogeneous materials, fracture interaction with other physical and chemical effects have increasingly been investigated by atomistic simulation. This talk discusses achievements and shortcomings in regard to fracture criteria, potential models, initial and boundary conditions, temperature control and multi-scale simulation. An atomistic simulation of the displacement-controlled fracture process of a single-walled carbon nanotube (SWNT) is given as an example highlighting the essential steps of the methodology.

Predavanje bo:

v četrtek, dne 20. januarja 2011 ob 16:00 v svečani dvorani FGG, Jamova 2.

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prof. dr. Matej Fischinger, l.r.