Irradiation-Induced Superplasticity of Graphene and Carbon Nanotubes

ZHUHUA ZHANG, YU LIN, Department of Materials Science and Nanoengineering, and the Smalley Institute for Nanoscale Science and Technology, Rice University, Houston, TX 7700, FENG DING, Institute of Textiles and Clothing, Hong Kong Polytechnic University, Kowloon, Hong Kong, Peoples Republic of China, BORIS I. YAKOBSON, Department of Materials Science and Nanoengineering, and the Smalley Institute for Nanoscale Science — The superplasticity of carbon nanotubes has been related to the dynamics of pentagon-heptagon (5/7) dislocations, but the mechanism remains elusive in light of prohibitively high barrier (~ 7 eV) of dislocation migration [1,2]. Here, we reveal the key role of electron irradiation in facilitating the dislocation migration and promoting nanotube plasticity. Atomistic simulations show that irradiation-induced adatoms and monovacancies diffuse towards the sessile 5/7 dislocations and switch them into a mobile radical state with a migration barrier as low as 1.6 eV, thereby significantly enhancing the plastic flow. The radical dislocations also act as defect scavengers to prevent lattice disorder in the tube wall, in agreement with experimental phenomena. Further, a formula is derived to quantify the plasticity in terms of irradiation intensity, aimed to guide the irradiation engineering of plasticity of carbon nanomaterials.


Zhuhua Zhang
Dept of Materials Science and Nanoengineering, and the Smalley Institute for Nanoscale Science and Technology, Rice University, Houston, TX 7700

Date submitted: 14 Nov 2014