Mechanism for Superelongation of Carbon Nanotubes at High Temperature\textsuperscript{1} CHUN TANG, Department of Physics & High Pressure Center, University of Nevada, Las Vegas, WANLIN GUO, Institute of Nano Science, Nanjing University of Aeronautics & Astronautics, CHANGFENG CHEN, Department of Physics & High Pressure Center, University of Nevada, Las Vegas — Recent discovery of superelongation of carbon nanotubes (CNTs) at high temperature raises fundamental questions about the deformation mechanism of these normally brittle materials. Here we report extensive molecular dynamics simulations that identify two key factors for this intriguing phenomenon: (1) activation of defects all over the tube at the elastic limit and continued emergence of additional defects at increasing strain that impede the formation of localized predominant instability and facilitate homogeneous deformation; (2) large-scale defect evolution that produces multistage necking and kink motion. Intricate interplay between CNT sizes and temperature activated defect nucleation and motion plays a key role in determining the overall deformation pattern.

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