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Nanosurgery in Carbon Nanotubes: Efficient Elimination of Pentagon-Heptagon Defects Using Femtosecond Laser Pulses MARTIN GARCIA, Institute of Physics, Universitaet Kassel, Germany, ALDO ROMERO, FELIPE VALENCIA, MAURICIO TERRONES, HUMBERTO TERRONES, Advanced Materials Department, IPICYT, SLP, Mexico, HARALD JESCHKE, Department of Physics, Johann Wolfgang — Using non-adiabatic molecular dynamics simulations we demonstrate that femtosecond laser pulses are able to eliminate pentagon-heptagon defects within carbon nanotubes. We conclude that ultrafast healing of zig-zag and armchair nanotubes can be achieved with pulse durations of 50 fs within a wide range of laser intensities. This nonthermal transition occurs at a relatively low lattice temperature (∼450 K) and is driven by the electronic entropy, which is dramatically increased by the action of the laser pulse, thus causing 5-7-5-7 defects to become unstable at very high electronic temperatures. The intermediate steps of the inverse Stone-Wales-type transformation are qualitatively different from those occurring in thermally driven phenomena.

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