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Stability and mechanical properties of partially unzipped carbon nanotubes[1] CHUN TANG, Department of Physics & High Pressure Science and Engineering Center, University of Nevada, Las Vegas, WANLIN GUO, Institute of Nano Science, Nanjing University of Aeronautics & Astronautics, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada Las Vegas — We have explored the stability and mechanical properties of partially unzipped carbon nanotubes using molecular dynamics simulations. Our results show that due to the presence of dangling bonds created by the unzipping process, the unzipped graphene ribbon region becomes unstable with increasing temperature. The dangling bonds can seamlessly self-heal to form nanotube structure at sufficiently high temperatures. These results suggest that temperature treatment that passivates the dangling bonds could be a useful tool in tailoring these nanoscale structures in nanoelectronic applications. Tensile tests show that the partially unzipped structure has a Young's modulus of 700 GPa, comparable to that of SWCNTs and graphene nanoribbons. Size and chirality effects are also discussed.

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