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Thermal activation of interlayer bonding and its effect on properties of multiwalled carbon nanotubes¹ 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 Science and Engineering Center, University of Nevada Las Vegas — We report molecular dynamics simulations of multiwalled carbon nanotubes (MWCNTs) at high temperatures. Our results show that thermally activated interlayer bonding have significant influence on structural, mechanical and electronic properties of MWCNTs and lead to new behaviors with implications for their applications. We examine the effect of strain and temperature conditions on the formation of interlayer bonding in MWCNTs and unveil the underlying atomistic mechanisms.

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