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Substantial reduction of thermal conductivity of defected carbon nanotubes CEM SEVIK, Artie McFerrin Dept of Chemical Engineering, Laboratory of Computational Engineering of Nanomaterials Texas A&M University, College Station, TX , HALDUN SEVINCLI, Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany, JUSTIN B. HASKIN, ALPER KINACI, Artie McFerrin Dept of Chemical Engineering, Laboratory of Computational Engineering of Nanomaterials Texas A&M University, College Station, TX , GIANAURELIO CUNIBERTI, Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany, TAHIR CAGIN, Artie McFerrin Dept of Chemical Engineering, Laboratory of Computational Engineering of Nanomaterials Texas A&M University, College Station, TX , TEXAS A&M UNIVERSITY TEAM, DRESDEN UNIVERSITY OF TECHNOLOGY TEAM — The influence of the structural details and defects on the thermal transport properties of carbon nanotubes (CNTs) are explored by molecular dynamics and real-space Kubo methodologies. A variety of randomly oriented and distributed defects, (mono- and di-vacancies, Stone Wales defects) on lattice thermal conductivity and anharmonic phonon mean free paths are studied for model systems in sizes up to 1000 nm. Substantial reduction in thermal conductivity, up to $\sim$80% reduction compared to the pristine CNTs, is observed for $\sim$0.5\% defect concentrations. Additionally, nearly the same saturation value of lattice thermal conductivity for CNTs with different type of defects is predicted.

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