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Mechanical properties of metal-repaired defective carbon nanotubes GUANGPING ZHENG, Hong Kong Polytechnic University, Kowloon, Hong Kong — Carbon nanotubes (CNs) are promising in the producing of strong and light structural materials because of their unique mechanical properties such as ultrahigh mechanical strength and large ultimate tensile strain. However, CNs are not defect free. Instead, several types of intrinsic defects exist, hence the mechanical strength and ductility of CN can be significantly lower than those of an ideal one. In this study, 3d transition-metal atoms (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn) or clusters are filled into the defective sites of single-walled (SW) CN containing vacancy defects, resulting in stable repaired SWCN. The mechanical and electronic properties of the repaired SWCNs are investigated by spin-polarized density functional theory. The results indicate that the 3d transition-metal atoms acting as substitutional defects can substantially modify the electronic structure and magnetization of an un-deformed CN. Compared with defective SWCN, the metal-repaired CN shows significant enhancements in mechanical strength and ductility that are close to or even better than those of pristine CNs. The underlying physics of these behaviors are analyzed by the structural transformation, electronic structures and spin and charge distributions during the tensile tests. Strong magneto-mechanical coupling effect is found to be responsible for the enhanced mechanical behaviors of metal-CN hybrid structures.

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