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The effect of carbon vacancies on the electrical conductance of carbon nanotubes ALEX TAEKYUNG LEE, Department of Physics, KAIST, YONG-JU KANG, Samsung Elec. Co. Korea , KEE JOO CHANG, Department of Physics, KAIST, THEORETICAL CONDENSDED MATTER PHYSICS GROUP TEAM — Defects such as carbon vacancy strongly affect the electronic properties of graphene and carbon nanotubes. It is known that divacancies are one of the most common defects generated under ion irradiation. Based on first-principles matrix Green's function calculations, we study the effect of various carbon vacancies on the electrical conductance of (5,5) and (9,0) carbon nanotubes. For vacancy clusters V_n ($n \leq 4$), where n is the number of missing atoms, conductance generally decreases due to the formation of topological defects. When vacancies are randomly distributed, resistances exhibit the localization behavior. The localization lengths are found to be smaller for vacancies with n = even integer due to scattering by the 7- or 8-membered ring. This length is also reduced in the zigzag tube as defect levels lie closer to the Fermi point, as compared to the armchair tube. For large vacancy clusters with $n \geq 5$, the electrical conductance is mainly affected by the local gap opening induced by the tube shrinkage. The overall behavior of electrical conductance in zigzag tubes is similar to that of armchair tubes.

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