# Molecular Dynamics analysis on crack initiation and extension of defective single walled carbon nanotube

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By employing molecular dynamic (MD) simulations based on COMPASS potential, we simulate a series of tensile tests of defect-free and defective single-walled carbon nanotubes (SWNTs). Young's modulus and linear stress-distance curves of defect-free SWNTs with different chirality have been calculated by our MD models. By monitoring the stress distribution on the SWNTs, we find out tensile stress concentration on vacancy-related defects cause cracks initiation and extension on SWNT under tensile loading. A new method of MD simulating crack propagation on the surface of SWNT based on a maximum stress criterion is proposed and applied. The results show that the convert from vacancyrelated defect to a circumferential penetrating crack is continuous and spontaneous under tensile loading. Tensile strengths of SWNTs with different defects are predicted and some deleterious defects have been identified. The effect of vacancy-related defects' characteristics on the SWNT strength is analyzed.

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## Figures

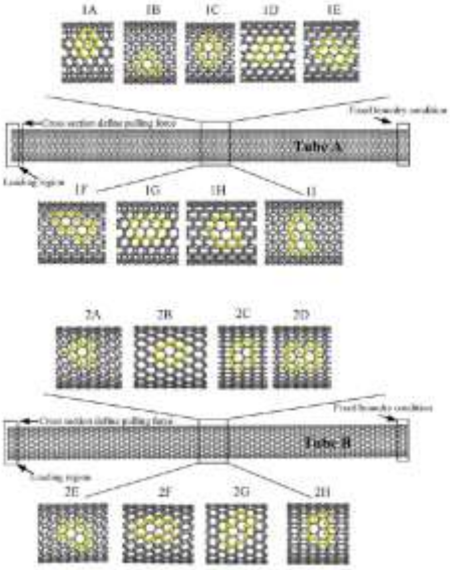

Figure 1 SWNT Defects

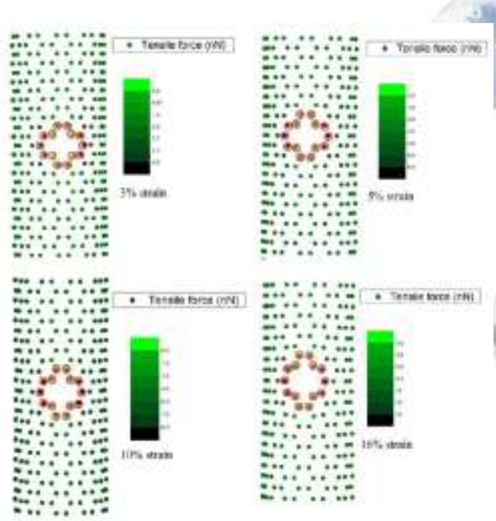

Figure 2 Tensile stress distributions on a two-atom vacancy (1C) and stress concentration on vacancy defect edge

Figure 3 Crack propagation of the vacancy (1C) defect SWMT induced by tensile stress concentration

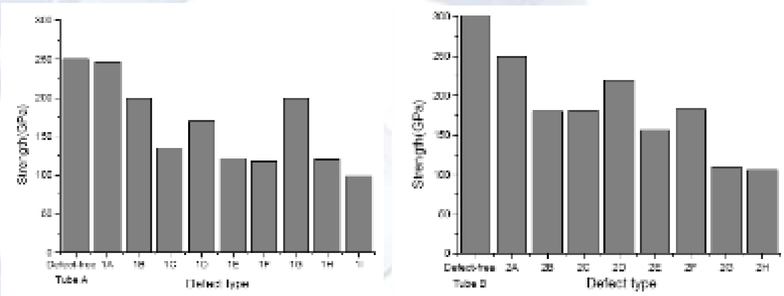

Figure 4 Tensile stresses of defect-free and defective SWNTs

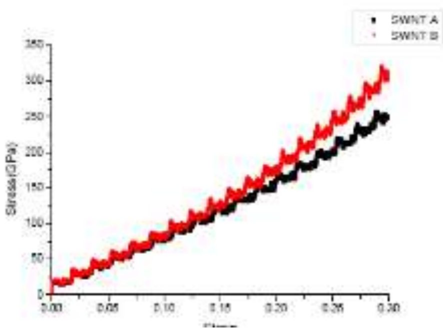

Figure 5 Stress-strain curves