

Joint CQSE and CASTS Seminar

Weekly Seminar
Mar. 15, 2013 (Friday)

TIME Mar. 15, 14:30 ~ 15:30
TITLE Investigations on the Thermo-physical Characteristics of Carbon Nanomaterials
SPEAKER Dr. Jian-Ming Lu
National Center for High Performance Computing
PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

Using both the molecular dynamics simulation method with the Tersoff potential and the concept of the thermal noise, which is based on nanostructure's characteristics, the Young's modulus of a single- and multi-walled carbon nanotube is performed under thermal-mechanical loadings. Moreover, buckling patterns and buckling strains of a single- and multi-walled carbon nanotube and the effect from fixed boundary layers are investigated. As for graphene, which is one of the hottest topic in academic research still now, is also performed. The graphene with and without defect loaded by two-sides external tension is performed. The tensile fracture damage undergoes four stages such as defects initiation, bonds breaking and defects growth, crack propagation, and ultimate catastrophic failure. In this talk, the thermo-physical characteristics of both carbon nanotube and graphene will be discussed and concluded.

Keywords: molecular dynamics, Young's modulus, buckling, tensile fracture, thermo-physical

