DeMEASS IV
March 27–30th, 2011,
Chateau dUrspelt, Luxembourg

Use of Molecular Dynamic Analysis to Build Accurate Structural Models for CNTs

C. Campisi, S. Brischetto, E. Carrera, M. Cinefra, E. Zappino
Department of Aeronautics and Space Engineering, Politecnico di Torino,
M.A. Deriu,
Department of Mechanics, Politecnico di Torino,
Torino, Italy

February 2, 2011

Nanotechnology and nanosciences are the keywords of what is likely to become one of the major scientific and technological revolutions of the 21st century. Working with atomic or near-atomic precision, various breakthroughs have already been achieved, but drastically more are still expected to come. In this work, we present two approach of molecular mechanics models to studies the mechanical and vibrational properties of single-walled carbon nanotubes. The mechanical properties of single walled CNTs are investigated via free vibration normal modes using with two computer code, Gromacs and Tinker. Normal mode calculations for single walled carbon nanotubes were presented based on the time averaged Hessians. The vibrational response of the single-walled carbon nanotubes, zigzag and arm-chair are investigated by numerical simulation method. We studied the change of the mechanical parameters to various lengths at 60, 100 toInfine abbiamo 210 nm are considered for each nanotube. The natural frequencies and their corresponding modes of deformation versus the change of the geometry are determined for the nanotubes. Geometry properties of CNT are in this table:

Type of CNT	(n,m)	n° Atoms	r	ρ	l
Zigzag	$(5,0)$	280	1.869	3.738	55.425
	$(10,0)$	1120	3.716	7.432	112.969
	$(16,0)$	2880	5.939	11.878	181.303
Armchair	$(5,5)$	840	3.222	6.444	97.043
	$(8,8)$	2144	5.146	10.292	155.261
	$(9,9)$	2700	5.787	11.574	173.879

Table 1: (Geometry of CNT).

Mechanical properties extrapolated by means of dynamic molecular analysis are used for carried out some analysis using the continuum mechanic approach. A higher order beam theory and a shell model, have been employed to represent the nanotube structure the results from dynamic molecular analysis have been compare with those from continuum mechanic With molecular dynamics we study the mechanical properties of single-walled carbon nanotubes (SWCNTs) with various radiuses under tensile, compressive loads are considered. Stress−strain curve, elastic modulus, tensile, compressive and pressure of different zigzag and armchair SWCNTs are investigated figure out the effect of radius and chirality on mechanical properties of nanotubes.

References

[1] S.S. Gupta, R.C. Batra, *Continuum structures equivalent in normal mode vibrations to single-walled carbon nanotubes*, Computational Materials Science 43 (2008) 715723

[2] Paras M. Agrawal, Bala S. Sudalayandi, Lionel M. Raff, Ranga Komanduri *A comparison of different methods of Youngs modulus determination for single-wall carbon nanotubes (SWCNT) using molecular dynamics (MD) simulations* Computational Materials Science 38 (2006) 271281.

[3] Yu.I. Prylutskyy, S.S. Durov, O.V. Ogloblya, E.V. Buzaneva, P. Schar *Molecular dynamics simulation of mechanical, vibrational and electronic properties of carbon nanotubes* Computational Materials Science 17 (2000) 352355.

[4] Berk Hess, David van der Spoel, and Erik Lindahl. *Gromacs: Groningen Machine for Chemical Simulations, USER MANUAL 4.5* 19912000: Department of Biophysical Chemistry, University of Groningen.

[5] Jay William Ponder. *Tinker: Software Tools for Molecular Design, USER MANUAL 4.2* Chemistry Department, University of New Mexico.