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Foundations of Nanotechnology

Volume 3
Mechanics of Carbon Nanotubes

Saeedeh Rafiei

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LIST OF ABBREVIATIONS

AACVD	Aerosol Assisted Chemical Vapor Deposition
AAO	Anodized Aluminum Oxide
ABC	Atomistic-Based Continuum
ACFs	Activated Carbon Fibers
ACs	Activated Carbons
AFM	Atomic-Force Microscope
APCVD	Atmospheric-Pressure Chemical Vapor Deposition
ASFEM	Atomic-Scale Finite Element Method
BCC	Body-Centered Cubic
BD	Brownian Dynamics
BOA	Born-Oppenheimer Approximation
CBR	Cauchy-Born Rule
C–C	Carbon–Carbon
CCVD	Catalytic Chemical Vapor Deposition
CG	Conjugate Gradient
CHC	Cahn–Hilliard–Cook
CNTs	Carbon Nanotubes
CRS	Compressed Row Storage
CVD	Chemical Vapor Deposition
DC-PECVD	Direct Current –PECVD
DFT	Density Functional Theory
DGEBA	Diglycidyl Ether of Bisphenol A
DMTA	Dynamic Mechanical Thermal Analyzer
DPD	Dissipative Particle Dynamics
ECBR	Exponential Cauchy-Born Rule
EDA	Electron-Donor-Acceptor
EMI	Electro Magnetic Induction
ERM	Effective Reinforcing Modulus
FCC	Face-Centered Cubic
FEM	Finite Element Method
FF	Force Field
FH	Ferrum–Hydrogen

GAC	Granular Activated Carbon
GDEs	Geodesic Differential Equations
GNFs	Graphite Nano fibers
HFCVD	Hot-Filament Chemical Vapor Deposition
H–T	Halpin–Tsai
ISS	Interfacial Shear Strength
LB	Lattice Boltzmann
LJ	Lennard-Jones
MC	Monte Carlo
MD	Molecular Dynamics
MH	Multi-scale Homogenization
MM	Molecular Mechanics
MM	Molecular Mechanics
MPECVD	Microwave Plasma Chemical Vapor Deposition
MWNT	Multi-Walled Carbon Nano Tube
MWPECVD	Microwave Plasma Enhanced Chemical Vapor Deposition
NM	Newtonian Mechanics
ODEs	Ordinary Differential Equations
OLED	Organic Light Emitting Diodes
PAC	Powdered Activated Carbon
PB	Prussian Blue
PCB	Printed Circuit Board
PE	Plasma Enhanced
PECVD	Plasma Enhanced Chemical Vapor Deposition
PLA	Polylactic Acid
PLD	Pulsed Laser Deposition
PMMA	Poly (Methyl Methacrylate)
PPV	Phenylenevinylene
PSNT	Polystyrene Target
QM	Quantum Mechanics
QM	Quantum Mechanics
RF-CVD	Radio Frequency Chemical Vapor Deposition
RVE	Representative Volume Element
RVE	Representative Volume Element
SD	Steepest Descent
SOCs	Synthetic Organic Compounds
SUSHI	Simulation Utilities for Soft and Hard Interfaces
SWNT	Single-Walled Carbon Nanotube

TB	Tight Binding
TDGL	Time-Dependent Ginsburg–Landau
TETA	TriethyleneTetramine
TPD	Temperature-Programmed Desorption
T–W	Tandon–Weng
vdW	van der Waals
VGCF	Vapor Grown Carbon Fiber

LIST OF SYMBOLS

A	set of all the atoms of the sheet
a	translational period of group L
a_1 and a_2	hexagonal lattice
B	body force per unit undeformed area
B	set of all the binary bonds between pairs of adjacent atoms
C	set of all the ordered couples of adjacent bonds
C	stiffness tensor
D	dissociation energy
E	function of spectroscopic constants
F	force vector
F	force applied to the cross-sectional area
H(i) and H(j)	Hamiltonian associated with the original and new configuration
n, m	number of steps along the unit vectors
P	non-equilibrium force vector
Pi	momentum of particle i
Q	empirical dielectric constant
S	average compliance
T	torque acting at the end of an SWNT
T	total torque applied on the nanotubes
Vnb	continuous Van der Waals energy double density

Greek Symbols

α	rotational angle at ends of beam
$A_0 = a_{CC}$	equilibrium bond length
B and B_0	Euclidean bases
B_X	ball centered at X with a radius that is function of potential cut-off radius
$B_{b[\psi]}$	vector related to the bond in Ω
d_g	diameter at the energy ground
Δr, $\Delta\theta$ and $\Delta\phi$	bond stretching increment

ΔL	axial stretching deformation
Δl	difference in length after the load
ΔU	change in the sum of the mixing energy and the chemical potential of the mixture
$\Delta\beta$	relative rotation between the ends of the beam
$\varepsilon_{\alpha\beta}$	mid-surface strains
Em	Young's modulus of the filler
Ef	Young's modulus of matrix
ε	predefined tolerance
$\vec{F_i}(t)$	force acting on the ith atom
F_{ij}^{c}	conservative force of particle j acting on particle i, γ and σ are constants
H_0	initial length
J_0	cross-sectional polar inertia of the SWNT
k_r, k_θ and k_τ	bond stretching force constant
k_l and k_p	stiffness coefficients
KB	Boltzmann constant
L_0	length of the tube
l_0	length on graphene sheet
l_g	length at energy ground for the tube
r_0	carbon-carbon distance
r_{ij}	distance between the atoms i and j
$\vec{r_i}$	atomic position
θ_{ijk}	angle between bonds i − j and i − k,
θ	angle of twist
v_f	volume fraction of filler
v_0	Poisson's ratio of the matrix
U^a, U^b and U^c	energies associated with truss elements
Uv	Hookian potential energy
U^{vdw}	covalent bond stretching
U_r	bond stretch interaction
U_θ	bond angle bending
U_ϕ	dihedral angle torsion
U_ω	improper (out-of-plane) torsion
U_{vdw}	non-bonded van der Waals interaction
Uv	Hookian potential energy
U_r and U_A	stretching energy
U_θ and U_M	bending energy

U_τ and U_T	torsional energy
V_R and V_A	repulsive and attractive pair terms
Vp(r)	potential function for bend stretch
vel_a	velocity function of the atom a • A
$\psi^{(0)}$	initial guess of equilibrium state
$\psi = \psi_e$	harmonic oscillator component
ψ_0	collision diameter
ν	Poisson ratio
ϕ	stands for double contraction of tensors
$\phi(m)$	Euler function
ε	dislocation energy
ζ_f	shape parameter depending on filler geometry
$(-\gamma P)$	dissipative
$(\sigma\, \zeta\, (t))$	random force terms
$\zeta(t)$	Gaussian random noise term
$\sigma(x)$	shape parameter
$\sigma(x)$	stress field
σ_v	vertical mirror plane
Λ	vibrational quantum number