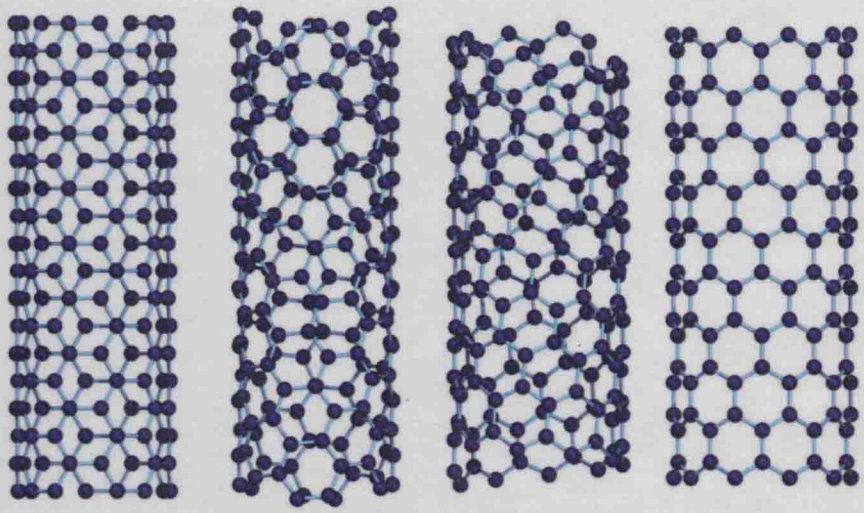
Carbon Nanotubes

Theoretical Concepts and Research Strategies for Engineers



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CARBON NANOTUBES

Theoretical Concepts and Research Strategies for Engineers

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LIST OF ABBREVIATIONS

A	Attractive Segment
AC	Activated Carbon
ACF	Activated Carbons Fibers
AF	Attractive Force
AFM	Atomic Force Microscopy
AP	Asymmetric Packing Segment
APP	Asymmetric Packing Process
ASA	Adsorption Stochastic Algorithm
ATRP	Atom Transfer Radical Polymerization
BD	Brownian Dynamics
BET	Brunauer-Emmet-Teller Method
CHC	Cahn–Hilliard–Cook
CNT	Carbon Nano Tube
CO	Carbon Monoxide
CPMD	Car–Parrinello molecular dynamics
CRTs	Cathode Ray Tubes
CS	Chitosan
CV	Cyclic Voltammeter
CVD	Chemical Vapor Decomposition
CVI	Chemical Vapor Infiltration
D	Directional Segment
DA	Dubinin-Astakhov Model
dE	Exact Differential Energy
DF	Directional Force
DFT	Density Functional Theory
DOM	Dissolved Natural Organic Matter
DPD	Dissipative Particle Dynamics
dP_s	Differential Entropy for Macrosystems
DRS	Dubinin-Radushkevich-Stoeckly Model
DS	Dubinin-Stoeckly Model
DTA	Differential Thermal Analysis
ED	External Force-Induced Directional factor
EDLC	Electric Double-Layer Capacitor

EF-F	External Force-Specific Functional Segment
ERM	Effective Reinforcing Modulus
F-BU	Fabrication Building Unit
FE-SEM	Field-Emission Scanning Electron Microscopy
FED	Field Emission Displays
FEM	Finite Element Method
FET	Field Effect Transistors
FOM	Federation Object Model
GCMC	Grand Canonical Monte Carlo Simulation
GIC	Graphite Intercalation Compounds
H–T	Halpin–Tsai
HK	Horvath-Kawazoe Model
HLA	High Level Architecture
HOPG	High Pyrolitic Graphite
HREM	High-Resolution Electron Microscopy
HRTEM	High Resolution Transmission Electron Microscopy
IHK	Improved Horvath-Kawazoe Model
ISS	Interfacial Shear Strength
ITO	Indium Tin Oxide
JG	Janus Green B
LB	Lattice Boltzmann
LDFT	Local Version of Density Functional Theory
LJ	Lennard-Jones Potential Function
M–T	Mori–Tanaka
MB	Methylene Blue
MC	Monte Carlo
MD	Molecular Dynamics
MDS	Molecular Dynamics Simulation
MFC	Microbial Fuel Cells
MH	Multi-Scale Homogenization
MO	Metal Oxide
MSA	Molecular Self-Assembly
MSC	Molecular Sieving Carbon
MSD	Micropore Size Distribution
N-CE	Nano-Communication Element
N-ME	Nano-Mechanical Element
N-PE	Nano-Property Element

N-SE	Nano-Structural Element
ND	Nguyen and Do method
NLDFT	Non Local Density Functional Theory
OMT	Object Model Template
OOP	Object-Oriented Programming
OPLS-AA	Optimized Potential for Liquid Simulations All-Atom
PA	Polyamide
PALS	Positron Annihilation Lifetime Spectroscopy
PC	Polycarbonate
PSA	Pressure Swing Adsorption
PSD	Pore Size Distribution
PVA	Polyvinyl Acetate
PVP	Poly Vinyl Pyridine
R	Repulsive Segment
R-BU	Reactive Building Unit
RF	Repulsive Force
RISC	Reduced Instruction Set Computer
RTI	Runtime Infrastructure
RVC	Reticulated Vitreous Carbon
RVE	Representative Volume Element
SA-BU	Self-Assembly Building Unit
SAM	Self-Assembled Monolayer
SANS	Small-Angle Neutron Scattering
SAXS	Small-Angle X-Ray Scattering
SOCs	Synthetic Organic Chemicals
SOM	Simulation Object Model
STM	Scanning Tunneling Microscopy
SUSHI	Simulation Utilities for Soft and Hard Interfaces
T&O	Taste and Odor
TDGL	Time-Dependent Ginsburg–Landau
TEM	Transmission Electron Microscopy
TEP	Thermoelectric Power
TETA	Triethylene Tetramine
TGA	Thermo-Gravimetric Analysis
Th	Thionine
TSA	Temperature Swing Adsorption
TVFM	Theory of Volume Filling of Micro pores

UFF	Universal Force Field
VLS	Vapor-Liquid-Solid
VSM	Vibrating Sample Magnetometer
XPS	X-Ray Photoelectron Spectroscopy
XRD	X-Ray Diffraction

LIST OF SYMBOLS

$\overline{\sigma}$	stress
v_f	volume fraction of filler
$\Pi_1 \& \Pi_2$	characterize the strength of surface forces field
A_{pot}	free energy of adsorption in Dubinin–Astakhov isotherm equation
$(L - d_a)_{p,max}$	pore width related to maximum value of function
ΔG_{m}	transformation from austenite to ferrite
A_{HK}	constant of HK method
a_m	monolayer capacity
$A_{max}, \bar{A} \& \sigma_A$	proportional to the parameter
a_{mi}	equilibrium amount adsorbed in micro pores
C_1, C_2, C_3, C_4	constants for adsorb ate-adsorbent system
C_{BET}	BET constant on flat surface
c_s	complete filling concentration
d_a	diameter of the adsorbate molecule
d_A	diameter of the adsorbent atom
D_c^{γ}	diffusion constant of C in austenite
$D_{in} \& \chi(D_{in})$	differential PSD function
d_{γ}	austenite grain size after reheating of slab
$\frac{dA}{dx}$	derivative of adsorption potential
f_d	downstream fugacities
f_u	upstream fugacities
$\dot{G}$	grow rate

I_s	nucleation rate at unit area
$L_{av,I}$	average effective width of primary porous structure
$L_{av,II}$	average effective width of secondary porous structure
$L_{av,tot}$	average effective width of primary and secondary porous structure
L_{av}	average pore width
$\frac{L-d_a}{d_A}$	reduced effective pore width
$(L-d_a)$	effective pore width
n_0	number of austenite grains at a unit volume
N_{DRS}	values of adsorption
N_{mDRS}	values of maximum adsorption
$\dot{N}$	nucleation rate for unit volume
p_0	standard state pressure
P_e	permeability of membrane
p_s	saturation pressure of an adsorbate
q^{diff}	differential heat of adsorption
$S_{c,\alpha}$	total specific surface area calculate by high-resolution αs-plot
S_{DFT}	surface of pores calculated for all pores
S_g	molar entropy of gas
V_{HK}	micropore volumes determined from HK
V_{m}	molar volume
V_m	molar volume of the adsorbent
W_0	Dubinin–Radushkevich isotherm equation
$W_{exp,tot}$	maximum value of the experimental adsorption
X_{dyn}	fraction dynamically recrystallized
X_e, Y_e	extended volume fraction
$X_{mi}(A)$	potential distribution in micro pores
z_{max} , $\bar{z}\&\sigma_z$	structural heterogeneity of microporous solids
γ_∞	surface tension of bulk fluid
γ_{me}	amount adsorbed at relative pressure per unit area of mesopore surface
γ_s	unit area of nonporous reference adsorbent surface
ε_0	adsorption characterized energy of standard state
$\lambda_1\&\lambda_2$	range of structural forces action
ρ_b^*	reduced number density of bulk fluid

v	velocity
ψ	wave function
δQ_{in}	inexact differential amounts of heat
δW_{in}	inexact differential amounts of work
Δx	spatial extension
ΔG^{ads}	free energy of adsorption equal to $RT \ln(p/p_s)$
ΔH^{ads}	enthalpy of adsorption
ΔH^{vap}	enthalpy of vaporization
ΔS^{ads}	entropy of adsorption
A	adsorption potential
a	total amount adsorbed
A, B	planes
a(k)	distribution of wave numbers
a^0_{mes}	monolayer capacity of mesopore surface
a^0_{mi}	maximum amount adsorbed in micro pores
a^0_s	monolayer capacity of reference adsorbent from standard adsorption isotherm
a_{mes}	amount adsorbed on mesopore surface
$a_{mes(p/p_0)}$	amount adsorbed on mesopore surface in relative pressure
a_{mic}	amount adsorbed on micro pore surface
$a_{mic}(p/p_0)$	amount adsorbed on micro pore surface in relative pressure
$a_s(0.4)$	amount adsorbed on surface of reference solid at pressure 0.4
$a_s(p/p_0)$	amount adsorbed on surface of reference adsorbent
b	an equilibrium adsorption constant
B	temperature-independent structural parameter of micropore sizes
c	average interstitial concentration
C	stiffness tensor
Ch	chiral vector
D	diffusion coefficient of C in austenite
d	tube diameter
D_0	constant Number
d^3r	volume element
D_{max},D_{min}	minimum and Maximum pore size in kernel of NLDFT
dP	probability
E_0	characteristic energy of adsorption for reference vapor

erf(W)	error function of w parameter
ε(x)	non-uniform in polymer
F	conversion factor for N_2 adsorption
f	fluid fugacity
$f(H)$	pore size distribution function
$f(z)$	intrinsic molecular Helmholtz free energy of adsorbate phase
$F[\rho(r)]$	intrinsic Helmholtz free energy function
F(B)	Gaussian distribution function of the structural parameter B
F(L)	PSD of the heterogeneous solid adsorbent
F(Z)	distribution function characterizing heterogeneity of microporous structure
ω	frequency
h_{cr}	critical capillary film thickness
H_{max}	width of largest pore
H_{min}	width of smallest pore
I	intensity
J	local molar flux
$J(L-d_a)$	effective pore size distribution
J(X)	micro pore size distribution
k	structural parameter
k	wave vector
L	micropore width
L/d_A	reduced pore width
M	mass
M	mobility of interface
m	proportionality constant
$m = (\beta\kappa)^{-2}$	proportional coefficient
mic	calculated only for the range of micro pores
N_A	Avogadro number
p/p_o	relative pressure
q_1-q_l	difference heat of condensation and adsorption
r	average size of precipitates
R	universal gas constant
$r(p/p_0)$	pore radius
r/R	ratio of distance to radius

r_{cr}	critical capillary radius
S	entropy for nano/small systems
S_{BET}	surface area of BET method
S_{meso}	total surface area of mesopores
S_{mi}	total surface area of micropores
S_t	slope of low pressure of α_s-plot
suffix i	all elements in the system
T	time
t-plot	T-curve method
$t\left(\frac{p}{p_0}\right)$	statistical thickness of the film
V(A)	characteristic adsorption curve
V(r)	interaction potential of the fluid molecule
V_{meso}	mesopore volume
V_{micro}	micropore volume
V_t	maximum volume adsorbed
V_t–v	unoccupied pore volume
W^0_{mi}	limiting volume of adsorption
λ	wavelength
x	fractions of elements
x	pore mole fraction in binary systems
X, Y	actual volume fraction
X(A)	adsorption potential distribution function
$X^*(A)$	non- normalized adsorption potential distribution function
x_0	micropore half width at the maximum of adsorption curve
$X_{mi}(A)$	micropore adsorption potential distribution function
y	bulk mole fraction in binary systems
Z	quantity associated with the micropore size
α	ferrite
β	similarity coefficient
γ	Austenite
Γ	Euler gamma function
δ	displacement of surface
δ, Δ	dispersion
ΔH	differential enthalpy

ΔS	differential entropy
ε	adsorption characterized energy
ε_{FC}	Len–Jones interaction parameter
ζ	constant equal to $\left(\frac{1}{\kappa^n}\right)$
η	Slope of linear segment of the α_s-plot
θ	chiral angle
Θ	degree of micropore filling
$\theta(L,P)$	local adsorption isotherm (kernel)
$\theta=a/a^0_{mi}$	relative adsorption
$\theta_{mes}\ (p/p_0)$	relative surface coverage of mesoporous reference adsorbent
$\theta_{mi}\ (p/p_0)$	relative surface coverage of micro porous reference adsorbent
$\theta_{mic}(z,A)$	local isotherm in uniform micropores
$\theta_s\ (p/p_0)$	relative surface coverage of nonporous reference adsorbent
μ	chemical potential
ν	liquid molar volume
ν	parameter for the gamma distribution function
ρ	parameter of gamma distribution function
$\rho(z)$	local density of the adsorbed fluid
$\rho(P,H)$	density of N_2 at pressure P in a pore of width H
ς	proportionality constant
σ_{FC}	Len–Jones interaction parameter
τ	time when the new phase nucleates at plane B
$\Phi(r)$	external potential function
$\varphi ij\ (r)$	pair potential between 2atoms
$\chi(D_{in})$	normalized differential PSD function
$\Omega[\rho(z)]$	grand potential function
ω, Ω	cross-sectional area