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Foundations of Nanotechnology

Volume 2
Nanoelements Formation and Interaction

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LIST OF ABBREVIATIONS

A	Attractive Segment
AF	Attractive Force
AFM	Atomic Force Microscope
AP	Asymmetric Packing Segment
APP	Asymmetric Packing Process
BAMs	Bulk-Amorphous Metals
BD	Brownian Dynamics
BSA	Bovine Serum Albumin
CNT	Carbon Nanotube
D	Directional Segment
DC	Direct Current
DF	Directional Force
DOD	Dynamic Oblique Deposition
DPD	Dissipative Particle Dynamics
DSMC	Direct Monte Carlo Simulation
E	Energy of the System
ED	External Force-Induced Directional Factor
EF-F	External Force-Specific Functional Segment
F-BU	Fabrication Building Unit
FET	Field Effect Transistors
LEDs	Light Emitting Diodes
M&S	Modeling and Simulation
MC	Monte Carlo
MCP	Mechanochemical Processing
MD	Molecular Dynamics
MEMS	Micro Electromechanical Systems
MMT	Montmorillonite
MRI	Magnetic Resonance Imaging
MSA	Molecular Self- Assembly
MWCNT	Multi Wall Carbon Nanotube
N-CE	Nano-Communication Element
NEMS	Nano Electromechanical Systems
N-ME	Nano-Mechanical Element

N-PE	Nano-Property Element
NSC	National Science Foundation
N-SE	Nano-Structural Element
NSET	Nanoscale Science, Engineering, and Technology
PEM	Proton Exchange Ma
PMMA	Polymethyl Methacrylate
PSL	Polystyrene Latex
PZT	Plumbum Zirconate Titanate
R	Repulsive Segment
R-BU	Reactive Building Unit
RF	Repulsive Force
RISC	Reduced Instruction Set Computer
RVE	Representative Volume Element
SA-BU	Self-Assembly Building Unit
SAMs	Self-Assembled Monolayers
SOFC	Solid Oxide Fuel Cells
SWCNT	Single Wall Carbon Nanotubes
TBT	Tributyltin
UV	Ultraviolet
VLS	Vapor-Liquid-Solid

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LIST OF SYMBOLS

A	an arbitrary physical quantity
A_L	new liquid surface area
A_S	surface area of the solid destroyed
A_{SL}	new liquid/solid interfacial area
D	particle diameter
D	characteristic size of the nanoelement
d	diameter of the nanoparticles
E	tensile strain
$E»(f)$	second derivative of the energy density surface
E_{Ani}	anisotropic energy
E_{App}	energy associated with an applied magnetic field
E_{Dem}	demagnetization energy
E_{Exc}	exchange energy
$e^{-i\omega t}$	monochromatic excitation
F	force
$\vec{F}_i(t)$	a random set of forces at a given temperature
$F^{ke}_{X_1}, F^{ke}_{X_2} F^{ke}_{X_3},$	external forces acting on nanoelements
$F^{kj}_{X_1}, F^{kj}_{X_2} F^{kj}_{X_3},$	the interaction forces of nanoelements
F^C_{ij}	conservative force
F^D_{ij}	dissipative force
F^R_{ij}	random force
F_{max}	the maximal force of the interaction of the nanoparticles
G	acceleration of gravity
H	Planck's constant
$\hbar$	reduced Planck constant
H_0	an incident electromagnetic wave
H_a	anisotropy field
H_t	transverse oscillating field
H_{demag}	demagnetizing field
H_{ext}	external field
H_{int}	internal field

H_{res}	residual field
I	area in the direction of the bending motion
J	the magnetisation oscillation
$J^k_{z_1}, J^k_{z_2}, J^k_{z_3}$	moments of inertia of a nanoelement
K	bulk modulus
k'	wave number
L	width of the potential well
l	length of the pendulum rod
L_0	latent heat of melting
M	magnetization vector
m	mass of the particle
m_i	the mass of the -th atom
$M^{ke}_{z_1}, M^{ke}_{z_2}, M^{ke}_{z_3},$	external moments acting on nanoelements
$M^{kj}_{z_1}, M^{kj}_{z_2}, M^{kj}_{z_3},$	the moment of forces of the nanoelement interaction
M^k	a mass of a nanoelements
M_s	saturation magnetization
N	anisotropy
n	the number of interatomic interaction types
$\hat{n}$	normal vector
N_e	the number of nanoelements
N_k	the number of atoms forming each nanoparticle
P	hydrostatic pressure
ρ	density
$\vec{\rho}_{ij}$	radius-vector
R	nanosphere radius
r_1	the position vector of the center of mass of particle
S	entropy
S_c	distance between the centers of mass of the nanostructure nanoelements
T	melting point of the extended system
Γ	shear strain
T_0	melting temperature of the bulk material
T_i	torque
U	anisotropy energy
∪	total interaction energy
u(r,t)	macroscopic velocity
$V(\vec{r},t)$	varying potential influencing the particle's motion

V_i	the velocity vector of the center of mass of particle
V	the volume of the particle
v	velocity
V_L	volume of liquid
v_i	the translational velocity
$W_D(r_{ij})$ and $W_R(r_{ij})$	weighting functions
w_i	the angular velocity vector
$\overline{V}_{i0}, \overline{V}_i$	initial and current velocities of the -th atom
$\overline{x}_{i0}, \overline{x}_i$	original and current coordinates of the -th atom
x_{max}	arbitrary amplitude

GREEK SYMBOLS

$\psi(\vec{r})$	a function of space
Δ	dilatation
α	Gilbert damping constant
λ	longitudinal displacement of the nanospring
l'	mean free path
φ	mean magnetization direction
γ	surface tension
σ	tensile stress
DA	increment in surface area
DG_{Bulk}	free energy of the bulk material
s_L	surface energy of the liquid per unit area
γ_S	solid surface energy per unit area
γ_{SL}	solid/liquid interfacial energy per unit area
$\Theta_1, \Theta_2, \Theta_3,$	mutual orientation of the nanoelements
Ω_k	nanoelement area
α_i	the "friction" coefficient in the atomic structure
δ_{ij}	Kronecker delta
ζ_{ij}	stochastic variable inducing the random motion of particles
θ_{ij}	stochastic variable
ρ_j and ρ_i	density functions for microscopic states j and
σ^2	variance
Δn_i^B	rotational displacement
$\varepsilon(w)$	dielectric function
ε_0	dielectric constant of free space
τ	shear stress

τ	the relaxation time (dimensionless)
$\Phi\left(\vec{\rho}_{ij}\right)$	the potential depending on the mutual positions of all the atoms
δ	arbitrary initial phase angle
η	viscosity
ξ	friction coefficient
0-D	zero-dimensional
1-D	one-dimensional
2-D	two-dimensional
3-D	three-dimensional

PREFACE

One of the main tasks in making nanocomposites is building the dependence of the structure and shape of the nanoelements forming the basis for the composite of their sizes. This is because with an increase or a decrease in the specific size of nanoelements, their physical-mechanical properties, such as the coefficient of elasticity, strength, deformation parameter, etc., vary by over one order. The calculations show that this is primarily due to a significant rearrangement of the atomic structure and the shape of the nanoelement. The investigation of the above parameters of the nanoelements is technically complicated and laborious because of their small sizes. When the characteristics of powder nanocomposites are calculated, it is also very important to take into account the interaction of the nanoelements since the changes in their original shapes and sizes in the interaction process and during the formation of the nanocomposite can lead to a significant change in its properties and a cardinal structural rearrangement. In addition, the studies show the appearance of the processes of the ordering and self-assembling leading to a more organized form of a nanosystem. The above phenomena play an important role in nanotechnological processes. They allow nanotechnologies to be developed for the formation of nanostructures by the self-assembling method (which is based on self-organizing processes) and building up complex spatial nanostructures consisting of different nanoelements.

The study of the above dependences based on the mathematical modeling methods requires the solution of the aforementioned problem at the atomic level. This requires large computational aids and computational time, which makes the development of economical calculation methods urgent. The objective of this volume is the development of such a technique in various nanosystems.

— Sabu Thomas, Saeedeh Rafiei, Shima Maghsoodlou, and Arezo Afzali

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