

MATERIALS BEHAVIOR

Research Methodology
and Mathematical Models

Mihai Ciocoiu, PhD
Editor

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Edited by
Mihai Ciocoiu, PhD

A. K. Haghi, PhD, and Gennady E. Zaikov, DSc

Reviewers and Advisory Board Members



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MATERIALS BEHAVIOR

Research Methodology and
Mathematical Models

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LIST OF ABBREVIATIONS

ABS	Acrylonitrile–Butadiene–Styrene
ANOVA	Analysis of Variance
BPE	Branched Polyethylenes
CCD	Central Composite Design
CD	Cross-Direction
CNT	Classical Nucleation Theory
CV	Coefficient of Variation
CSC	Crystallites with Stretched Chains
DSC	Differential Scanning Calorimetry
EDANA	European Disposables and Nonwovens Association
EP	Epoxy Polymer
EVA	Ethylene-co-Vinyl Acetate
FH	Fluorohectorite
FOD	Fiber Orientation Distribution
FT	Fourier Transform
HBP	Hyper Branched Polymer
HRR	Heat Release Rate
HRTEM	High Resolution Transmission Electron Microscopy
HT	Hectorite
HT	Hough Transform
I(e)	Informational Entropy
IP	Inclined Plates
IRD	Institutional Research Development Programme
LDHs	Layered Double Hydroxides
LDPE	Low Density Polyethylene
LOI	Loss on Ignition
MC	Monte Carlo
MD	Machine Direction
MD	Molecular Dynamics
MFI	Melt Flow Index
MMT	Montmorillonite
NRF	National Research Foundation
NSMs	Nano Structured Materials
PA	Polyurethane
PAr	Polyarylate
Pc	Phthalocyanines

PC	Polycarbonate
PET	Poly(ethylene terephthalate)
PGD	Pores Geometry Distribution
PHRR	Peak of Heat Release
PMMA	Poly(methyl methacrylate)
POSS	Polyhedral Oligomeric Silse Squioxaneo
PP	Polypropylene
PVD	Pore Volume Distributions
REP	Rarely Cross-Linked Epoxy Polymer
RSM	Response Surface Methodology
SEM	Scanning Electron Microscope
SR	Smoke Release
TBP	Tetrabenzoporphyrin
TEM	Transmission Electron Microscopy
TGA	Thermogravimetric Analysis
THR	Total Heat Release
TPC	Tetra Pyrrole Compounds
TPP	Tetraphenyl Porphyrin
TTI	Time to Ignition
VA	Vinyl Acetate
WL	Weight Loss
0DNSM	Zero-Dimensional Nanostructured Materials
1DNSM	One-Dimensional Nanostructured Materials
2DNSM	Two-Dimensional Nanostructured Materials

LIST OF SYMBOLS

a	the acceleration
a and b	integers
a_i	the acceleration of particle i
b	Burgers vector
c	speed of light in m/s
C_∞	characteristic ratio
d	dimension of Euclidean space
D_p	nanofiller particles diameter in nm
d_{surf}	nanocluster surface fractal dimension
d_u	fractal dimension of accessible for contact (“nonscreened”) indicated particle surface
d_w	dimension of random walk
E	the potential energy of the system
E_a	the distance from the surface acceptor level to the E_v
E_n and E_m	elasticity moduli of nanocomposites and matrix polymer, respectively
F	the force exerted on the particle
F_i	the force exerted on particle i
F_s	the distance from the Fermi level at the surface to E_v
G	shear modulus
G_∞	equilibrium shear modulus
G_c , G_m and G_f	shear moduli of composite, polymer matrix and filler, respectively
G_{cl}	the shear modulus
h	Planck constant
I	the scattering intensity
I_0	a reference value of intensity
I_{ph}	photocurrent in μA
k	Boltzmann constant
K_s	stress concentration coefficient
K_T	bulk modulus
L	filler particle size
l_0	main chain skeletal length
l_k	specific spatial scale of structural changes
l_{st}	statistical segment length
m	the mass
M	the total sampling number

m and n	exponents in the Mie equation
$m_{\text{absorbed water}}$	weight of the saturated condensed vapors of volatile liquid, g
M_{cl}	molecular weight of the chain part between cluster
M_{e}	molecular weight of chain part between entanglements
m_i	the mass of particle i
m_{sample}	weight of dry sample, g
N	the number of atoms in the system
N_A	Avogadro number
n_{cl}	statistical segments number per one nanocluster
N_{α} and N_{β}	the numbers of particles of the entities of type α and β , respectively
p	solid-state component volume fraction
p_c	percolation threshold
q	the parameter
q	the wave number
Q_1 and Q_2	the charges
R	a hydrogen atom or an organic group
r	the position
R	universal gas constant
r_{ij}	the distance between a pair of atoms i and j
\mathbf{r}^N	the complete set of $3N$ atomic coordinates
S	macromolecule cross-sectional area
T , T_g and T_m	testing, glass transition and melting temperatures, respectively
$u(\mathbf{r})$	an externally applied potential field
v	the velocity
V	the volume of the system
W	absorbed light power W
w	activation energy of the transition to the charged form
W_n	nanofiller mass contents in mas.%,
Z_i	the effective charge of the i -th ion

Greek Symbols

$f_{\infty}^{(0)}$	the equilibrium distribution
$\langle \rangle$	ensemble average
σ_f^n	nominal (engineering) fracture stress
σ_f^c and σ_f^m	fracture stress of composite and polymer matrix, respectively
a	the efficiency constant
α_i	the electric polarizability of the i -th ion
β	coefficient
β_p and ν_p	critical exponents (indices) in percolation theory
ΔS	entropy change in this process course
ε	misfit strain arising from the difference in lattice parameters

ε_0	the permittivity of free space
ε_f	strain at fracture
ε_y	the yield strain
η	exponent
J	total concentration of adsorbed molecules
l	wavelength m
λ_b	the smallest length of acoustic irradiation sequence
λ_k	length of irradiation sequence
n	Poisson's ratio
v_{cl}	cluster network density
v_p	correlation length index in percolation theory
r	nanofiller (nanoclusters) density
ρ	polymer density
ρ_{cl}	the nanocluster density
ρ_d	the density if linear defects
ρ_α and ρ_β	the corresponding densities of α and β subsystems
τ	the relaxation time (dimensionless)
τ_{in}	the initial internal stress
t_{IP}	the shear stress in IP (cluster)
φ_n	nanofiller volume contents
c	the relative fraction of elastically deformed polymer
Γ	Euler gamma-function

