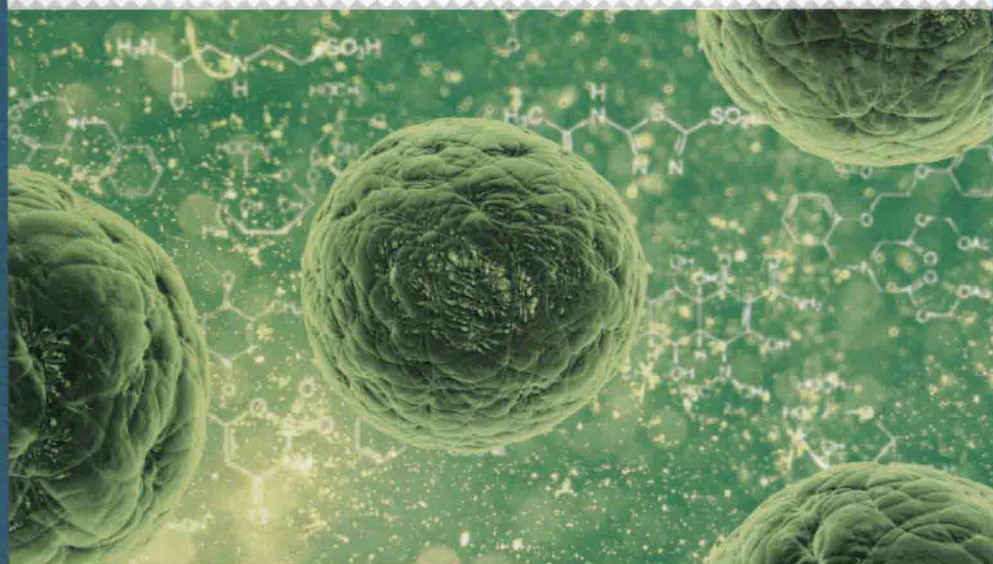


Volume 2

# Physical Chemistry Research for **Engineering** and **Applied Sciences**

Polymeric Materials and Processing



Editors

Eli M. Pearce, PhD

Bob A. Howell, PhD

Richard A. Pethrick, PhD, DSc

Gennady E. Zaikov, DSc

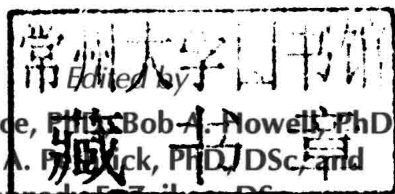
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## VOLUME 2

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Edited by  
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Richard A. P. Frick, PhD, DSc, and  
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**PHYSICAL CHEMISTRY  
RESEARCH FOR ENGINEERING  
AND APPLIED SCIENCES**

**VOLUME 2**

Polymeric Materials and Processing



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Dr. Eli M. Pearce was the President of the American Chemical Society. He served as Dean of the Faculty of Science and Art at Brooklyn Polytechnic University in New York as well as a Professor of Chemistry and Chemical Engineering. He was the Director of the Polymer Research Institute, also in Brooklyn. At present, he consults for the Polymer Research Institute. As a prolific author and researcher, he edited the *Journal of Polymer Science* (Chemistry Edition) for 25 years and was an active member of many professional organizations.

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Bob A. Howell, PhD, is a Professor in the Department of Chemistry at Central Michigan University in Mount Pleasant, Michigan. He received his PhD in physical organic chemistry from Ohio University in 1971. His research interests include flame-retardants for polymeric materials, new polymeric fuel-cell membranes, polymerization techniques, thermal methods of analysis, polymer-supported organoplatinum antitumor agents, barrier plastic packaging, bioplastics, and polymers from renewable sources.

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Professor R. A. Pethrick, PhD, DSc, is currently a Research Professor and Professor Emeritus in the Department of Pure and Applied Chemistry at the University of Strathclyde, Glasgow, Scotland. He was Burmah Professor in Physical Chemistry and has been a member of the staff there since 1969. He has published over 400 papers and edited and written several books. Recently, he has edited several publications concerned with the techniques for the characterization of the molar mass of polymers and also the study of their morphology. He currently holds a number of EPSRC grants and is involved with Knowledge Transfer Programmes involving three local companies involved in production of articles made out of polymeric materials. His current research involves AWE. He has acted as a consultant for BAE Systems in the area of explosives and a company involved in the production of anticorrosive coatings.

Dr. Pethrick is on the editorial boards of several polymer and adhesion journals and was on the Royal Society of Chemistry Education Board. He is a Fellow of the Royal Society of Edinburgh, the Royal Society of Chemistry, and the Institute of Materials, Metal and Mining. Previously, he chaired the 'Review of Science Provision 16-19' in Scotland and the restructuring of the HND provision in chemistry. He was also involved in the creation of the revised regulations for accreditation by the Royal Society of Chemistry of the MSc level qualifications in chemistry. For a many years, he was the Deputy Chair of the EPSRC IGDS panel and involved in a number of reviews of the courses developed and offered under this program. He has been a member of the review panel for polymer science in Denmark and Sweden and the National Science Foundation in the USA.

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Editors: Eli M. Pearce, PhD, Bob A. Howell, PhD,

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# LIST OF ABBREVIATIONS

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AFM	Atomic Force Microscopy
AP	Aromatic Polyesters
CNT	Carbon Nanotubes
CTZ	Polysaccharide Chitosan
DCV- GCMD	Dual-Volume GCMD
DM	Dibenzothiazole Disulphide
DP	Diamond Pore
DSC	Differential Scanning Calorimetry
EB	Electron Beam
ER	Epoxy Resin
F	Flexible
FG	Fiber Glass
GCMD	Grand Canonical Molecular Dynamics
HR	Heat Radiation
HTS	High Temperature Shearing
IUPAC	International Union of Pure and Applied Chemistry
LDPE	Low Density Polyethylene
LQPS	Liquid-Crystal Polyesters
MC	Monte Carlo
MD	Molecular Dynamics
MF	Microfiltration
MSD	Mean-Square Displacement
MWCO	Molecular Weight Cut-Off
MWNT	Multi-Walled Carbon Nanotube
NBR	Acrylonitrile-Butadiene Rubber
NCN	National Science Centre Poland
NF	Nanofiltration
NR	Natural Rubber
OIT	Oxidation Induction Time
OOT	Oxidation Onset Temperature
PEG	Polyethylene Glycols
PFR	Phenoloformaldehyde Resin
PMS	Polymethyl-Silsesquioxane
PP	Polypropylene
PUE	Polyurethane Elastomers

R	Rigid
RESPA	Reference System Propagator Algorithm
RHR	Rate of Heat Release
RO	Reverse Osmosis
ROA	Rheometrics Optical Analyzer
SALS	Small Angle Light Scattering
SBR	Styrene-Butadiene Rubber
SE	Secondary Electron Signal
SEM	Scanning Electron Microscope
SFE	Surface Free Energy
SP	Straight Path
SWNT	Single-Walled Carbon Nanotube
TPES	Thermoplastic Elastomers
TS	Tensile Strength
UF	Ultrafiltration
US	Ultrasound
VACF	Velocity Autocorrelation Function
ZP	Zigzag Path

# LIST OF SYMBOLS

---

$\alpha_0$	amplitude of the initial disturbance
$\alpha_B$	amplitude of the instability
$\bar{u}$	average molecular speed
$A_{m's}$	coefficients of the Fourier expansion
$P_S^*$	constant
$C_{j\sigma}^+$	creation operators of electrons
$t_\Delta$	electron hopping integral
$\varepsilon_{l\sigma}$	energy of the electron by the impurity
$c_{j\sigma}$	Fermi annihilation
$f_s(\mathbf{p}, \mathbf{r})$	Fermi distribution function
$f_A$	fugacity
$V_{lj}$	matrix element of hybridization
$\xi_i$	random numbers generated for each trial
$C_h^*$	saturation constant
$D_A^*$	self-diffusion coefficient
$\Gamma$	surface tension
$\eta_m$	viscosity of the matrix material
$A$	proportionality constant
$\mathbf{a}_1$ and $\mathbf{a}_2$	unit vectors
$aq$	energy barrier
$B$	hole affinity constant
$c(x)$	concentration
$c_A$	concentration of diffusant A
$D$	pore diameter
$\mathbf{e}_1, \mathbf{e}_2$ and $\mathbf{e}_3$	coordinates in the current configuration
$eV$	electron energy
$F$	applied external force
$G_1, G_2$	material coordinates of a point in the initial configuration
$J$	molecular flux
$K$	temperature dependent Henry's law coefficient
$K_n$	Knudsen number
$K_0$	proportionality constant
$K_p$	henry's law constant
$L$	membrane thickness
$M$	molecular mass



$m_{\text{sample}}$	sample weight
$M_{\eta}$	molecular weight
$N$	number of carbon atoms in the lattice
$n$	quantization number
$N_a$	the number of molecules
$N_{\text{imp}}$	number of adsorbed hydrogen atoms
$P$	permeability
$p_x$	parallel component of the graphene sheet
$Q$	heat of adsorption
$R$	radius of the modeled SWCNT
$R_0$	initial radius of the undisturbed fibril
$r_p$	pore radius
$S$	solubility coefficient
$T$	thickness of the adsorbate film
$T_0$	constants depending on some quantum mechanical values
$T_{\text{melt}}$	melting point of polyamide
$U$	constant of the Coulomb repulsion
$V$	center-of-mass velocity component
$V$	hybridization potential
$V'', V'$	volumes of polysaccharide
$V_L$	molecular volume of the condensate
$X$	position across the membrane
$\Gamma$	interfacial tension
$\Delta p$	pressure drop across the membrane
$\Delta S$	entropy change
$\Delta H$	fusion heat
$\Theta$	time-lag
$\lambda$	mean free path of molecules
$\rho(x)$	an arbitrary probability distribution function
$\rho'', \rho'$	density of polysaccharide
$T$	pore tortuosity
$\Omega$	known function of the viscosity ratio