

Index

Note: Page numbers in *italics* and **bold** refers to figures and tables respectively.

a

Advanced Photon Source (APS) 145
amorphous PP 12
Andreeva and Gel'fandbein model 178
anharmonic term 40–41
anisotropic specimen 132, 133
anisotropy index 264
Arthur and Coulson model 173
atactic polystyrene (aPS) 122
atom 90
atomic force microscopy (AFM) 160, 231–232
average coefficient of linear thermal expansion
(CLTE_{AV}) 32, **74**, 75, 130, **135**
average coefficient of volume thermal expansion
(CVTE_{AV}) 32, 117, 135, **135**

b

Bekkedahl method 116
bellows method 120–128, 120, 122–125, **127**
bending mode 107
Bloch theorem 100

c

Cahn-Hilliard theory 14
carbon nanotubes (CNTs) 243–247, 243–246
multi-walled CNT (MWCNT) 243–246,
243–246
single-walled CNT (SWCNT) 243, 245, 247
cell model (CM) 43, 65, 126
Chamberlain model 176
characteristic ratio (C_{∞}) 3–4, **4**
chemical cross-linking 258–259, 259–261
Chow model 173–174
coefficient of linear thermal expansion
(CLTE) 34, 74, 76–77, 128–129, 129, 130,
178, 228, 233
expansion/compression mode 129
measurement of 128–135

penetration mode 131–135, 131–134, **135**
tension mode 130, 131
coefficient of volume thermal expansion
(CVTE) 115, 174, 208
bellows method 120–128, 120,
122–125, **127**
measurement of 115–128
piston-die method 119–120, 119
PVT behavior measurement 118–128
volume dilatometry 115–118, 116, 117, **118**
comonomers 4–5
complementary energy density 183
composite theory
Chow model, linear and volume thermal
expansion coefficients 205–208, 206,
208–209
Mori-Tanaka theory 208–223
polymer composites, thermal expansion
theories of 169–180
spherical shell model, polymer blends with
layered shells 200–205, 202, 204
thermal expansion theory, Schapery 180–195
Wang-Kwei model, polymer composites
195–200, 196, 197, 199–200, **199–200**
compression-molded specimens 132–135, 133,
134, **135**
conformation 5
constant strain distribution 184
core/sheath model 272
Craft and Christensen model 177
Cribb model 173
crystalline polymers 59–60
Grüneisen parameter 60–68, 63, 67, 69, 70
lattice parameters, linear thermal expansion
coefficients of 68–69
crystal systems 8, **10**
cylindrical-shaped inclusion, thermal expansion
of 175–180

d

data accuracy 121
 Debye distribution 67–68
 differential coefficient of linear thermal expansion
 ($CLTE_{dif}$) 32, 34, 36, 130, 135
 differential coefficient of volume thermal
 expansion ($CVTE_{dif}$) 32, 117
 digital image correction (DIC) 155–160,
 157–158, 156–160
 dilatometer 115–117, 116
 distribution function 46–47, 46, 47
 Doolittle's viscosity formula 52

e

efficiency factor 178
 Einstein's relation 51
 elastomers 273–287, **274**, 275–280, 282–283
 electrostatic interactions 10
 ellipsoidal filler 205–206
 ellipsoidal inclusions 205–208, 206, 208
 Eshelby equivalent inclusion method 209–213,
 210–212
 Eshelby's tensor 211, 213–215
 ethylene-co-octene rubber (EOR) 276
 ethyleneoctene copolymer (EO) 33
 Euler's theorem 15
 European Synchrotron Radiation Facility
 (ESRF) 145
 external stress 213

f

fiber-reinforced composites, thermal expansion
 of 175–180
 filler-filled systems 258
 fillers
 negative thermal expansion (NTE) 251–258,
253
 reduction of thermal expansion by 227–230,
 229
 surface 23–25
 flexible network 252–255, 253–255
 Flory-Huggins equation 15–16, 20
 Flory-Huggins theory 18–23, 18–20, 22, 78
 Flory model (FM) 54, 56, 126
 Flory's equation 56
 flow direction (FD) 135, 147, 230–232
 free volume 42, 49–50, 49–51
 contribution of 51, 57–59, 58, **59**
 equation of state 53–57, **54**
 theory 49, 51–53

g

gas, thermal expansion of 47–48, **48**
 Gibbs-Bogoliubov inequality 101
 Gibbs free energy density 183
 glass fiberreinforced plastics (GFRP) 157–158,
 158, 160, 160
 glass transition temperature (T_g) 49

GNOMIX Inc. 120
 graphene 247–251, 247–250, **251**
 graphene oxide (GO) 247
 grazing incidence X-ray diffraction (GIXD) 146
 Grüneisen parameter 60–68, 63, 67, 69, 70
 Grüneisen theory 108–109
 gypsum powders 158–159

h

Hamiltonian 92, 93, 95, 96, 99
 harmonic term 40–41
 heating device 159, 159
 Helmholtz free energy 14, 182
 high brightness light 145
 Hole theory 42

i

infrared image correction (IIC) 157–158
 injection-molded isotactic polypropylene 33–34,
 33–36
 injection-molded specimens 132–135, 133, 134,
135
 intercrystalline bridge volume
 fraction 273
 internal rotational potentials 9
 intrinsic anharmonic model 94–95
 isotactic poly(methyl methacrylate)
 (I-PMMA) 117–118
 isotactic polypropylene (iPP) 12, 12, 33–34,
 33–36, 72–77, 125, 147
 isotropic specimens 132, 133

k

Kerner model 172, 239

l

lamellae 8
 laser interferometry 153–155, 153–155
 lattice theory 43–46, 44, 45
 Lennard-Jones and Devonshire theory 45
 linear chain model 89
 CLTE of chain growth direction 93–95
 CLTE of transverse to chain growth
 direction 95–98, 98
 modeling 89–93, 89–91
 linear elastic theory 182
 linear thermal expansion 31–33, 40–41
 amorphous and crystalline phase 144–152
 linear thermal expansion coefficients
 68–69, 252
 Chow model 205–208, 206, 208–209
 isotactic polypropylene 72–77, 73, **74–76**,
 74, 76
 lattice parameters 68–69
 polyethylene 69–72, 71–72, **72**
 randomly oriented SF composites 177
 thermal expansion theory 190–195, **193**,
 193, 195

linear variable differential transformer (LVDT) 121, 129
 liquid state
 distribution function 46–47, 46, 47
 lattice theory 43–46, 44, 45
 thermal expansion of material of 41–43, 42
 long-range interaction/excluded volume effect 7
 loop-train-tail model 25, 25
 lower critical solution temperature (LCST) 18, 19

m

macromolecules 1
 magnetovolume effect 255–258, 256–257
 maleic anhydride modified polystyrene (MA-SEBS) 282–284
 Marom and Weinberg model 177–178
 mercury 116
 modified cell model (MCM) 126, 128
 molecular dynamics (MD) simulation 259
 molecular weight (M_e) 1, 3–4, 4
 montmorillonite (MMT) 230–235, 231–233, 235
 Mori-Tanaka mean field theory 215, 216
 basic idea of 215–217
 basic theory and general expression of 217–219
 model comparison 220–223, 221–223
 thermal expansion coefficient, explicit expressions of 219–220
 thermal expansion of polymer composite 217–223
 Mori-Tanaka (M-T) model 220
 Schapery model 220–223, 221, 223
 Turner model 220–223, 221, 222
 Mori-Tanaka theory 208
 Eshelby equivalent inclusion method 209–213, 210–212
 Eshelby's tensor 213–215
 Mori-Tanaka mean field theory 215–223, 216
 self-consistent model 223–224, 223
 multi-walled CNT (MWCNT) 243–246, 243–246

n

nano-clay 230–236, 231–235
 nanocomposites 23
 nano-fillers 230
 carbon nanotube 243–247, 243–246
 graphene 247–251, 247–250, 251
 nano-clay 230–236, 231–235
 nano-silica 236–243, 236–242
 nano-silica 236–243, 236–242
 n-butane 5–6, 5
 negative thermal expansion (NTE) 98, 103, 108, 228, 251
 flexible network 252–255, 253–255
 magnetovolume effect 255–258, 256–257
 reduction of thermal expansion, fillers 251–258, 253

Nernst theorem 37
 nonbonded atomic interaction 9
 normal direction (ND) 230
 Noryl™ resin 14, 18
 n-pentane 6, 7
 nylon 6, 6, 13, 13

o

oriented molecules 266–273, 267–269, 271–272
 ortho-Ps (o-Ps) 139–142, 140, 142

p

parameters of polyoxymethylene (POM) 62, 63
 para-Ps (p-Ps) 139
 perturbed strain 213
 phase diagram 14
 of polymer blend 77–80, 78–79, 79
 of PS/PB mixture 18, 18
 of PS/PVME mixture 18, 19
 of PS/SBR 18–19, 19
 phase-separated system 78–80, 78, 79
 piston-die method 119–120, 119, 121
 Poisson contraction 109
 Poisson's ratio 192
 poly(alkyl methacrylate) with poly(cyclohexyl methacrylate) (PCHMA) 117–118
 poly(cyclopentyl methacrylate) (PCPMA) 117–118
 poly(dimethylsiloxane) (PDMS) 126
 poly(ethylene-co-octene) (EO) 132
 poly(hydroxypropyl ether of bisphenol A) (PO) 126
 poly(p-phenylene terephthalamide) (PPTA) 130
 polyamide 6 (PA6) 282
 polybutadiene (PBD) 18
 polycarbonate (PC) 141–143, 143
 polyethylene (PE) 4, 11, 11, 69–72, 91, 122, 266
 polyethylene terephthalates (PETs) 50
 polyimide film 154–155, 154–155
 polymer
 defined 1
 higher-order structure 5, 7–13, 8, 9, 10
 molecular weight 1–4, 2, 3, 4
 phase diagram and Flory-Huggins theory 18–23, 18–20, 22
 polymer alloy and blend 14–18, 14, 16, 17
 polymer composite 23–28, 24, 25
 primary structures 4–5
 secondary structures 5–7, 5–7
 polymer alloy 14–18, 14, 16, 17
 polymer blend 14–18, 14, 16, 17
 phase diagram of 77–80, 78–79, 79
 polymer composite 23–28, 24, 25
 Chow model, linear and volume thermal expansion coefficients of 205–208, 206, 208–209
 Mori-Tanaka Theory 217–223
 thermal expansion theories of 169–180
 Wang-Kwei model for 195–200, 196, 197, 199–200, 199–200

- polymer liquids 53–54, **54**
- polymer-polymer miscibility 19–20, 19–20
- polymethyl methacrylate (PMMA) 16, 66–68, 69
- polypropylene (PP) 11, 122, 266
- polystyrene (PS) 2, 66–68, 69, 126, 140–144
- polystyrene-polybutadiene copolymer 19
- polyvinyl alcohol (PVA) 9
- polyvinyl methyl ether (PVME) 18, 19
- positron annihilation lifetime spectroscopy (PALS) 50, 57, 136
 - free volume size 51
 - temperature evaluation of free volume 136–144, 137–144
- positronium (P_s) 139–140
- positrons 136–139
- PRD49 fiber 110–111
- pressure-volume-temperature (PVT) 115, 123
 - behavior measurement 118–128
 - bellows method 120–128, 120, 122–125, **127**
 - piston-die method 119–120, 119
- pseudo-equilibrium modulus 2
- q**
- quasi-harmonic approximation (QHA) 61
- r**
- radial distribution function 46
- random oriented SF composites 177
- reduction technologies
 - composite by fillers with negative thermal expansion 251–258, **253**
 - fillers 227–230
 - oriented molecules 266–273, 267–269, 271–272
 - polymer blends, elastomers 273–287, **274**, 275–280, 282–283
 - structural constraints into polymer backbone 258–266
 - using nano-fillers 230–251
- rigid functional group 260, 262–264, 262–263, **263–264**, 265–266
- rotational isomer 5, 5
- rule-of-mixtures (ROM) 170–171, 170, 188, 192–193, 230, 258
- s**
- scaling law 27
- scanning electron microscope (SEM) 237
- Schapery model 173, 175–176, 220–221
- Schneider model 176–177
- self-consistent harmonic model 98
 - experimental data, comparison of 102–103, 103
 - modeling 99–102
- self-consistent model 223–224, 223
- Shanghai Synchrotron Radiation Facility (SSRF) 145
- shear lag theories 177–179, 179–181, **179**
- short fiber (SF) reinforced composites 177–179, 179–181, **179**
- short-range/four-bond interaction/pentane effect 5
- single-walled CNT (SWCNT) 243, 247
- skeletal approximation 99
- small-angle X-ray scattering (SAXS) 147–148, 148, 149
- solid state (crystal lattice), thermal expansion of 38–41, 38–40
- spherical particle reinforced composites 171–175, 175
- spherical shell model 200–205, 202, 204
- spring-in-medium model 103–104, 104
 - experimental data, comparison of 107–110
 - thermal expansion model, preparation construction of 104–107, 104
- stress 201–202
- stress-strain relationship 183
- Strobl-Schneider method 148, 149
- structural constraints
 - chemical cross-linking 258–259, 259–261
 - reduction of thermal expansion 258–266
 - rigid functional group 260, 262–264, 262–263, **263–264**, 265–266
- Super Photon Ring-8 (Spring-8) 145
- synchrotron radiation 144–152, 147, 145–152
- syndiotactic PP (sPP) 12
- synthetic polymers 169
- t**
- Takahashi model 174, 176
- temperature-variable AFM 160–164, 161, 163, 164
- temperature-variable x-ray scattering 144–152, 145–152
- tetramethyl bisphenol-A polycarbonate (TMPC) 141–143, 143
- thermal expansion 136
 - coefficient of linear thermal expansion 128–135, 129, 130
 - coefficient of volume thermal expansion 115–119
 - contribution of free volume 51, 57–59, **58, 59**
 - crystal lattice in crystalline polymers 59–69
 - definition of 31–37, 31, 33–38
 - digital image correlation method 155–160, 156–160
 - emerging technologies of 136–160
 - equation of state 53–57, **54**
 - free volume 49–53, 49–51
 - fundamentals of 31–83
 - gas state 47–48, **48**
 - Grüneisen parameter 60–68, 63, 67, 69, 70
 - laser interferometry 153–155, 153–155
 - linear thermal expansion coefficients 68–69
 - liquid state 41–47, **42**
 - material mechanism of 38–47, 39
 - measurement of 115–164

thermal expansion (*Cont.*)

- PALS, temperature evaluation of free volume 136–144, 137–144
- polymer blend, phase diagram of 77–80, 78, 79, 79
- polymers mechanism of 48–69
- reduction technologies of. *see* reduction technologies
- solid state (crystal lattice) 38–41, 38–40
- temperature-variable AFM 160–164, 161, 163, 164
- temperature-variable x-ray scattering 144–152, 145–152
- thermal stress 80–83, 80–82
- two materials combined phenomenon 77–83
- thermal expansion coefficient 32, 37, 203
- thermal expansion stress 280
- thermal expansion theories. *see also* composite theory
 - cylindrical-shaped inclusion/fiber-reinforced composites 175–180
 - experimental data, comparison of 110–112, 112
 - linear chain model 89–98
 - linear thermal expansion coefficient 190–195, 193, 193, 195
 - polymer composites 169–180
 - random oriented SF composites, linear thermal expansion coefficient 177
 - rule-of-mixtures 170–171, 170
 - Schapery 180–195
 - self-consistent harmonic model 98–103
 - shear lag theories to calculate 177–179, 179–181, 179
 - spherical particle reinforced composites 171–175, 175
 - spring-in-medium model 103–110, 104
 - thermoelastic energy principles 182–185
 - unidirectional fiber composites 175–177
 - volume thermal expansion coefficient 185–189, 189, 190
- thermal stress 80–83, 80–82
- thermoelastic energy principles 182–185
- thermomechanical analysis (TMA) 128–129, 129, 130

- coefficient of linear thermal expansion 130–135
- expansion/compression mode 129
- measurement of 128–135
- penetration mode 131–135, 131–134, 135
- tension mode 130, 131
- tie molecules 8
- transmission electron microscopy (TEM) 134, 231
- transverse-to-flow direction (TD) 230–232
- Tummala and Friedberg model 172
- Turner model 171, 221
- Turner's formula 258
- two-component system 172

U

- unidirectional fiber composites 175–177
- unit cell 8, 11
- upper critical solution temperature (UCST) 18, 18

V

- van der Waals forces 9, 13, 53–54, 95–96
- viscoelastic function 1–3
- volume dilatometry 115–118, 116, 117, 118
- volume fraction 19, 20, 26, 27, 53, 59, 201
- volume thermal expansion coefficient 185–189, 189, 190, 203, 205–208, 206, 208–209

W

- Wang-Kwei model 173
- spherical composites 195–200, 196, 197, 199–200, 199–200
- wide-angle X-ray scattering (WAXS) 147–148, 148, 150, 151
- WLF formula 52–53

X

- X-ray absorption fine structure (XAFS) 146
- X-ray diffraction (XRD) 97, 98, 103, 249

Y

- Young's modulus 80