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Review

Effective thermal conductivity of polymer composites: Theoretical models and simulation models

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ABSTRACT

Polymer composites of highly effective thermal conductivity (ETC) are commonly used in various industries, for renewable energy systems and Electronic Systems. Owing to the low thermal conductivity (TC) of polymers, inserting particles with ultra-high TC into the polymer matrix makes it possible for polymer composites to possess high ETC. The ETC of polymer composites is determined by several factors, including the particle and matrix properties and microscopic structures. Modelling methods are powerful tools to understand how these factors influence the ETC of polymer composites. Modelling methods can be combined with experimental data and can be used to qualitatively and quantitatively analyse the impact of various factors on the ETC. Moreover, modelling methods can be used as a guide for the choice and design of particle-filled composites for engineering applications. Herein, we review the recent research on ETC models of polymer composites. First, the classical theoretical models of ETC for polymer composites are introduced. Then, novel theoretical and simulation models are described. We focus on the influence of the theoretical models and the simulation models of polymer composites at multiple scales. Finally, we conclude and give an outlook regarding the ETC models of polymer composites.

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Nomenclature

Symbols

f	volume fraction of particle (vol%)
R_I	interfacial thermal resistance between particle and matrix ($K \cdot m^2/W$)
k_{eff}	effective thermal conductivity of composites (W/m·K)
k_m	thermal conductivity of matrix (W/m·K)
k_p	thermal conductivity of particle (W/m·K)
k_p^{eff}	effective thermal conductivity of particle adding the effect of R_I
r	radius of particle
j	phase of B–L model or EMT
L_i	depolarization factor
$k_{eff,i}$	effective thermal conductivity of composites along the i-axis (i = x, y and z)
$\overline{k_{eff}}$	effective thermal conductivity tenser of composites
$\overline{k_m}$	thermal conductivity tenser of matrix
$\overline{k_p}$	thermal conductivity tenser of particle
$\overline{s_p}$	Eshelby tensor of particle
$\overline{I}$	identity tensor
p	aspect ratio of particle
B_0, B_1, B_2	experimental coefficients
ξ, ζ, η	transformational coordinates
α	orientation angle of h-BN
k_η^c, $k_{\xi-\zeta}^c$	effective thermal conductivities of the unit cell along the η direction and in the $\xi - \zeta$ plane
L, W, H	length, width, height of unit cell
a, b	size of h-BN
$\overline{s_{(i)}}$	second-rank Eshelby tensor common to the ith heterogeneity and all of its layers
$f_{(i)_{\alpha_i}}$	volume fraction of the α_ith layer of the ith heterogeneity
$\overline{A}_{(i)}^{(\alpha_i)}$	global strain concentration tensor
h	thickness of particle
n	number of layers of Multilayer graphene
h_m	thickness of monolayer graphene
C	specific heat
v	phonon velocity
Λ_{eff}	effective phonon mean free path
Λ	phonon mean-free path
D	lateral sizes of multilayer graphene
$k_{eff}(n)$	layer-dependent effective thermal conductivity of composites
$k_P(n)$	layer-dependent thermal conductivity of graphene
$k_i^c(n)$	equivalent thermal conductivity of composites along the i-axis (i = x, y and z)
$R_I(n)$	layer-dependent interface resistance
F	flatness ratio
L^e	Equivalent length of graphene nanoplate or carbon nanotube
k_p^e	equivalent thermal conductivity of graphene nanoplate or carbon nanotube
L_{CNT}	length of carbon nanotube
L_{GNP}	length of graphene nanoplate
$H(p)$	geometrical factor
y_a	amplitude of the wavy penny-shaped ellipsoidal heterogeneity
λ	length of the wavy penny-shaped ellipsoidal heterogeneity
$\overline{k_{11}}$, $\overline{k_{12}}$, $\overline{k_{22}}$	components of the effective compliance tensor
s	synergistic effect parameter
$k_{m,equ}$	equivalent thermal conductivity of unit cell
a_K	Kapitza radius, $k_m \cdot R_I$
θ_{opt}	optimal particle ratio
$k_{p,i}$	thermal conductivity of particle i
f_i	volume fraction of particle i
f_m	mass fraction of particle (wt%)
f_c	critical volume fraction of particle or percolation threshold
k_{nc}	effective thermal conductivity of the dead-end particle
f_{nc}	volume fraction in the dead-end particle
k_a	effective thermal conductivity the single aggregate
f_b	volume fraction of the backbone particles
f_a	volume fraction of the aggregates
f_{int}	volume fraction of the particles in an aggregate
k_1	effective thermal conductivity in parallel with the direction of the heat flow
k_o, k_r	thermal conductivity of the layer with the oriented and random graphite flakes
ρ, ρ_o, ρ_r	density of the composite and the oriented and randomly graphite flakes
$k_{p,e}$	thermal conductivity of the element
f'_{void}	effective fraction of pores
f_{void}	volume fraction of the pore
k_m^{eff}	effective thermal conductivity of the effective matrix
k'_{eff}	effective thermal conductivity of the porous composite
p_{void}	shape factor of pores
f_{matrix}	volume fraction of the matrix
k_{void}	thermal conductivity of the pore
f_{max}	maximum volume fraction
ρ_p, ρ_m	densities of the particle and matrix
k_s	thermal conductivity of the solid phase
f_s	volume fraction of the solid phase
k_{v-l}	thermal conductivity of the gas and liquid phases
k_x^c, k_z^c	effective thermal conductivity of the cell in-plane and through-thickness

Abbreviations

TC	thermal conductivity
ETC	effective thermal conductivity
EMA	effective medium approximation
M-G	Maxwell–Garnett
H–J	Hasselman–Johnson
B–H	Bruggeman–Hanai
IE	integral embedding
ITR	interfacial thermal resistance
B–L	Bruggeman–Landauer
EMT	effective medium theory
M-T	Mori–Tanaka
MWCNT	multi-walled carbon nanotube
MD	molecular dynamics
GNP	graphene nanoplate
CNT	carbon nanotube
SWCNT	single-walled carbon nanotube
CTR	contact thermal resistance
SEM	scanning electron microscopy
MC	Monte Carlo
FEM	finite element method
EMD	equilibrium molecular dynamics
NEMD	non-equilibrium molecular dynamics
RNEMD	reverse non-equilibrium molecular dynamics
DPD	dissipative particle dynamics
LBM	lattice Boltzmann method
LGA	lattice gas automata
SPH	smoothed particle hydrodynamics
TIM	thermal interface materials
FDM	finite difference method
EFG	element-free Galerkin