

ON SOME GENERAL IMPERFECT INTERFACE MODELS FOR CONDUCTIVITY PROBLEM

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Abstract. Three general imperfect interface models for thermal conduction are presented. The discontinuity of the microscopic field is described through the interface parameters: one characterizes the temperature jump, and another controls the heat flux jump. These models include the highly and lowly conducting ones as particular cases. The effective conductivity of composite materials with imperfect interfaces is derived from several effective medium approximations. Unlike the perfect interface, the effective conductivity of a composite containing imperfectly bonded inclusions depends on the size of the particles. The results for these models are illustrated by numerical calculations. Some discussions are also presented.

Keywords: general imperfect interface, interface parameters, effective conductivity.

1. INTRODUCTION

The interface between the components is one of the factors affecting the effective properties as well as the microscopic fields of the composite material. In the context of thermal conduction, four kinds of interfaces are discussed. The first is the perfect interface, which is widely adopted in conventional composites, assuming that both the temperature and heat flux are continuous across the interface. The second one is the well-known Kapitza's thermal resistance model, also called the lowly conducting interface model (LC), according to which the temperature is discontinuous while the normal heat flux component is continuous and proportional to the temperature jump across the

interface. Dual to the lowly conducting model, the highly conducting interface model (HC) assumes that the normal heat flux is discontinuous across the interface while the temperature is continuous across it. The last and most complex model is the general imperfect interface one when both the temperature and heat flux are discontinuous.

While previous studies have mainly focused on the thermal resistance or highly conducting cases, the general imperfect interface model remains an object for further research. In [1], Pavanello et al. used the two dual T and Π models to describe the interface between different phases. Another general imperfect interface model was proposed in the works of Gu et al. [2] and Le-Quang [3]. In these works, the interface is considered as the limiting case of an ultra-thin isotropic interphase situated between the inhomogeneity and the matrix. The discontinuity of both local conduction fields is described through two interface material parameters, which depend on the isotropic conductivity of the interphase. Recently, Pham and Nguyen [4] constructed a general imperfect interface model for thermal conduction based on the compound sphere assemblage involving an intermediate anisotropic thin coating. The aim of this study is to provide a summary of general interface models and compare them with each other.

The paper is structured as follows. Section 2 presents three general imperfect interface models. In Section 3, the effective conductivity of composite materials with imperfect interfaces is constructed from several effective medium approximations. In Section 4, the numerical calculations are shown. The discussion and some remarks are provided in the last part.

2. GENERAL IMPERFECT INTERFACE MODELS

2.1. Pavanello's model

Pavanello et al. proposed two dual schemes to describe the complex behavior of the interface. These two models are initiated from the classical T and Π electric lattice structures. The T-model consists of three thin layers between the inclusion and the matrix: an internal lowly conducting (L), an intermediate highly conducting (H), and an external lowly conducting layer (L), which can be called the *LHL* model, while the dual Π -model is the *HLH* one (Fig. 1). The discontinuities of temperature and heat flux are described by the following expressions [1]

$$[[T]] = -\alpha(J^+ + J^-), \quad (1)$$

$$[[J]] = c_s \alpha \Delta_s J^- + c_s \Delta_s T^-, \quad \text{for T-model}, \quad (2)$$

$$[[T]] = -\alpha J^- + \alpha c_s \Delta_s T^-, \quad (3)$$

$$[[J]] = c_s \Delta_s (T^+ + T^-), \quad \text{for } \Pi\text{-model}, \quad (4)$$

in which $(\bullet)^+$ and $(\bullet)^-$ stand for the values of the quantity $(\bullet)$ on the sides of the inclusion and the matrix, respectively. $\Delta_s(\bullet)$ is the surface Laplacian of the quantity $(\bullet)$. c_s denotes the surface conductivity with dimension W/K, while α designates the Kapitza thermal resistance with dimension $\text{m}^2\text{K}/\text{W}$.

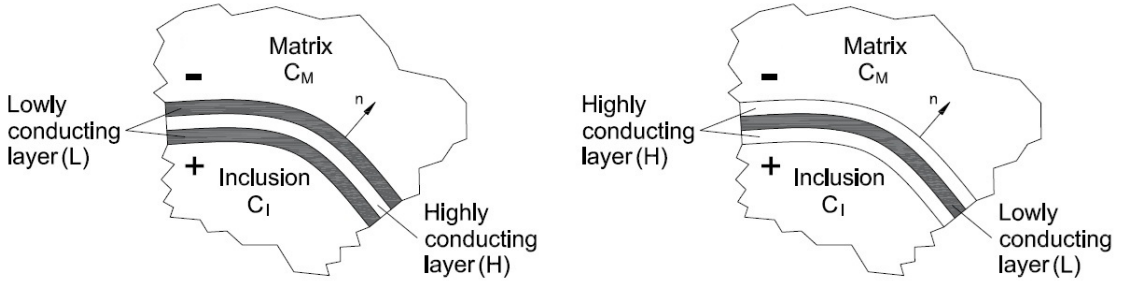


Fig. 1. The dual imperfect interfaces: T-model (left) and Π -model (right)

2.2. Gu's model

Gu et al. [2] consider a configuration in which an inclusion phase $\Omega^{(i)}$ is embedded in the matrix phase $\Omega^{(M)}$ via a thin interphase of uniform thickness h . The interfaces between the interphase and the matrix, as well as between the interphase and the inclusion, are assumed to be perfect. The interphase is replaced by a zero-thickness imperfect interface located at the middle surface Γ of the interphase, and the matrix phase and inclusion are extended up to Γ (Fig. 2). By requiring that the temperature and normal flux jumps across the interphase be equal to the corresponding jumps across the interface, and by applying Taylor expansion [5], the jumps across the interface are characterized by the relations

$$[[T]] = h\gamma\langle J \rangle, \quad (5)$$

$$[[J]] = h\beta\Delta_s\langle T \rangle, \quad (6)$$

in which $\langle \bullet \rangle$ is the interfacial average operator defined by $\langle \bullet \rangle = \frac{\bullet^+ + \bullet^-}{2}$, and γ, β are two interface material parameters defined by

$$\gamma = \frac{1}{2} \left(\frac{1}{c_M} + \frac{1}{c_I} - \frac{2}{c_{Inter}} \right), \quad (7)$$

$$\beta = \frac{1}{2} (2c_{Inter} - c_I - c_M), \quad (8)$$

where c_I, c_{Inter}, c_M are the conductivities of the inclusion, interphase, and matrix, respectively.

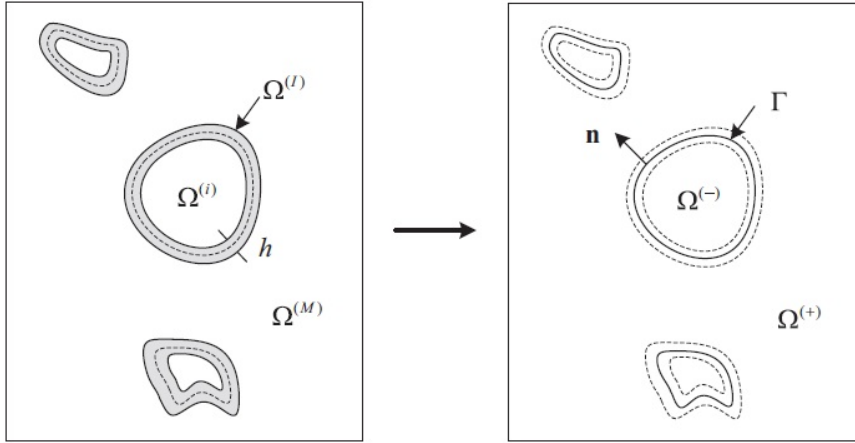


Fig. 2. Gu's imperfect interface model [2]

2.3. Pham's model

Consider a compound sphere consisting of a spherical inhomogeneity of radius R with conductivity c_I , which is coated by an anisotropic coating with conductivity in the normal direction c_N and in the transverse direction c_T . This compound is finally coated by a spherical matrix shell with conductivity c_M . Here, the coating is composed of m ultra-thin coatings of high conductivity $c_2 = \frac{2c_s}{h}$ alternating with m ultra-thin coatings of low conductivity $c_3 = \frac{h}{2\alpha}$ (Fig. 3). In the limit $m \rightarrow \infty$ and the ratio between the thickness of the coating and the radius of the inhomogeneity tends to zero, $\frac{h}{R} \rightarrow 0$, one obtains

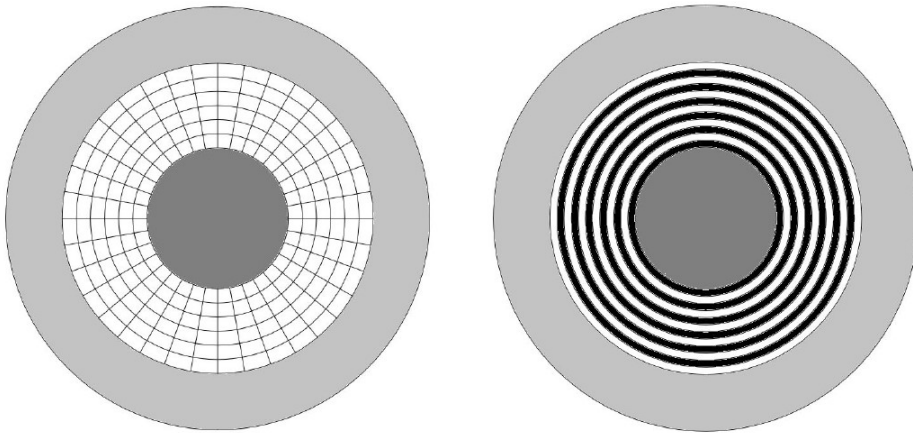


Fig. 3. A compound sphere with anisotropic coating (left), the anisotropic coating is modelled by alternating highly and lowly conducting shells (right)

$$v_c = 2v_2 = 2v_3 = \frac{dh}{R}v_I, \quad (9)$$

$$c_T = \frac{c_s}{h}, \quad c_N = \frac{h}{\alpha}. \quad (10)$$

The jumps of temperature and normal heat flux are characterized by the following relations [4]

$$T^+ - T^- = \frac{h}{4} \left(\frac{1}{c_M} + \frac{1}{c_I} - \frac{2}{c_N} \right) (J^+ + J^-), \quad (11)$$

$$J^+ - J^- = \frac{h}{4} (2c_T - c_I - c_M) (\Delta_s T^+ + \Delta_s T^-). \quad (12)$$

In the limit of a zero-thickness interface ($h \rightarrow 0$), it is easy to obtain the relations for the interface in the form

$$[T] = -\frac{\alpha}{2} (J^+ + J^-) = -\alpha \langle J \rangle, \quad (13)$$

$$[J] = \frac{c_s}{2} (\Delta_s T^+ + \Delta_s T^-) = c_s \Delta_s \langle T \rangle. \quad (14)$$

3. EFFECTIVE CONDUCTIVITY OF COMPOSITE WITH IMPERFECT INTERFACE

3.1. Effective conductivity for Pavanello's model

When the interfaces are described by Eqs. (1), (2) or Eqs. (3), (4), Pavanello et al. generalized the Maxwell approach to obtain the effective conductivity [1]

$$c^{eff} = c_M \left[1 + \frac{dv_I B}{C - (d-1)v_I B} \right]^{-1}, \quad (15)$$

where $d = 2$ or $d = 3$ for circular or spherical inhomogeneity, v_I is the volume fraction of the inhomogeneity, and the parameters B and C are defined as follows

$$B = c_M - c_I + \frac{2\alpha c_I c_M}{R} - (d-1) \frac{c_s}{R} \left(1 - \frac{\alpha c_M}{R} \right) \left(1 + \frac{\alpha c_I}{R} \right), \quad (16)$$

$$C = c_I + (d-1) \left\{ c_M + \frac{2\alpha c_I c_M}{R} + \frac{c_s}{R} \left[1 + (d-1) \frac{\alpha c_M}{R} \right] \left(1 + \frac{\alpha c_I}{R} \right) \right\}, \quad (17)$$

for the T-model, and

$$B = c_M - c_I + \frac{\alpha c_I c_M}{R} - (d-1)^2 \frac{c_s^2 \alpha}{R^3} - \frac{(d-1)c_s}{R} \left(2 - \frac{\alpha c_M}{R} + \frac{\alpha c_I}{R} \right), \quad (18)$$

$$C = c_I + (d-1) \left\{ c_M + \frac{\alpha c_I c_M}{R} + (d-1) \frac{c_s^2 \alpha}{R^3} + \frac{c_s}{R} \left[2 + (d-1) \frac{\alpha c_M}{R} + \frac{\alpha c_I}{R} \right] \right\}, \quad (19)$$

for the Π -model.

3.2. Effective conductivity for Gu's model

With the model of interface (5), (6), Gu et al. [2] used several effective medium approximations (EMA) such as the dilute distribution (DD), Mori–Tanaka (MT), self-consistent (SC), and generalized self-consistent (GSCM) schemes to estimate the effective conductivity of the composite. In this subsection, we present only the expression for the GSCM scheme

$$c_{GSCM}^{eff} = c_M \left[1 + \frac{3v_I[\Psi + (1 - c_M/c_I)]}{3(c_M/c_I - \delta\gamma c_M) + (1 - v_I)[\Psi + (1 - c_M/c_I)]} \right], \quad (20)$$

in which $\delta = h/R$ and $\Psi = \delta(\gamma c_M + 2\beta/c_I)$. Note that the expression (20) is identical to the one from the Mori–Tanaka scheme [2].

3.3. Effective conductivity for Pham's model

By using the differential substitution scheme (see more details in [6]), the effective conductivity of the compound sphere can be obtained. This scheme starts with the inclusion. At each step of the procedure, a volume amount $\Delta v = \frac{1}{2m} \frac{dhv_I}{R}$ of a spherical coating shell of conductivity $c_2 = \frac{2c_s}{h}$ (or $c_3 = \frac{h}{2\alpha}$) is alternatively added to the already constructed compound sphere from the previous step. When the added volume reaches $v_c = \frac{dhv_I}{R}$, we obtain the effective conductivity as follows [4]

$$c^{eff} = \left[\frac{v_I}{c_{Is} + (d-1)c_M} + \frac{1-v_I}{dc_M} \right]^{-1} - (d-1)c_M, \quad (21)$$

in which c_{Is} is the function of the inhomogeneity radius R such as

$$c_{Is} = \left[c_I + \frac{(d-1)c_s}{R} \right] \left[1 + \frac{\alpha c_I}{R} \right]^{-1}, \quad (22)$$

where c_s and α are the interface parameters presented in the previous subsection.

4. NUMERICAL CALCULATION

In this section, the effective conductivity of a composite with a general imperfect interface is calculated. We take the parameters as in Gu's paper [2]: the thermal conductivities of the inhomogeneity and matrix are $c_I = 0.1 \text{ W/m/K}$ and $c_M = 1 \text{ W/m/K}$, respectively. The interface parameters c_s and α are chosen to be equivalent to those in [2] ($c_s = \frac{hc_{Inter}}{2}$ and $\alpha = \frac{h}{2c_{Inter}}$, with $h = 50 \text{ nm}$ and c_{Inter} designating the thickness and isotropic conductivity of the interphase, respectively), and are shown in Table 1.

Table 1. Parameters of interface

	Gu et al. [2]	Pham's model	
	c_{Inter} (W/m/K)	c_s (W/K)	α (m ² K/W)
Case 1	10^2	2.5×10^{-6}	2.5×10^{-10}
Case 2	5×10^{-3}	1.25×10^{-10}	5×10^{-6}
Case 3	5×10^{-2}	1.25×10^{-9}	5×10^{-7}

Figs. 4–6 present the effective conductivity as a function of the inhomogeneity volume fraction v_I . One can see that when $c_{Inter} \gg c_I$ and c_M , or equivalently $c_s \gg \alpha$, the effective conductivity is an increasing function of the volume fraction v_I , as in the case of the highly conducting HC (Fig. 4). The reason is that the superconducting effect is predominant. Conversely, when $c_{Inter} \ll c_I$ and c_M , or $c_s \ll \alpha$, the effective conductivity is a decreasing function of the volume fraction v_I , as in the case of the lowly conducting LC (Fig. 5). In this case, the thermal resistance effect dominates. When c_{Inter} , c_I , c_M , or c_s , α are of the same order, the macroscopic conductivity can be an increasing or decreasing function, depending on the specific values of the interface parameters (Fig. 6).

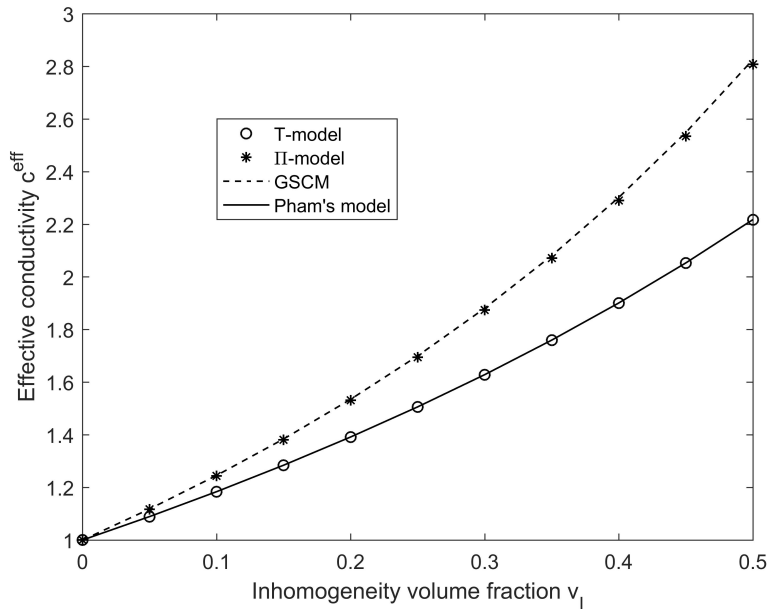


Fig. 4. The effective conductivity as a function of the inhomogeneity volume fraction v_I with radius $R = 1 \mu\text{m}$, HC case

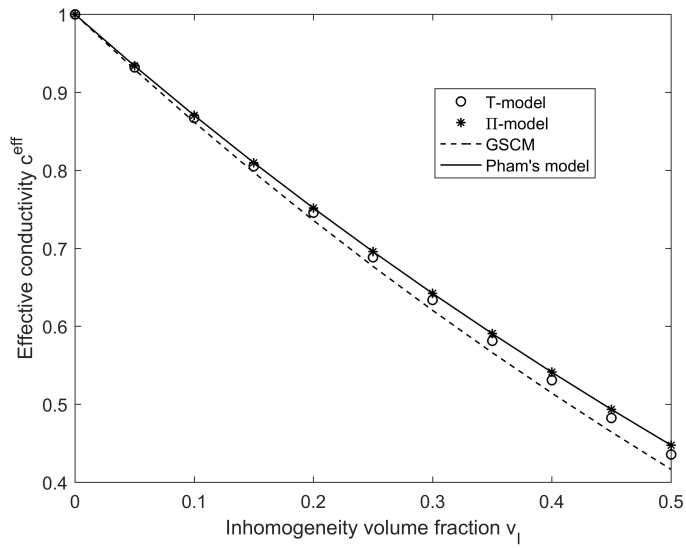


Fig. 5. The effective conductivity as a function of the inhomogeneity volume fraction v_I with radius $R = 1 \mu\text{m}$, LC case

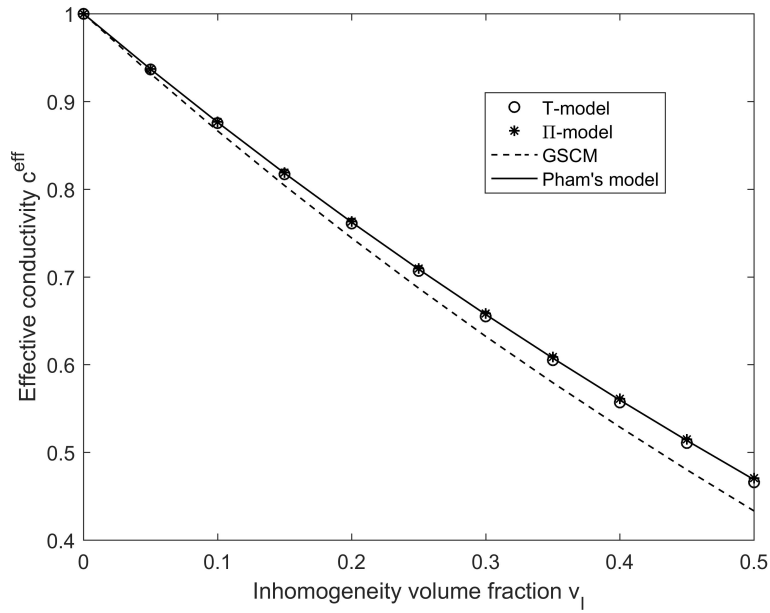


Fig. 6. The effective conductivity as a function of the inhomogeneity volume fraction v_I with radius $R = 1 \mu\text{m}$, intermediate case

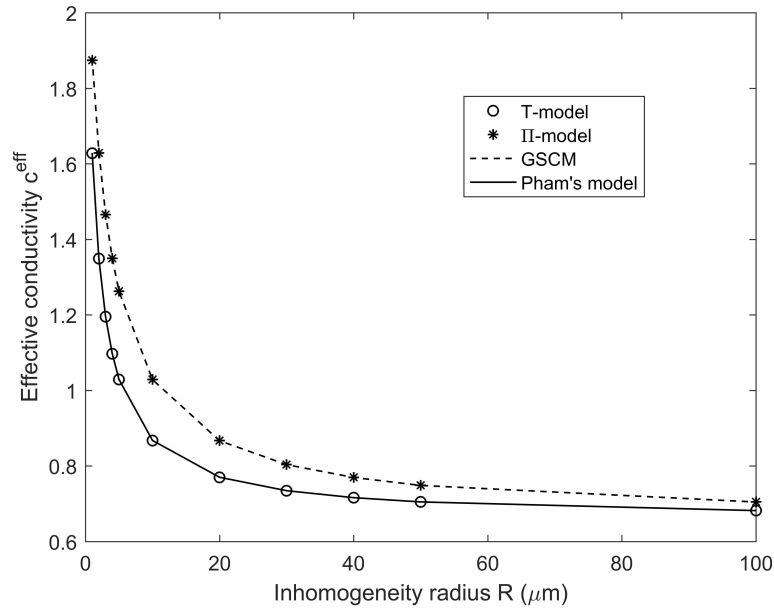


Fig. 7. The effective conductivity as a function of the inhomogeneity radius R with volume fraction $v_I = 0.3$, HC case

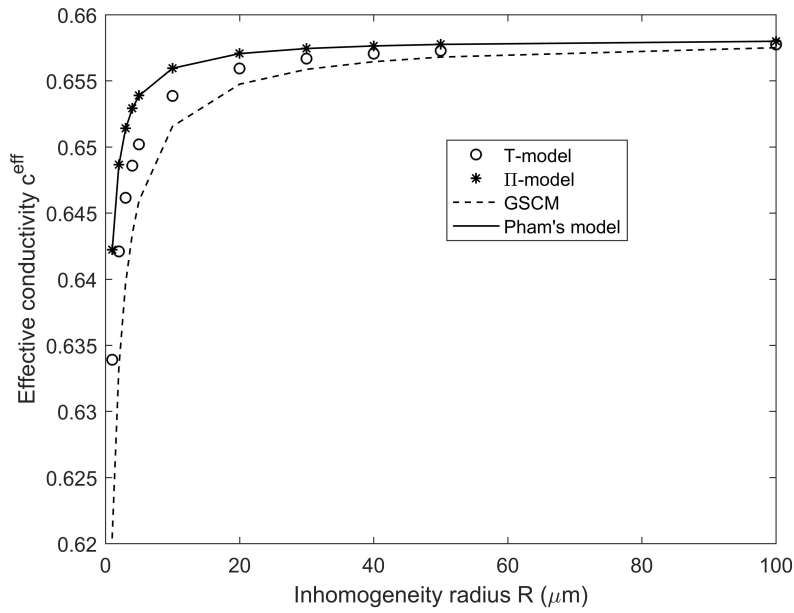


Fig. 8. The effective conductivity as a function of the inhomogeneity radius R with volume fraction $v_I = 0.3$, LC case

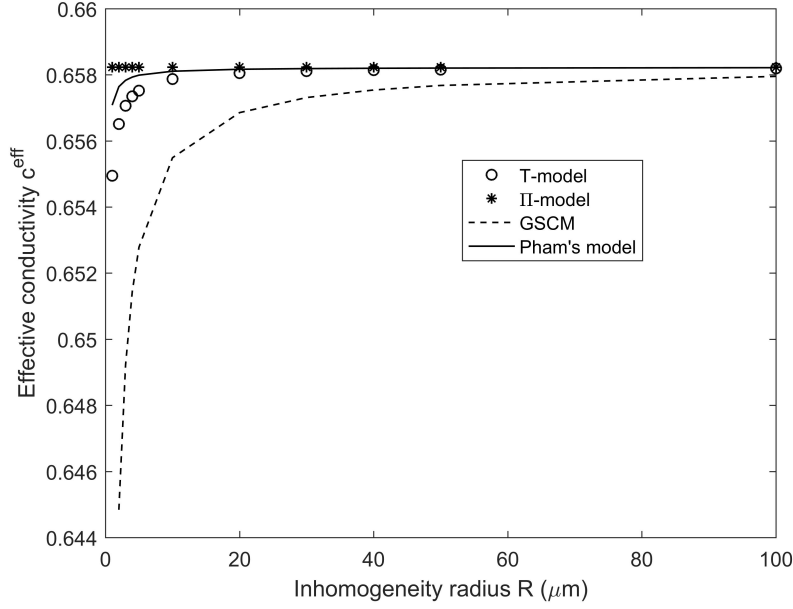


Fig. 9. The effective conductivity as a function of the inhomogeneity radius R with volume fraction $v_I = 0.3$, intermediate case

In contrast to the perfect interface, the effective conductivity of a composite containing imperfectly bonded inclusions depends on the size of the particles. Figs. 7–9 show the variation of macroscopic conductivity as a function of the inhomogeneity radius R for the three cases, respectively. The effective conductivity decreases as the radius R increases for the HC case (Fig. 7), and the effective conductivity increases as the radius R decreases for the LC case (Fig. 8). One can see that the results for these models are comparable.

5. DISCUSSION

One can observe that all three models presented in the previous section include the lowly conducting (LC) and highly conducting (HC) cases as specific examples. For Pavanello's model and Pham's model, the highly conducting imperfect interface can be reproduced if the Kapitza thermal resistance $\alpha = 0$

$$\begin{aligned}
 \llbracket T \rrbracket &= 0, \\
 \llbracket J \rrbracket &= c_s \Delta_s T^-, & \text{for T-model,} \\
 \llbracket J \rrbracket &= c_s \Delta_s (T^+ + T^-), & \text{for II-model,} \\
 \llbracket J \rrbracket &= c_s \Delta_s T, & \text{Pham's model,}
 \end{aligned} \tag{23}$$

while the lowly conducting case can be obtained if the surface conductivity $c_s = 0$

$$\begin{aligned} \llbracket J \rrbracket &= 0, \\ \llbracket T \rrbracket &= -\alpha(J^+ + J^-), & \text{for T-model,} \\ \llbracket T \rrbracket &= -\alpha J^-, & \text{for II-model,} \\ \llbracket T \rrbracket &= -\alpha J, & \text{Pham's model.} \end{aligned} \quad (24)$$

It is easy to see that in the HC case, the jump of normal heat flux depends only on the temperature on the matrix side for the T-model, while in the LC case, the jump of temperature depends only on the heat flux on the matrix side for the II-model.

For Gu's model, the cases of a highly or lowly conducting interface are obtained when the conductivity of the interphase is much larger or smaller than that of its surrounding phases. Indeed, when the interphase is highly conducting, $c_{Inter} \gg c_M$ and $c_{Inter} \gg c_I$, the general imperfect interface conditions (5), (6) degenerate into the HC model as follows

$$\begin{aligned} \llbracket T \rrbracket &= 0, \\ \llbracket J \rrbracket &= hc_{Inter}\Delta_s T. \end{aligned} \quad (25)$$

Conversely, when the interphase is lowly conducting, $c_{Inter} \ll c_M$ and $c_{Inter} \ll c_I$, the general imperfect interface (5), (6) reduces to the LC model described by

$$\begin{aligned} \llbracket J \rrbracket &= 0, \\ \llbracket T \rrbracket &= -\frac{h}{c_{Inter}}J. \end{aligned} \quad (26)$$

One can see that cases 1 and 2 are equivalent to the HC and LC models, respectively, while case 3 can be considered as an intermediate situation.

In Gu's model, the two interface parameters γ and β depend on the conductivity of the isotropic interphase. In other words, only the conductivity of the interphase c_{Inter} drives the behavior of the interface. Pavanello's and Pham's models are more general, with two independent parameters, α and c_s . In Pham's model, an infinite number of ultra-thin layers with high and low conductivity are alternately arranged between the inhomogeneity and the matrix. That leads to an anisotropic interface in which the normal resistance (as in the lowly conducting case) and tangential conductance (as in the highly conducting case) are completely independent.

As mentioned above, the T-model is equivalent to the LHL model in the sense that the spherical inhomogeneity with conductivity c_I is coated by a thin shell of low conductivity $\frac{h}{\alpha}$, which in turn is coated by a thin shell of high conductivity $\frac{c_s}{h}$, and finally, it is coated by a thin shell of low conductivity $\frac{h}{\alpha}$. By applying the substitution scheme [6],

one obtains the conductivity of the equivalent inclusion (in the limit $h \rightarrow 0$) as follows

$$c_{ILHL} = \frac{c_I + (d-1)\frac{c_s}{R} + (d-1)\frac{c_s\alpha}{R^2}c_I}{1 + \frac{2\alpha}{R}c_I + (d-1)\frac{c_s\alpha}{R^2} + (d-1)\frac{c_s\alpha^2}{R^3}c_I}. \quad (27)$$

Similarly, the equivalent inclusion for the Π -model (or HLH model) has the following expression

$$c_{IHLH} = \frac{c_I + 2(d-1)\frac{c_s}{R} + (d-1)\frac{c_s\alpha}{R^2}c_I + (d-1)^2\frac{c_s^2\alpha}{R^3}}{1 + \frac{\alpha}{R}c_I + (d-1)\frac{c_s\alpha}{R^2}}. \quad (28)$$

If these equivalent inclusions are embedded in a spherical matrix shell with conductivity c_M , the effective conductivity c_T^{eff} for the T-model or c_{Π}^{eff} for the Π -model can be obtained by formulation (21), in which c_{Is} is replaced by c_{ILHL} or c_{IHLH} , respectively, as follows

$$c_T^{eff} = \left[\frac{v_I}{c_{ILHL} + (d-1)c_M} + \frac{1-v_I}{dc_M} \right]^{-1} - (d-1)c_M, \quad (29)$$

$$c_{\Pi}^{eff} = \left[\frac{v_I}{c_{IHLH} + (d-1)c_M} + \frac{1-v_I}{dc_M} \right]^{-1} - (d-1)c_M. \quad (30)$$

Comparing (27) and (28), one can see that $c_{IHLH} > c_{ILHL}$. The consequence is that $c_{\Pi}^{eff} > c_T^{eff}$ because (21) is a monotonic function of the conductivity of the equivalent inclusion. This explains why all the curves of the Π -model always lie above the curves of the T-model, as seen in Figs. 4–9. Numerical results show that the curves of Pham's model always lie between those of the T and Π models.

Finally, the expressions (15), (21) can determine the effective conductivity for both circular (2D) or spherical (3D) inclusion composites, while the expression (20) determines the macroscopic conductivity only for the spherical inhomogeneity case.

6. CONCLUSION AND PERSPECTIVES

In recent analyses of nanocomposites, the behavior of the interface can not be simply described through the lowly or highly conducting models. In this work, three general imperfect interface models for thermal conduction are presented. Some conclusions are drawn:

- The temperature and heat flux jumps are characterized by two interface parameters;
- From the jump conditions of the microscopic fields at the interface, the effective conductivity of the composite material is derived using different effective medium approximations;
- All these models can be used to describe the complex behavior of the interface.

Due to the similarity in physical essence between the conductivity problem and other transport phenomena such as electricity and magnetism, these models can be applied to those problems. On the other hand, constructing a general imperfect interface model for the elastic problem is also a further research.

DECLARATION OF COMPETING INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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