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HIGHER-GRADE THEORY OF HEAT CONDUCTION AND SIZE EFFECTS

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Abstract: *It is experimentally evident that size-dependent effects are observed in small samples of nano/micro-scale dimensions. On the other hand, the classical theory of heat conduction is scale invariant. Incorporation of higher-order gradients of primary field variables into constitutive relationships yields a qualitative explanation of size-effects. Study of stationary heat conduction in bi-layer is rather simple 1D problem which can be solved analytically even within the higher-grade theory despite the high-order differential equations. Having known the exact solution, one can get a reliable analysis of size-effects with avoiding any numerical uncertainties. The influence of boundary conditions, material coefficients and geometrical dimensions on the temperature distribution in bi-layer is studied and discussed in this paper.*

Keywords: Fourier law, Gibbs free energy, Higher-grade theory, Heat flux, Additional boundary densities

1. Introduction

Thermal conductivity has always been described using a local theory. However, the local theory was unable to explain certain experimental observations occurring mainly in micro/nano length scale devices. Energy is transported by many different kinds of particles or excitations. The process is inherently nonlocal, since the particles or excitations arrive at a point in space having brought the energy from other points. Generally, a nonlocal theory of transport is required whenever the mean free path of particles or excitations is long compared to the distance scale of variations in the driving force (temperature gradient). Mahan and Claro (1988) developed nonlocal theory of thermal conductivity by phonons and shown that the need for nonlocal theory does not depend on whether ∇T is large or small. Instead, it depends on whether $\nabla^2 T$ varies rapidly on the distance scale of a phonon mean free path. Since the constitutive law in nonlocal theory is given by functional relationship between the heat flux and temperature gradient, the gradients of ∇T play a role inside the area of nonlocality (Sladek et al, 2022).

2. Heat conduction equation within higher-grade theory

Making use the 1st and 2nd law of thermodynamics, one can show that the rate of density of the Gibbs free energy for classical heat conduction process is given as (Sladek et al, 2022)

$$\dot{g}(\dot{T}, \nabla T) = -\sigma \dot{T} + \kappa_{ij} T_{,i} T_{,j} / 2T_0 \tag{1}$$

where T, T_0, σ, κ_{ij} stand for the temperature, reference value of temperature, entropy density, tensor of heat conduction coefficients, respectively. Furthermore, the Gibbs free energy is decreasing under irreversible processes, when the system is not in equilibrium, while in equilibrium reaches its minimum. Thus, minimization of the Gibbs free energy can serve as the variation principle for derivation of complete

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formulation of the heat conduction process. In the classical theory, the heat flux vector (the amount of heat that flows through a unit area per unit time) is expressed by the Fourier law $\lambda_i = -\kappa_{ij} T_{,j}$. It is known that consideration of higher-grade gradients of field variables in continua models gives rise to scale dependent solutions and possible explanation of size effects observed in small size samples. Incorporating the 2[nd] order gradients of temperature into the Gibbs free energy functional (1), this becomes

$$\dot{g}(\dot{T}, \nabla T, \nabla^2 T) = -\sigma \dot{T} + \kappa_{ij} T_{,i} T_{,j} / 2T_0 + \alpha_{ijkl} T_{,ij} T_{,kl} / 2T_0 \tag{2}$$

with α_{ijkl} being the tensor of higher order thermal conductivity coefficients, and $\mu_{ij} = \alpha_{ijkl} T_{,kl}$ is the energetically conjugated field to $T_{,ij}$. For simplicity, we assume isotropic materials ($\kappa_{ij} = \kappa \delta_{ij}$) and $\alpha_{ijkl} = l^2 \delta_{kl} \kappa_{ij}$ with l being the microstructural-length scale parameter. Now, application of the variation principle to 2D stationary heat conduction problems with the functional corresponding to the Gibbs free energy density (2) yields the governing equation (Sladek et al, 2022)

$$\kappa\left(1 - l^2 \nabla^2\right) \nabla^2 T = 0 \text{ , in } \Omega \tag{3}$$

and the possible boundary conditions for two pairs of boundary densities (Λ, T) and (η, χ):

$$\Lambda\big|_{\Gamma_f} = \overline{\Lambda} \quad \text{or} \quad T\big|_{\Gamma_T} = \overline{T} \quad \text{with} \quad \Gamma_T \cup \Gamma_\Lambda = \partial\Omega \ ; \quad \eta\big|_{\Gamma_\eta} = \overline{\eta} \quad \text{or} \quad \chi\big|_{\Gamma_\chi} = \overline{\chi} \text{ with } \quad \Gamma_\chi \cup \Gamma_\eta = \partial\Omega \ ,$$

with the heat flux $\Lambda = -\kappa n_i \left(1 - l^2 \nabla^2\right) T_{,i}$ and additional boundary densities $\eta := n_i n_j \mu_{ij}$, $\chi := n_k T_{,k}$.

2.1. Bi-layer composite system

Consider two infinite layers A and B with perfect contact on their interface $x = 0$ and prescribed temperature values T_a on their outer surfaces with h_a being the layer thickness for $a \in \{A, B\}$. Then $x \in [-h_A, 0] \cup [0, h_B]$. Introducing the dimensionless coordinate, temperature and heat conduction coefficients by $y = x / h_B$, $\theta = (T - T_0) / T_0$, $k_a = \kappa_a / \kappa_0$ with T_0 and κ_0 being arbitrarily chosen, we have the general solution of the considered 1D problem is given as

$$\theta(y) = \begin{cases} B_1 + c_1 \left(\dfrac{l_B}{h_B} \right)^2 \left(B_3 + B_4 \right) + \dfrac{\kappa_B}{\kappa_A} B_2 y + f(y), & y \in \left[-h_A / h_B, \, 0 \right] \\ B_1 + B_2 y + \left(\dfrac{l_B}{h_B} \right)^2 \left(B_3 \mathrm{e}^{-(h_B y / l_B)} + B_4 \mathrm{e}^{(h_B y / l_B)} \right), & y \in [0, \, 1] \end{cases} \tag{4}$$

where $f(y) := \dfrac{1}{2} \dfrac{l_A}{h_B} \left\{ \left[-c_1 B_2 + \dfrac{l_B}{h_B} \left(c_3 B_3 + c_2 B_4 \right) \right] \mathrm{e}^{-(h_B y / l_A)} + \left[c_1 B_2 + \dfrac{l_B}{h_B} \left(c_2 B_3 + c_3 B_4 \right) \right] \mathrm{e}^{(h_B y / l_A)} \right\}$

The integration constants $B_\bullet$ are specified for two kinds of boundary value problems (Sladek et al, 2022):

$\theta(1) = \theta_B$, $\theta(-h_A / h_B) = \theta_A$, (i) $\eta(1) = 0$, $\eta(-h_A / h_B) = 0$; (ii) $\chi(1) = 0$, $\chi(-h_A / h_B) = 0$.

2.2. Illustration of size-effects

In this section, we illustrate the differences between the temperature distributions by the classical and higher-grade theory of heat conduction in bi-layer system represented by two infinite layers with perfect contact on interface. Furthermore, we discuss the conditions under which the size-effects occurs.

Fig. 1 shows that no size-effect occurs in case of b.c. (i) for any values of the l_a / h_a parameters in contrast to the case of b.c. (ii) as long as $\kappa_A = \kappa_B$.

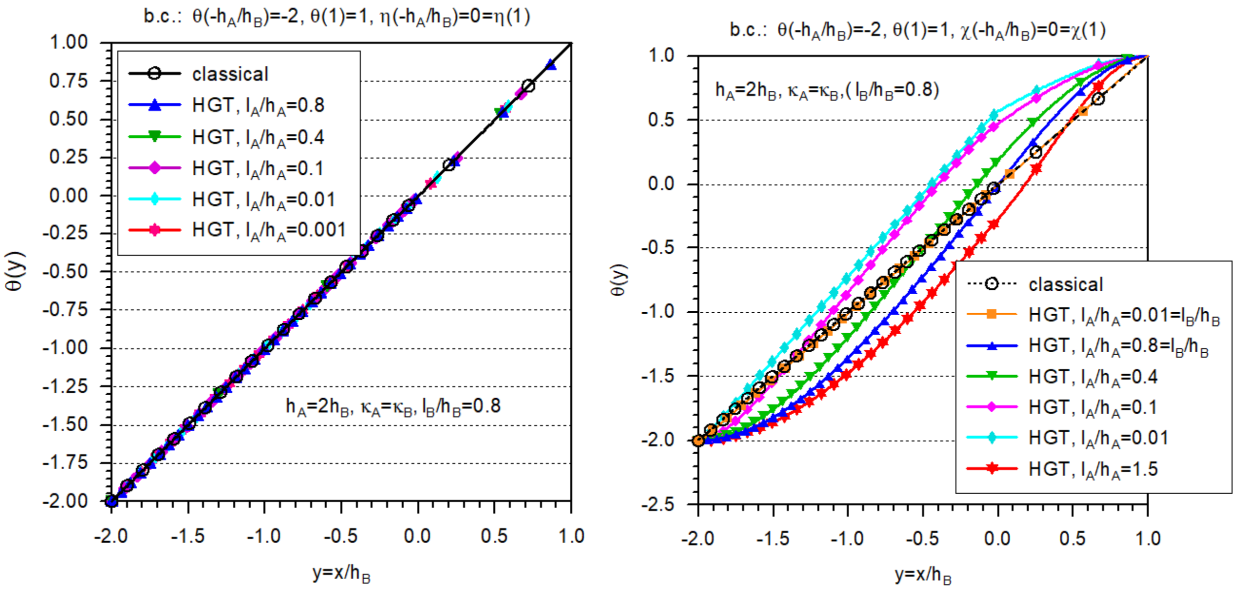

Fig.1: Temperature distributions for two kinds of b.c.(variant (i) – left; variant (ii) – right) and various values of l_A / h_A parameter in the bi-layer with $\kappa_A = \kappa_B$

In the composite bi-material layered system with $\kappa_A \neq \kappa_B$ and $l_B / h_B = \text{const} = 0.8$ (Fig.2), the size-effect occurs in case of both variants of b.c. and it is diminishing with decreasing l_A / h_A only in case of b.c. (i).

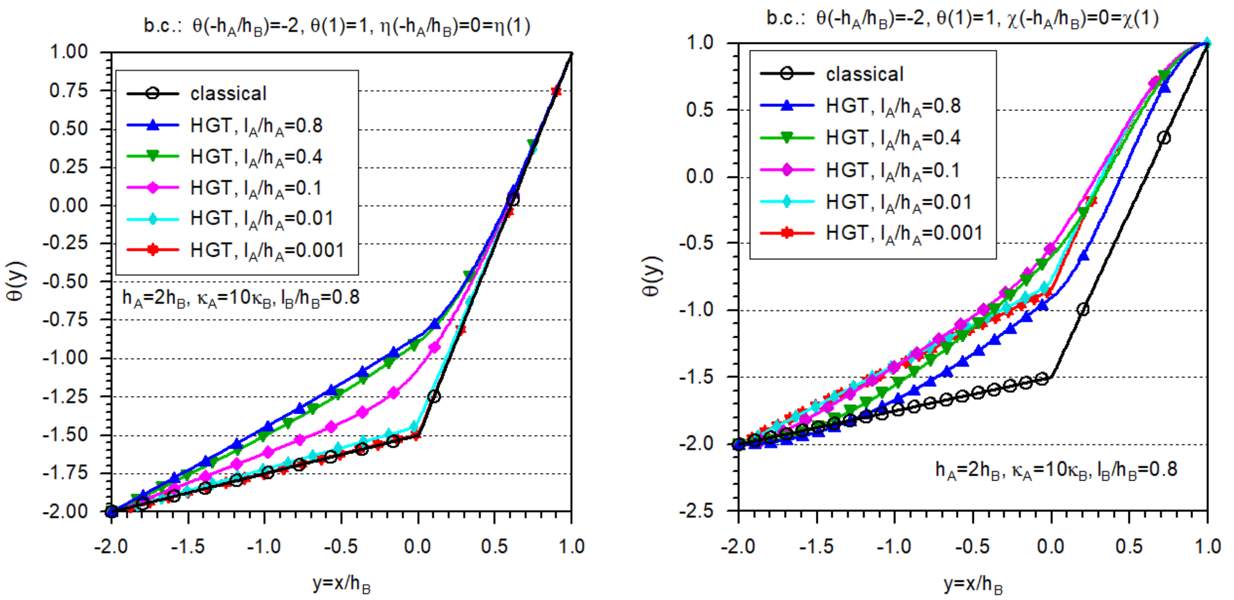

Fig.2: Temperature distributions for two kinds of b.c.(variant (i) – left; variant (ii) – right) and various values of l_A / h_A parameter in the bi-layer with $\kappa_A = 10\kappa_B$, $l_B / h_B = \text{const} = 0.8$

As long as at least one of the micro-length scale parameter l_a / h_a is small (Fig.3), the size-effect is negligible in case of b.c. (i), while the size-effects is diminishing only very slowly with decreasing both l_a / h_a parameters in case of b.c. (ii).

The role of the ratio κ_A / κ_B on the size-effect for temperature distribution in bi-layer with fixed rather large value of $l_A / h_A = l_B / h_B = 0.8$ is shown in Fig.4 for both variants of additional b.c. in HGT.

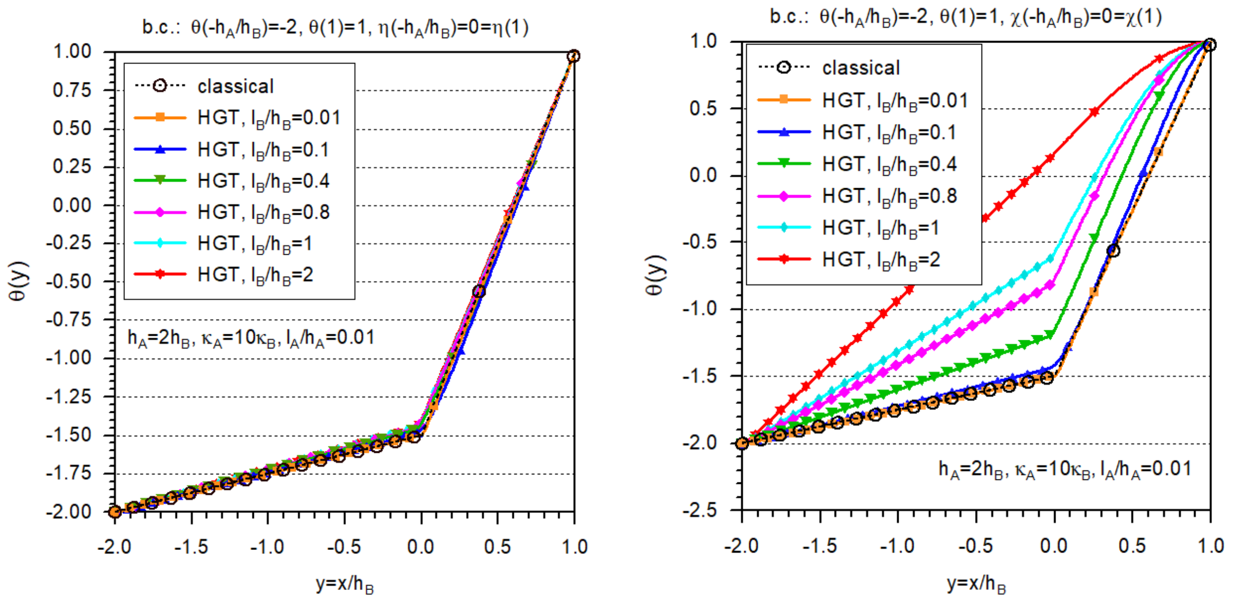

Fig.3: Temperature distributions for two kinds of b.c.(variant (i) – left; variant (ii) – right) and various values of l_A / h_A parameter in the bi-layer with $\kappa_A = 10\kappa_B$, $l_A / h_A = \mathrm{const} = 0.01$

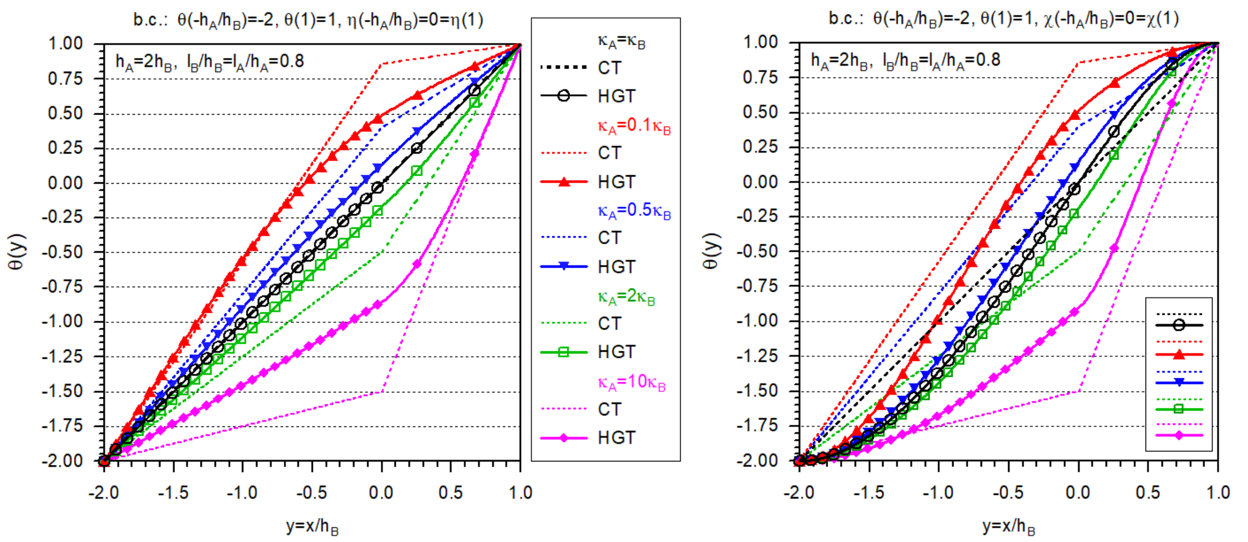

Fig.4: Temperature distributions for two kinds of b.c. with fixed $l_A / h_A = l_B / h_B = 0.8$ and various values of ratio κ_A / κ_B in the bi-layer

3. Conclusions

The main result of the study is revealing that the ratio l_a / h_a is not the only parameter which affects occurring the size-effect for distribution of temperature in bi-material layered structure. The classical material parameters (κ_a) as well as additional boundary conditions in HGT play a role.

Acknowledgement

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