



A thermodynamic model for heat transport and thermal wave propagation in graded systems



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ABSTRACT

We study the effects of a composition gradient and of a non-vanishing heat flux on the phase velocity of thermal waves along a graded system. We take into account non-local and non-linear effects by applying a generalized heat transport equation. We compare the results for high-frequency and low-frequency waves. For low frequency, we discuss the conditions in which thermal waves may propagate in $\text{Si}_x\text{Ge}_{1-x}$ and $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ systems. For high frequency, we discuss the influence of the relaxation of the flux of the heat flux on the heat wave propagation.

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1. Introduction

Graded materials are inhomogeneous materials, layered or continuous, which are increasingly used in technology, in such a way that the change of a material property with temperature may be compensated by its change with composition, in order to achieve optimization of some process [1–8]. A usual example is the alloy $\text{Si}_x\text{Ge}_{1-x}$, which has been much studied in semiconductor physics to engineer heat or current transport [9–13]. Other examples arise in thermoelectricity, where the maximization of ZT , with Z being the figure of merit and T being the absolute temperature, is important to optimize the efficiency of energy conversion from heat to electricity [14–18]. The figure of merit is defined as $Z = S^2\sigma/\lambda$, S being the Seebeck coefficient, σ the electrical conductivity and λ the thermal conductivity. Besides the difficulty in finding materials with high enough ZT , an additional difficulty is its variation with temperature, because usually σ increases with T while S decreases, in such a way that ZT has a maximum in a relatively narrow range of temperatures. Thus, the use of graded systems is very natural, namely to optimize ZT not only at one point, but along the whole system.

The thermoelectric materials that are most used for energy conversion are Bi_2Te_3 , Sb_2Te_3 and PbTe and/or their alloys $\text{Bi}_{2-2x}\text{Te}_{3-2x}\text{Pb}_x$ and $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ [1,10], with x changing along the longitudinal direction z . The alloys with x ranging in the interval

[0, 1], as, for instance, Bi_2Te_3 for $x=0$, and PbTe or Sb_2Te_3 , for $x=1$, are of special interest, as PbTe has a maximum of ZT around $T=400^\circ\text{C}$, Bi_2Te_3 around 200°C , and Sb_2Te_3 around $T=130^\circ\text{C}$. Consequently, their combination along a system allows us to improve the global efficiency of the energy conversion [19–21].

In this work we consider the practical consequences of the inhomogeneity of the composition on the evolution equation for the heat flux in graded materials, which allows us to obtain the temperature distribution along the system. This information is relevant for the optimization of the thermoelectric energy conversion. Furthermore, we explore the consequences of such evolution equation on thermal wave propagation, in order to infer which information could be obtained on the system by using low-frequency and high-frequency thermal waves as exploration technique [22]. To achieve that task, it is possible to take into account the influence of ∇x and, in the case of systems which are out of equilibrium, also of the heat flux due to a non vanishing superimposed heat flux \mathbf{q}_0 . The consequences of a non-monotonic dependence of the thermal conductivity on x on the behaviour of slow thermal waves are pointed out in Section 2. In Section 3, a generalized equation for heat transport, incorporating non-local and non-linear terms, is derived. Its consequences on the speed of high-frequency heat waves are considered in Sections 4–6.

2. Heat waves in a graded system: Maxwell–Cattaneo approach

In this preliminary section, we use the Maxwell–Cattaneo equation for the heat flux \mathbf{q} as a model of generalized heat transport equation yielding finite wave speed for high-frequency

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heat waves, and we search the speed of thermal waves, in the presence of a composition gradient ∇x and of an initial heat flux \mathbf{q}_0 . The Maxwell–Cattaneo equation is [23–25]

$$\tau \dot{\mathbf{q}} + \mathbf{q} = -\lambda \nabla T, \tag{1}$$

with τ being the heat flux relaxation time. Combined with the energy balance equation in the absence of external sources, namely

$$\rho \dot{u} = \rho c \dot{T} = -\nabla \cdot \mathbf{q}, \tag{2}$$

with $u = cT$ being specific internal energy, ρ mass density and c specific heat per unit mass, one gets

$$\tau \rho c \frac{\partial^2 T}{\partial t^2} + \rho c \frac{\partial T}{\partial t} = \lambda \nabla^2 T + \frac{\partial \lambda}{\partial x} (\nabla x) \cdot \nabla T + \frac{\partial \lambda}{\partial T} \nabla T \cdot \nabla T. \tag{3}$$

We explore the consequences of this equation on the heat wave propagation, a topic of much interest in non-equilibrium thermodynamics [22–34].

2.1. Propagation along an equilibrium state ($\mathbf{q}_0 = 0$)

We consider small-amplitude temperature perturbations $\delta T = \delta T_0 \exp[i(\omega t - \kappa z)]$, with δT_0 being a constant reference temperature, ω the frequency of the perturbation and κ the component of the wave-vector along z . First, we neglect the non-linear term in $(\nabla T)^2$, because we consider propagation along an equilibrium state. In such condition it is logical to suppose that (∇T) is very small, in such a way that $(\nabla T)^2$ may be considered negligible. Then, by Eq. (3) one gets for the dispersion relation

$$\chi \kappa^2 - Bi \kappa + (i\omega - \tau \omega^2) = 0, \tag{4}$$

with $\chi = \frac{\lambda}{\rho c}$, $B = \frac{1}{\rho c} \frac{\partial \lambda}{\partial x} \nabla_x x$. From here, one obtains

$$\kappa = \frac{Bi \pm \sqrt{B^2 i^2 - 4\chi(i\omega - \tau \omega^2)}}{2\chi}. \tag{5}$$

Thus, the phase speed

$$v_p \equiv \omega / \text{Re}(\kappa), \tag{6}$$

reads

$$v_p = \frac{\sqrt{2\chi\omega}}{\sqrt{\tau\omega - \frac{B^2}{4\chi\omega} + \sqrt{\left(\tau\omega - \frac{B^2}{4\chi\omega}\right)^2 + 1}}}. \tag{7}$$

For $B=0$, from Eq. (7) we get the classical expression of the phase speed corresponding to Maxwell–Cattaneo equation, well-known in the literature [24–26]. For $B \neq 0$ and low-frequency waves ($4\chi\tau\omega^2 \ll B^2$) we obtain

$$v_p = B \sqrt{1 - \frac{4\chi\tau}{B^2} \omega^2} \approx B. \tag{8}$$

Thus, the presence of a composition gradient yields a propagatory character to low-frequency heat waves, which otherwise, would proceed with speed $v_p = \sqrt{2\chi\omega}$, vanishing for $\omega \rightarrow 0$.

Since $B = (1/\rho c)(\partial\lambda/\partial x)\nabla x$, it turns out that the phase speed is positive (i.e., the speed will propagate to the right-hand side) for positive gradient of λ . Moreover, the higher $\nabla\lambda$, the higher v_p , so that the waves proceed faster in regions with higher inhomogeneity in the thermal conductivity. This result could be also interpreted in terms of the Le Châtelier–Braun principle [35], according to which the system reacts against perturbations; in this case, since heat diffuses faster in regions with high thermal conductivity, going towards such direction will provide the most

efficient way to react against the perturbation. For $\omega \rightarrow \infty$, in Eq. (7) one has

$$v_p(\omega \rightarrow \infty) = \sqrt{\frac{\lambda}{\rho c \tau}}, \tag{9}$$

which is the usual expression of high-frequency wave speed for Maxwell–Cattaneo equation [23–26].

By Eq. (5) we also obtain the attenuation length

$$A = -\frac{1}{\text{Im}(\kappa)} = -\frac{1}{\frac{B}{2\chi} - \sqrt{\frac{\omega}{\chi} \sqrt{-\tau\omega + \frac{B^2}{4\chi\omega} + \sqrt{\left(\tau\omega - \frac{B^2}{4\chi\omega}\right)^2 + 1}}}}. \tag{10}$$

For $B \neq 0$, and in the limit of low-frequency waves, the expression above reduces to

$$A = \frac{1}{\frac{B}{2\chi} - \omega \sqrt{\frac{1}{B^2 - \tau\omega^2 4\chi}}} \approx \frac{2\chi}{B}. \tag{11}$$

2.2. Propagation along a non-equilibrium steady state ($\mathbf{q}_0 \neq 0$)

In a non-equilibrium steady state, characterized by a non-vanishing heat flux \mathbf{q}_0 , the term $\frac{\partial \lambda}{\partial T} \nabla T \cdot \nabla T$ is no longer negligible. However, up to the first-order approximation in ∇T , it may be linearized as $-\frac{2}{\lambda} \frac{\partial \lambda}{\partial T} \mathbf{q}_0 \cdot \nabla T$. Then, Eq. (3) becomes

$$\tau \rho c \frac{\partial^2 T}{\partial t^2} + \rho c \frac{\partial T}{\partial t} = \left[\frac{\partial \lambda}{\partial x} (\nabla x) - \frac{2}{\lambda} \frac{\partial \lambda}{\partial T} \mathbf{q}_0 \right] \cdot \nabla T + \lambda \nabla^2 T. \tag{12}$$

From this expression one gets the dispersion relation still in the form (4), with

$$B = \frac{1}{\rho c} \left(\frac{\partial \lambda}{\partial x} \nabla_x x - \frac{2}{\lambda} \frac{\partial \lambda}{\partial T} q_0 \right), \tag{13}$$

where q_0 denotes the scalar value of \mathbf{q}_0 . The phase speed v_p is still given by Eq. (7), with B given by this expression above. When $B \neq 0$ and $\omega \rightarrow 0$, it reduces to Eq. (8).

It is worth observing that B contains now both the contributions of ∇x and of \mathbf{q}_0 . When $\mathbf{q}_0 = \mathbf{0}$, one recovers Eq. (7). Finally, in the high-frequency limit, Eq. (9) is recovered.

Thus, we conclude that in this model ∇x and \mathbf{q}_0 influence the low-frequency speed but not the high-frequency speed.

2.3. Illustration in $\text{Si}_x\text{Ge}_{1-x}$, and in $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ alloys

Eq. (8) yields $v_p = \frac{1}{\rho c} \frac{\partial \lambda}{\partial x} \nabla_x x$. For many systems $\lambda(T, x)$ is a non-monotonic function of x because crystals with atoms with different atomic masses disperse phonons more intensely than uniform crystals. Thus, the value of $\partial\lambda/\partial x$ may be positive or negative. For instance, at $T=300$ K, in the system $\text{Si}_x\text{Ge}_{1-x}$, $\lambda(T, x)$ has $\lambda_{\text{Si}}(300) = 148$ W/m K, $\lambda_{\text{Ge}}(300) = 60$ W/m K and has a minimum near $x=0.4$ with $\lambda_{\text{Si}_{0.4}\text{Ge}_{0.6}} = 15$ W/m K [9], and in the system $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$, $\lambda(T, x)$ has $\lambda_{\text{Bi}_2\text{Te}_3}(300) = 1.75$ W/m K, $\lambda_{\text{Sb}_2\text{Te}_3}(300) = 1.70$ W/m K and has a minimum near $x=0.5$ with $(\text{Bi}_{0.5}\text{Sb}_{0.5})_2\text{Te}_3 = 0.2$ W/m K [19]. In Fig. 1 we plot a sketch of them. For the alloy $\text{Si}_x\text{Ge}_{1-x}$, for x between 0 and 0.4, $\partial\lambda/\partial x < 0$, and for x between 0.4 and 1, $\partial\lambda/\partial x > 0$. Then, the low-frequency waves will propagate to the left-hand side (from $\text{Si}_{0.4}\text{Ge}_{0.6}$ to Ge) in the former case, and to the right-hand side (from $\text{Si}_{0.4}\text{Ge}_{0.6}$ to Si) in the latter case. These situations are sketched in Fig. 2(a).

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