



## Heat reduction by thermal wave crystals

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### ABSTRACT

Non-Fourier heat conduction models assume wave-like behavior does exist in the heat conduction process. Based on this wave-like behavior, thermal conduction controlled in a one-dimensional periodical structure, named thermal wave crystal, has been demonstrated through both theoretical analysis and numerical simulation based on the Cattaneo-Vernotte (CV) heat-conduction model. The transfer matrix method and Bloch theorem have been applied to calculate the complex dispersion curves of thermal wave propagating in thermal wave crystals. And the temperature responses are obtained by using the FDTD method. The results show that the band gaps with pronounced heat reduction do exist in non-Fourier thermal transfer process because of the Bragg scattering. The mid-gap frequency is well predicted analytically based on the Bragg scattering mechanism. Finally, the key parameters determining the band gaps are presented and discussed. This study shows the potential applications of these materials in heat isolation and reduction.

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### 1. Introduction

Traditional Fourier conduction law with implicit assumption of instantaneous thermal propagation is no longer applicable under specific conditions such as ultralow temperature, micro scale and biological tissues. In 1958, Cattaneo [1] and Vernotte [2] separately proposed a model with a time lag between the heat flux vector and the temperature gradient. In the one-dimensional (1D) case, the Cattaneo-Vernotte (CV) heat-conduction model can be written as

$$q + \tau_q \frac{\partial q}{\partial t} = -\kappa \frac{\partial T}{\partial x}, \quad (1)$$

where  $q$  and  $T$  are heat flux and temperature, respectively;  $\tau_q$  is the relaxation time for the phonon collision; and  $\kappa$  is the thermal conductivity. The equation of energy conservation is given by [3]

$$\frac{\partial q}{\partial x} = -\rho c_p \frac{\partial T}{\partial t} + Q, \quad (2)$$

where  $Q$  is the internal energy generation rate;  $\rho$  is the mass density; and  $c_p$  is the specific heat. Substitution of Eq. (1) into Eq. (2) yields [3]

$$\frac{1}{\tau_q} \frac{\partial T}{\partial t} + \frac{\partial^2 T}{\partial t^2} = \frac{\kappa}{\rho c_p \tau_q} \frac{\partial^2 T}{\partial x^2} + \frac{1}{\kappa} \left( Q + \tau_q \frac{\partial Q}{\partial t} \right). \quad (3)$$

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It is noted that Eq. (3) is a hyperbolic heat wave conduction equation. The heat propagates in the medium with a finite speed:

$$C_{CV} = \sqrt{\kappa(\rho c_p \tau_q)^{-1}} \quad [3].$$

The CV model is the simplest but rather rough model in describing the non-Fourier heat conduction. In order to describe the physical process more precisely, more generalized models were proposed, e.g. the dual phase lag model [4,5], the thermomass model [6,7] and the EIT model [8,9]. Due to the peculiarity of the hyperbolic wave equations in these models, efforts have been exerted on the wave-like behavior in the past several decades. Reviews of thermal propagation in the non-Fourier theory were given by Joseph et al. [10], Tzou et al. [11], Xu et al. [12] among others. Wang et al. [13] examined the non-Fourier thermal oscillation and resonance in a 1D homogeneous medium analytically with oscillatory temperature boundary conditions. Zhao et al. [14] analyzed the non-Fourier thermal behavior in a solid sphere. Ma et al. [15] studied the non-Fourier thermal process in functional graded materials. Furthermore, Moosaie et al. [16–19] presented the non-Fourier effect under periodical boundary and non-periodical boundary conditions in 1D or a hollow sphere homogeneous medium analytically.

It is well known that wave manipulation is an eternal, important and challenging issue. In past decades, control of electromagnetic waves by photonic crystals [20,21] and control of acoustic or elastic waves by phononic crystal [22–24] have been received considerable attention. We refer to Refs. [25–27] for detailed reviews

in these fields. Analogously, based on the fact that thermal conduction can be modeled by ballistic phonon transport in micro-scale, control of thermal conduction by using periodic micro-scale structures has attracted considerable attention. Early, thermal conduction in superlattices was considered [28–31]. Recently, Maldovan proposed a concept of “thermocystal” based on nano-scale phononic crystals which can manage the thermal energy flow [32–35]. Similar studies were undertaken by Zen et al. [36], Nomura et al. [37], Davis et al. [38], Lacatena et al. [39], and Anufriev et al. [40] among others with focus on reducing the thermal conductivity by using nano-scale phononic crystals. It is noted that the aforementioned studies are limited to micro-scale because the ballistic phonon transport model of thermal conduction and coherent thermal transfer is applied. Tzou [41] develop a way to relate micro-scale to macro-scale heat transfer, where the wave-like behavior (i.e. thermal wave) was included in the process of thermal transfer based on the fact of the finite time required for completing the interactions between particles. The CV model, equations (1)–(3), can describe this kind of wave-like behavior although it is rather rough. In this Article, we will discuss thermal wave propagation through a periodically layered structure based on the CV model and Bloch theory [42]. Band gaps with pronounced heat reduction are found in the spectrum. This new class of artificial thermal material will be named ‘thermal wave crystal’ which can control heat wave analogy to a photonic crystal for control of electromagnetic waves [43] and a phononic crystal for control of acoustic or elastic waves [27]. It is expected to have a variety of applications in manipulating heat waves including heat isolation or reduction [44].

## 2. Problem formulation

Consider a periodically layered structure with bilayer unit-cells as shown in Fig. 1. Each unit-cell consists of layer (sub-cell) A with thickness  $l_A$  and layer B with thickness  $l_B$  (the unit-cell’s thickness  $l = l_A + l_B$ ). All material properties  $\{\kappa, \tau_q, \rho, c_p, C_{CV}\}$  of the two layers are distinguished by subscripts A and B. The coordinate  $(x, y)$  is shown in the figure. We number an arbitrary unit-cell as the  $j$ th unit-cell. Its left and right boundaries coordinates are  $x_L^j = jl$  and  $x_R^j = (j+1)l$ , respectively; and the coordinate of the interface between layers A and B is  $x_{AB}^j = jl + l_A$ .

A 1D thermal wave propagates in the periodic structure without any internal heat source or loss (i.e.  $Q = 0$ ). For a time-harmonic thermal wave with angular frequency  $\omega$ , the temperature and heat flux fields may be written as  $\{T(x, t), q(x, t)\} = \{\hat{T}(x), \hat{q}(x)\}e^{-i\omega t}$  with  $\hat{T}(x)$  satisfying

$$\hat{T}''(x) + \frac{\omega^2 + i\omega/\tau_q}{C_{CV}^2} \hat{T}(x) = 0, \quad (4)$$

where  $i = \sqrt{-1}$ . The general solution of equation (4) is

$$\hat{T}(x) = A_1 e^{i\gamma x} + A_2 e^{-i\gamma x}, \quad (5)$$

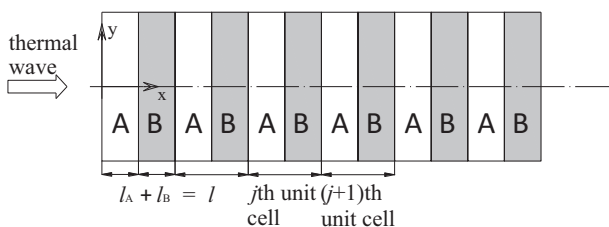


Fig. 1. Schematic diagram of a 1D thermal wave crystal.

where  $A_1$  and  $A_2$  are unknown coefficients, and

$$\gamma = \sqrt{\frac{\omega^2 + i\omega/\tau_q}{C_{CV}^2}}, \quad (6)$$

of which the real part demonstrates propagating of the thermal wave and the imaginary part characterizes the attenuation. The heat flux  $\hat{q}(x)$  is obtained by following Eq. (2),

$$\hat{q}(x) = -A_1 \frac{i\kappa\gamma}{1 - i\omega\tau_q} e^{i\gamma x} + A_2 \frac{i\kappa\gamma}{1 - i\omega\tau_q} e^{-i\gamma x}. \quad (7)$$

For conciseness, the following state vector is introduced,

$$\mathbf{S}(x) = \{\hat{T}(x), \hat{q}(x)\}^T = \mathbf{M}(x)\{A_1, A_2\}^T, \quad (8)$$

where the superscript T denotes the transpose, and

$$\mathbf{M}(x) = \begin{pmatrix} 1 & 1 \\ -\frac{i\kappa\gamma}{1 - i\omega\tau_q} & \frac{i\kappa\gamma}{1 - i\omega\tau_q} \end{pmatrix} \begin{pmatrix} e^{i\gamma x} & 0 \\ 0 & e^{-i\gamma x} \end{pmatrix}. \quad (9)$$

The above solution holds for both layers A and B, and is denoted as  $\mathbf{S}_A^j(x) = \mathbf{M}_A^j(x)\{A_1, A_2\}^T$  (with  $x_L^j < x < x_{AB}^j$ ) in layer A of the  $j$ th unit-cell or  $\mathbf{S}_B^j(x) = \mathbf{M}_B^j(x)\{B_1, B_2\}^T$  (with  $x_{AB}^j < x < x_R^j$ ) in layer B. The matrix  $\mathbf{M}_A^j(x)$  and  $\mathbf{M}_B^j(x)$  are obtained from equation (9) by replacing  $\kappa, \tau_q, \gamma, C_{CV}$  with those with the subscripts of A and B, respectively.

Next the transfer matrix method [45,46] is used to calculate dispersion relations. Introduce the state vectors at the left and right boundaries of layers A and B:  $\mathbf{S}_{AL}^j = \mathbf{S}_A^j(x_L^j)$ ,  $\mathbf{S}_{AR}^j = \mathbf{S}_A^j(x_{AB}^j)$ ,  $\mathbf{S}_{BL}^j = \mathbf{S}_B^j(x_{AB}^j)$  and  $\mathbf{S}_{BR}^j = \mathbf{S}_B^j(x_R^j)$ . Then from equation (8) it is easy to obtain the relations:

$$\mathbf{S}_{AL}^j = \mathbf{M}_A^j(x_L^j)\{A_1, A_2\}^T, \mathbf{S}_{AR}^j = \mathbf{M}_A^j(x_{AB}^j)\{A_1, A_2\}^T; \\ \mathbf{S}_{BL}^j = \mathbf{M}_B^j(x_{AB}^j)\{B_1, B_2\}^T, \mathbf{S}_{BR}^j = \mathbf{M}_B^j(x_R^j)\{B_1, B_2\}^T.$$

Eliminating  $\{A_1, A_2\}^T$  from the first two equations and  $\{B_1, B_2\}^T$  from the last two yields

$$\mathbf{S}_{AR}^j = \mathbf{M}_{AR}^j(\mathbf{M}_{AL}^j)^{-1} \mathbf{S}_{AL}^j, \mathbf{S}_{BR}^j = \mathbf{M}_{BR}^j(\mathbf{M}_{BL}^j)^{-1} \mathbf{S}_{BL}^j, \quad (10)$$

where  $\mathbf{M}_{AL}^j = \mathbf{M}_A^j(x_L^j)$ ,  $\mathbf{M}_{AR}^j = \mathbf{M}_A^j(x_{AB}^j)$ ,  $\mathbf{M}_{BL}^j = \mathbf{M}_B^j(x_{AB}^j)$  and  $\mathbf{M}_{BR}^j = \mathbf{M}_B^j(x_R^j)$ .

The temperature and heat flux are continuous at the interface between two adjacent sub-layers, which states

$$\mathbf{S}_{AR}^j = \mathbf{S}_{BL}^j, \mathbf{S}_{BR}^j = \mathbf{S}_{AL}^{j+1}. \quad (11)$$

Substitution of Eq. (10) into Eq. (11) yields

$$\mathbf{M}_{AR}^j(\mathbf{M}_{AL}^j)^{-1} \mathbf{S}_{AL}^j = \mathbf{S}_{BL}^j, \mathbf{M}_{BR}^j(\mathbf{M}_{BL}^j)^{-1} \mathbf{S}_{BL}^j = \mathbf{S}_{AL}^{j+1}.$$

Eliminating  $\mathbf{S}_{BL}^j$  from the above two equations, we have

$$\mathbf{S}_{AL}^{j+1} = \mathbf{M}_{BR}^j(\mathbf{M}_{BL}^j)^{-1} \mathbf{M}_{AR}^j(\mathbf{M}_{AL}^j)^{-1} \mathbf{S}_{AL}^j, \quad (12)$$

which gives the relationship between the state vectors of the  $j$ th and  $(j+1)$ th unit-cells. The matrix  $\mathbf{M}_{BR}^j(\mathbf{M}_{BL}^j)^{-1} \mathbf{M}_{AR}^j(\mathbf{M}_{AL}^j)^{-1}$  is the transfer matrix between two consecutive unit-cells, which is the same for any value of  $j$  and therefore is denoted as  $\mathbf{M}_{Transfer}$ .

It was found by Felix Bloch [47] that the electron wave governed by the Schrödinger’s equation in a periodic potential field is modulated by the periodicity and propagates with the form of  $\varphi(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$  where  $\varphi(\mathbf{r})$  is a periodic function with the same periodicity as the potential field. This is the so-called Bloch theorem; and the wave is called Bloch wave with  $\mathbf{k}$  being Bloch wave vector [48]. The Bloch theorem was proved to hold for general wave equations including those for classical waves (e.g. lattice wave [48], electromagnetic wave [47], acoustic or elastic wave [27], etc.).

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