Complex band structure of thermal wave crystals: The plane-wave method

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In this paper, we present an extension of the plane-wave method (PWM) to compute the complex band structure of thermal wave crystals (TWCs). The structural periodicity of TWC allows the possibility to manipulate non-Fourier heat *via* wave interference. While the Cattaneo-Vernotte (CV) heat conduction theory accurately models oscillatory wave-like propagation of heat in TWCs, obtaining an eigenvalue equation for frequency using the CV wave equation is not possible. To overcome this limitation, we propose a novel approach that solves a complex eigenvalue equation for the Bloch wave vectors.

Keywords: Heat; non-Fourier; crystal.

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1. Introduction

Thermal Wave Crystals (TWCs), which were first proposed by A-Li Chen *et al* in 2018, have attracted a lot of interest for the existence of band gaps when heat flow is of oscillatory nature [1]. The fact that TWCs exhibit band gaps for their oscillatory behavior motivated the development of numerous studies aimed at exploring their properties and potential applications [2-6]. For instance, the presence of band gaps within a TWC structure has the potential to reduce heat propagation by means of interference [1]. The ability to control heat flow as a wave could have significant implications in managing heat in electronic devices, which is crucial to their performance [7].

The classical Fourier conduction law, which is based on a parabolic-type heat equation, describes only diffusive heat propagation [8]. On the other hand, TWC materials follow the Cattaneo-Vernotte (CV) model, which is based on a hyperbolic heat equation that describes thermal waves [8]. Therefore, TWCs possess a remarkable potential to manipulate and guide heat flow as waves, analogous to how photonic crystals (PtCs) and phononic crystals (PnCs) control electromagnetic and mechanical waves, respectively. The wave-like behavior in TWCs has inspired to carefully study them as a promising platform for developing novel thermal management devices and applications [9,10].

Before introducing our approach, let us discuss the framework surrounding our proposal. When PtCs are studied considering only dielectric materials, the Plane Wave Method (PWM) can be directly applied to solve the wave equation [11,12]. This results in a matrix problem with real frequency eigenvalues dependent on the Bloch wave vector, $\omega(\mathbf{k})$ [13]. However, if at least one material in the unit cell is a metal or semiconductor with a complex dielectric function where exist absorption, obtaining an eigenvalue problem for a real frequency is no longer possible [14]. To study dispersive materials, several methods have been explored to obtain a complex frequency as the eigenvalue [15-17].

In recent years, researchers made progress in formulating the PWM to study dispersive PtCs. Rather than proposing the frequency as a function of the wave vector, they sought to use the Bloch wave vector as a function of the frequency, $\mathbf{k}(\omega)$. Brand *et al* were the first to report on this reformulation of the PWM in 2007. They used it to determine the effective plasma frequency of two-dimensional arrays of metal rods modeled with the Drude dielectric function [18]. In 2016, Guevara-Cabrera *et al* applied the reformulated PWM to determine the complex band structure of a 2D array of cylinders modeled with the Lorentz dielectric function [19]. Similar ideas have been recently implemented in PnCs to model viscoelastic materials. In 2023, Schalcher *et al* proposed a reformulation of the PWM for a standard solid material to obtain a matrix problem with the Bloch wave vector as the eigenvalue [20]. The goal of this work is to determine the band structure of TWC by applying PWM for the first time in a heat transfer problem using a non-Fourier model.

The first calculation of band gaps for one-dimensional (1D) TWCs was carried out using an analytical formula obtained via the Transfer Matrix Method (TMM) [1]. Here, we present a new approach using the PWM to calculate the Thermal Wave Band Structure (TWBS). There are at least two important reasons for developing the PWM for calculating complex band structures in TWC. Firstly, PWM can be applied to study two- or three-dimensional structures, as has been previously reported for PtCs [21,22]. Second, the PWM's adapt-

ability in developing homogenization theories that have been published for PtCs and PnCs and that can also be adapted to investigate TWC [23].

2. Method

The CV model proposes a modification of Fourier's law of thermal conduction by introducing a time lag between the heat flux vector and the temperature gradient [24,25]. In the case of a one-dimensional periodic structure, the heat conduction model is

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

where $q(x,t)$ and $T(x,t)$ are the time-dependent heat flux and temperature, respectively. There are two position-dependent material parameters, $\tau(x)$ and $\kappa(x)$ that are the relaxation time and thermal conductivity, respectively. The conservation of energy in the absence of heat sources is given by the equation

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

where $\rho(x)$ and $c_p(x)$ are the position-dependent mass density and specific heat at constant pressure, respectively. By combining Eqs. (1) and (2) we obtain a wave equation in the time-domain as

$$\frac{\partial}{\partial x}\left[\frac{1}{\rho(x)c_p(x)}\frac{\partial}{\partial x}q(x,t)\right] = \frac{1}{\kappa(x)}\frac{\partial}{\partial t}q(x,t) + \frac{\tau(x)}{\kappa(x)}\frac{\partial^2}{\partial t^2}q(x,t). \tag{3}$$

Considering the Fourier Transform

$$q(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} q(x,\omega)e^{-i\omega t}d\omega, \tag{4}$$

we obtain a wave equation in the frequency domain

$$\frac{\partial}{\partial x}\left[\frac{1}{\rho(x)c_p(x)}\frac{\partial}{\partial x}q(x,\omega)\right] = -i\omega\frac{1}{\kappa(x)}q(x,\omega) - \omega^2\frac{\tau(x)}{\kappa(x)}q(x,\omega). \tag{5}$$

The conventional approach of formulating an eigenvalue problem to obtain the frequency as a function of the Bloch wave vector [$\omega(K)$] is no longer applicable to Eq. (5). In this paper, we propose a method to solve the eigenvalue problem that results from the implementation of the PWM where the Bloch wave vectors $k(\omega)$ are the eigenvalues.

The PWM is a straightforward method that operates in the Fourier space. It requires the expansion of periodic material parameters in the form of a Fourier series, as follows:

$$\frac{1}{\rho(x)c_p(x)} = \sum_G \alpha_G e^{iGx}, \tag{6}$$

$$\frac{1}{\kappa(x)} = \sum_G \beta_G e^{iGx} \tag{7}$$

and

$$\frac{\tau(x)}{\kappa(x)} = \sum_G \gamma_G e^{iGx}. \tag{8}$$

In Eqs. (6)-(8) the summation extends over the infinite reciprocal lattice vectors of amplitude $G = (2\pi n)/d$, where $n = ..., -2, -1, 0, 1, 2, ...$ The period d is the length of the unit cell. To solve Eq. (5) we apply the Bloch theorem, which states that in a periodic medium, the fields can be written as the product of two functions. The first is a periodic function and the second is a wave-like part that defines the series

$$q(x,\omega) = \sum_G Q_G e^{i(G+K)x}, \tag{9}$$

where K is the one-dimensional Bloch wave vector. The substitution of the Fourier series defined by Eqs. (6)-(9) in Eq. (5) allows us to obtain, after some algebraic manipulations, the equation

$$\sum_{G'}\left[k^2 A_{G,G'} + kB_{G,G'} + C_{G,G'}\right]Q_{G'} = 0, \tag{10}$$

where the matrix elements are

$$\begin{aligned} A_{G,G'} &= \alpha_{G-G'}, \\ B_{G,G'} &= \alpha_{G-G'}(G+G'), \\ C_{G,G'} &= GG'\alpha_{G-G'} - i\omega\beta_{G-G'} - \omega^2\gamma_{G-G'}. \end{aligned} \tag{11}$$

If all the points of the reciprocal lattice are considered, then we obtain an infinite set of equations that is convenient to write in the form

$$\left(K^2\mathbb{A} + K\mathbb{B} + \mathbb{C}\right)\vec{Q} = 0, \tag{12}$$

where $\mathbb{A}$,$\mathbb{B}$ and $\mathbb{C}$ are matrices and $\vec{Q}$ is a vector. Equation (12) defines a Quadratic Eigenvalue Problem, which can be used to accurately investigate periodic systems with absorption. Many years ago, research on PtCs composed of absorbent materials established the efficacy of this theoretical approach [26]. Conductivity was added via PWM, in particular for materials with a complex frequency-dependent dielectric function. The complex band structure is calculated by solving the quadratic eigensystem, which is then linearized into an ordinary eigenvalue problem. In this manner, it is possible to find the allowed values for the Bloch wave vector K if we write Eq. (12) in the form of a generalized eigenvalue problem as

$$\begin{pmatrix} \mathbb{C} & \mathbb{B} \\ \mathbb{O} & \mathbb{I} \end{pmatrix}\begin{bmatrix} \vec{Q} \\ K\vec{Q} \end{bmatrix} = K\begin{pmatrix} \mathbb{O} & -\mathbb{A} \\ \mathbb{I} & \mathbb{O} \end{pmatrix}\begin{bmatrix} \vec{Q} \\ K\vec{Q} \end{bmatrix}, \tag{13}$$

where $\mathbb{I}$ and $\mathbb{O}$ are the identity matrix and the zero matrix, respectively. The complex eigenvalues K are obtained by a process of numerical diagonalization.

To solve the matrix problem, we need to know the Fourier coefficients of the periodic material parameters $1/(\rho(x)c_p(x))$, $1/\kappa(x)$ and $\tau(x)/\kappa(x)$. We consider a unit cell of thickness $d = d_a + d_b$ formed by two different materials a and b of thickness d_a and d_b, respectively. The material a is at the center of the unit cell. The unit cell is in the range $-d/2 < x < d/2$. The periodic materials parameters are described by the analytical function

$$\frac{1}{\rho(x)c_p(x)} = \frac{1}{\rho_b c_{p,b}} + \left(\frac{1}{\rho_a c_{p,a}} - \frac{1}{\rho_b c_{p,b}}\right) \Theta\left(\frac{d_a}{2} - |x|\right), \tag{14}$$

$$\frac{1}{\kappa(x)} = \frac{1}{\kappa_b} + \left(\frac{1}{\kappa_a} - \frac{1}{\kappa_b}\right) \Theta\left(\frac{d_a}{2} - |x|\right), \tag{15}$$

and

$$\frac{\tau(x)}{\kappa(x)} = \frac{\tau_b}{\kappa_b} + \left(\frac{\tau_a}{\kappa_a} - \frac{\tau_b}{\kappa_b}\right) \Theta\left(\frac{d_a}{2} - |x|\right) \tag{16}$$

where $\Theta(x)$ is the Heaviside function ($\Theta = 1$ for $x \geq 0$, $\Theta = 0$ for $x < 0$). The Fourier coefficients defined by Eqs. (6)-(8) are

$$\alpha_G = \frac{1}{d}\int_{-d/2}^{d/2} \frac{1}{\rho(x)c_p(x)} e^{-iGx} dx, \tag{17}$$

$$\beta_G = \frac{1}{d}\int_{-d/2}^{d/2} \frac{1}{\kappa(x)} e^{-iGx} dx, \tag{18}$$

$$\gamma_G = \frac{1}{d}\int_{-d/2}^{d/2} \frac{\tau(x)}{\kappa(x)} e^{-iGx} dx. \tag{19}$$

The explicit form of the Fourier coefficients are

$$\alpha_G = \left[\frac{1}{\rho_b c_{p,b}} + f\left(\frac{1}{\rho_a c_{p,a}} - \frac{1}{\rho_b c_{p,b}}\right)\right]\delta_{G,0} + \left[f\left(\frac{1}{\rho_a c_{p,a}} - \frac{1}{\rho_b c_{p,b}}\right)\frac{\sin(Gd_a/2)}{Gd_a/2}\right] \times (1 - \delta_{G,0}), \tag{20}$$

$$\beta_G = \left[\frac{1}{\kappa_b} + f\left(\frac{1}{\kappa_a} - \frac{1}{\kappa_b}\right)\right]\delta_{G,0} + \left[f\left(\frac{1}{\kappa_a} - \frac{1}{\kappa_b}\right)\frac{\sin(Gd_a/2)}{Gd_a/2}\right] \times (1 - \delta_{G,0}), \tag{21}$$

and

$$\gamma_G = \left[\frac{\tau_b}{\kappa_b} + f\left(\frac{\tau_a}{\kappa_a} - \frac{\tau_b}{\kappa_b}\right)\right]\delta_{G,0} + \left[f\left(\frac{\tau_a}{\kappa_a} - \frac{\tau_b}{\kappa_b}\right)\frac{\sin(Gd_a/2)}{Gd_a/2}\right](1 - \delta_{G,0}), \tag{22}$$

where $f = d_a/d$ is the filling fraction of material a within the unit cell.

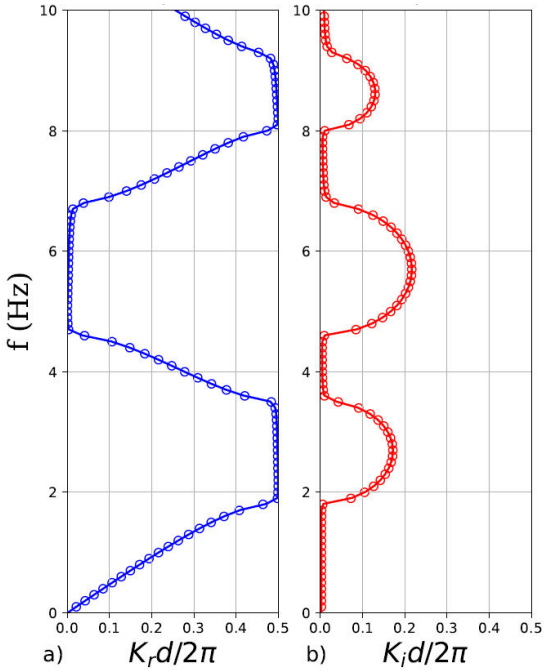

FIGURE 1. Complex band structure of a 1D-TWC, composed of alternating layers of dermis and stratum with equal layer widths and a period of $d = 20$ μm. The solid curves represent the results obtained using the PWM, and the open circles correspond to the TMM calculations. a) The real part of the wave vector is displayed in blue, and b) the imaginary wave vector is displayed in red in panel. We used 101 plane waves for the PWM in this calculation.

3. Results

To validate our method, as a first test, we have computed the TWBS with the analytical formula given by Eq. (17) in Ref. [1], where it was obtained using the TMM. The multilayer consists of a layer a of Stratum-like material, and a layer b of Dermis-like material [1]. For the material a we have the following parameters: thermal conductivity $\kappa_a = 0.235$ W/m K, specific heat $c_a = 3600$ J/kg K, density $\rho_a = 1500$ kg/m^3, and relaxation time $\tau_a = 1$ s. For the material b we have the following parameters: thermal conductivity $\kappa_b = 0.445$ W/m K, specific heat $c_b = 3300$ J/kg K, density $\rho_b = 1116$ kg/m^3, and relaxation time $\tau_b = 20$ s. The period of the unit cell is $d = 20$ μm and the filling fraction is $f = 0.5$.

In Fig. 1, the band structure obtained with the TMM is presented with open blue and red circles for the real (K_r) and imaginary (K_i) part of the wave vector, respectively. Our results obtained with the PWM are presented with blue and red lines for the real (K_r) and imaginary (K_i) part of the wave vector. We have found an excellent agreement between the TMM and PWM results.

For a second test of our method, we analyze a semiconductor multilayer composed of silicon (Si) and germanium (Ge). The multilayer consists of a layer a of Si, and a layer b of Ge [7]. For the material a we have the following parameters: thermal conductivity $\kappa_a = 150$ W/m K, specific

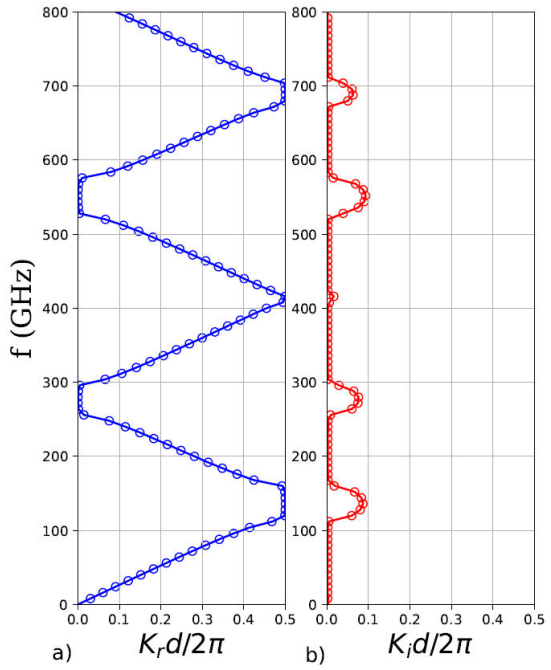

FIGURE 2. Complex band structure of a 1D-TWC, composed of alternating layers of Si and Ge with equal layer widths and a period of $d = 2$ nm. The solid curves represent the results obtained using the PWM, while the open circles correspond to the TMM calculations. a) The real wave vector is displayed in blue, b) while the imaginary wave vector is displayed in red. We used 101 plane waves for the PWM in this calculation.

heat $c_a = 710$ J/kg K, density $\rho_a = 2330$ kg/m^3 and relaxation time $\tau_a = 150$ ps. For the material b we have the following parameters: thermal conductivity $\kappa_b = 60$ W/m K, specific heat $c_b = 310$ J/kg K, density $\rho_b = 5300$ kg/m^3 and relaxation time $\tau_b = 200$ ps. The period of the unit cell is $d = 2$ nm and the filling fraction is $f = 0.5$. It is found that the semiconductor multilayer has band gaps in the GHz range. It is important to point out that recently it has been reported the experimental observation of thermal waves for Ge at room temperature [27]. The existence of band gaps for thermal waves in semiconductor multilayer opens up new possibilities to manipulate the flow of heat in electronic devices. We have computed the TWBS with the analytical formula given by Eq. (3) in Ref. [7]. In Fig. 2, the TWBS obtained with the TMM is presented with open blue and red circles for the real (K_r) and imaginary (K_i) part of the Bloch wave vector, respectively. Our results obtained with the PWM are presented with blue and red lines for the real (K_r) and imaginary (K_i) part of the Bloch wave vector, respectively. We have found an excellent agreement between the TMM and PWM results.

4. Conclusions

In summary, we have successfully adapted the PWM to calculate the TWBS of TWCs. By solving the resulting eigenvalue equation, we can determine the complex Bloch wave vector as a function of the real frequency. Our results were compared to an analytical solution obtained by the TMM, and we found excellent agreement between the two methods. We applied our approach to two specific cases: a biological multilayer composed of dermis and stratum, which exhibits band gaps in the Hz range, and a semiconductor multilayer composed of Ge and Si, which exhibits band gaps in the GHz range.

The results presented in this paper validate the PWM's applicability for 1D thermal waves described by the CV model. The applicability of the PWM is expected to hold true for other thermal wave models as well as the investigation of 2D or 3D systems.

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