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Thermal Bragg Shields for Thermal Waves.

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ABSTRACT

Ultrafast heating processes do not follow Fourier's heat conduction law, but rather the proposed Cattaneo-Vernotte equation (CVe) which has wave-like solutions that have some important differences from other wave phenomenon. In a periodic system made of materials with different thermal conductivities, solutions of the CVe lead to a band-like structure in the dispersion relation. In this work, we show that highly reflective Bragg mirrors for thermal waves can be designed. Even for a mirrors with a few layers a very high reflectance is achieved ($> 90\%$). The mirrors are made of materials with large thermal response times, where thermal waves have been measured. A second alternative consists of adding a thin metallic film which also leads to an efficient thermal Bragg mirror. Finally, the role of defects in opening new thermal-stop bands is demonstrated.

1 Introduction

The sudden heating of materials leads to a deviation from the usual Fourier law of heat conduction due to a time delay between the temperature gradient and the heat flux. The time delay implies a finite velocity of heat propagation and the partial differential equation for the temperature is no longer a diffusion equation but a wave equation (hyperbolic partial differential equation) known as the Cattaneo-Vernotte equation (CVe)¹⁻⁴. The wave-like nature of the temperature and heat flux derived by Cattaneo's equation opens new possibilities for thermal management and can find analogies to wave phenomena in other areas of physics. For example, in the behavior of electromagnetic⁵⁻⁷ and acoustic waves⁸⁻¹⁰ in periodic structures. Experimentally, non-Fourier behavior has been shown in different materials like granular media^{3,11}, wet sand¹² and organic materials¹³, blood and porcine muscle¹⁴ and processed meat¹⁵. Skin bio-thermomechanics and bioheat transfer mechanisms also follow a non-Fourier behavior.¹⁶⁻¹⁸. Although solutions of the CVe are wave-like, there are differences with respect to the waves found in acoustics and electromagnetic theory, that have to be considered. An important difference is that the heat flux is not derived from a quadratic quantity unlike the case of acoustic or electrodynamics where the energy flow is described from quadratic quantities of the wave amplitude¹⁹. Several authors have discussed the differences and misconceptions of heat waves²⁰⁻²³. The wave-like behavior can be used to control the heat flux with systems that are similar to those used in optics or acoustics, for example designing thermal crystals²⁴ and metamaterials where concepts such as thermal cloaking have been proposed²⁵.

In this paper we show that it is possible to design thermal Bragg mirrors made of alternate layers of different materials that follow a non-Fourier behavior, with almost perfect reflectivity (larger than 90%), even for mirrors made of a few layers. To do this, we present in Section II a detailed analysis of the solution of CVe is presented as well as the transfer matrix formalism for the temperature and heat flux fields. In section III the results for periodic mirrors are shown as well as the role of defects on the mirrors. Finally, the conclusions and outlook.

2 Thermal waves. Cattaneo-Vernotte equation

In this section we review the basic principles of thermal waves as solutions of the Cattaneo-Vernotte equation (CVe). The CVe arises when there is a time delay τ between the application of a temperature gradient and the ensuing heat flux $\vec{q}(\vec{r}, t)$. In this case the heat flux is¹⁻⁴,

$$\vec{q}(\vec{r}, t) + \tau \frac{\partial \vec{q}(\vec{r}, t)}{\partial t} = -\kappa \nabla T(\vec{r}, t), \quad (1)$$

where κ is the thermal conductivity. Eq. (1) is written in terms of the temperature by considering the balance equation of the thermal energy density $u(\vec{x}, t)$ given by

$$\rho c_v \frac{\partial T(\vec{r}, t)}{\partial t} + \nabla \cdot \vec{q}(\vec{r}, t) = s(\vec{r}, t) \quad (2)$$

with s a source term. Here, c_v is the specific heat capacity at constant volume and ρ the mass density. Applying the divergence to Eq. (1) and using Eq. (2) in the absence of sources ($s(\vec{r}, t) = 0$) we obtain

$$\nabla^2 T(\vec{r}, t) = \frac{1}{\alpha} \frac{\partial T(\vec{r}, t)}{\partial t} + \frac{1}{v^2} \frac{\partial^2 T(\vec{r}, t)}{\partial t^2}, \quad (3)$$

where the thermal diffusivity is defined as $\alpha = \kappa/c_v$, and $v^2 = \alpha/\tau$. The parameter v is identified as the propagation speed of the thermal perturbation^{26,27}. In the limit $\tau \rightarrow 0$, the speed v goes to infinity, and Eq. (1) is the usual Fourier law for heat conduction^{22,28,29}.

Assuming a time harmonic dependence, the solution of Eq. (3) is

$$T(\vec{r}, t) = A e^{i(\vec{k} \cdot \vec{r} - \omega t)} + B e^{-i(\vec{k} \cdot \vec{r} + \omega t)}, \quad (4)$$

and the complex wave number is

$$k = \frac{\omega}{v} (1 + i) \sqrt{\frac{1}{2\omega\tau}}. \quad (5)$$

The heat equation Eq. (3) and the wave vector given by Eq. (5) have the same form as the electrodynamic telegrapher's equation. For example for a medium of electrical conductivity σ the wave number is $k = \frac{\omega}{c} (1 + i) \sqrt{\frac{4\pi\sigma}{2\omega}}$, with c the speed of light. Comparing with Eq. (5), we see that the reciprocal of the delay time is equivalent to the electrical conductivity. Similarly, for $\omega\tau \gg 1$ we can define the thermal wave skin depth $\delta = \tau v \sqrt{2/\omega\tau}$, again akin to the case of electromagnetic waves.

Using Eq. (4) in Eq. (1) for the heat flux we have

$$\vec{q}(\vec{r}, t) = -isk\hat{k} \left(A e^{i(\vec{k} \cdot \vec{r} - \omega t)} - B e^{-i(\vec{k} \cdot \vec{r} + \omega t)} \right), \quad (6)$$

with $s(\omega) = \frac{\kappa}{1 - i\omega\tau}$. We define $Y(\omega) = -is(\omega)k$ as the *thermal admittance* that can be expressed as

$$Y(\omega) = \frac{\kappa}{v\tau} \frac{1}{\sqrt{1 + i/\omega\tau}}. \quad (7)$$

The reciprocal of the admittance defines the thermal impedance³⁰, $Z(\omega) = T/\vec{q} \cdot \hat{n}$, where the normal vector to the interface is $\hat{n}$. We point out two limits of interest, when $\omega\tau \ll 1$ the CVe goes to the usual diffusion equation. When $\omega\tau \rightarrow \infty$, the wave vector Eq.(5) becomes real as well as the admittance and CVe is a non-damped wave equation.

The constant amplitudes A and B in Eq. (4) and Eq. (6) are determined from the boundary conditions that are the continuity (i) of the temperature and (ii) of the heat flux, both are consequences of assuming perfect thermal contact.

2.1 Heat waves in laminated systems

In this section we derive the transfer matrix and the reflectance coefficients for a layered media or thermal crystals²⁴.

Consider an array of N layers in a Cartesian coordinates system (x, y, z) where the x -axis is perpendicular to the interfaces. Each layer is of width d_j with thermal properties α_j, v_j as is shown in Fig. 1(a). The first interface is at $x_0 = 0$ and the last layer interface is at $x_N = d_1 + \dots + d_N = L$. Outside the layered structure, for $x < x_0$ there is a medium with thermal properties α_0, v_0 ; and for $x > x_N$ there is a substrate defined by α_s, v_s . We will consider normal incidence, thus $\vec{q}(\vec{r}, t) = q(x, t)\hat{x}$.

Within particular layer bounded between $x_L = x_j$ and $x_R = x_j + d_j$, the temperature and heat flux Eq. (4) and Eq. (6) can be written as

$$\begin{pmatrix} T(x, t) \\ q(x, t) \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ Y_j & -Y_j \end{pmatrix} \begin{pmatrix} e^{ik_j x} & 0 \\ 0 & e^{-ik_j x} \end{pmatrix} \begin{pmatrix} A_j \\ B_j \end{pmatrix} \\ = m_j(x) \begin{pmatrix} A_j \\ B_j \end{pmatrix}, \quad (8)$$

in the previous equation the time term $\exp(-i\omega t)$ is obviated.

Figure 1. (a) Finite layered system made of consecutive layers with different thermal properties. Each layer is characterized by its thickness d , thermal speed v and the thermal diffusivity α . The system is bounded by a substrate and outer medium. (b) Semi-infinite periodic system. The substrate is removed and the layered system extends indefinitely.

Following the usual transfer matrix formalism we can relate the fields at the first interface x_0 with those of the final interface at point in x_L by applying the continuity of the temperature and the heat flux at the interfaces, to obtain

$$\begin{pmatrix} T(L) \\ q(L) \end{pmatrix} = (M_N M_{N-1} \dots M_1) \begin{pmatrix} T(0) \\ q(0) \end{pmatrix}, \quad (9)$$

where the matrix M_j is given by⁹

$$M_j = \begin{pmatrix} \cos(k_j d_j) & -\frac{1}{Y_j} \sin(k_j d_j) \\ Y_j \sin(k_j d_j) & \cos(k_j d_j) \end{pmatrix}. \quad (10)$$

The matrix $M = \left(\prod_{j=0}^{N-1} M_{N-j} \right)$ in Eq. (9) is known as the Associated Transfer Matrix (ATM), which transfers the fields, in this case temperature and heat flux, through a given domain³¹. In terms of the total transfer matrix M , the reflectivity is given by^{9,31}

$$r = \frac{Y_0 - Y}{Y_0 + Y}, \quad (11)$$

where the surface admittance of the layered structure Y is written in terms of the admittance of the substrate Y_s and the components of the total transfer matrix as,

$$Y = \frac{M_{21} - Y_s M_{11}}{Y_s M_{12} - M_{22}}. \quad (12)$$

There is an important difference between the Cattaneo-Vernotte equation and other wave phenomena, such as electromagnetic or acoustic, when the reflectance is calculated. The intensity of the acoustic and electromagnetic waves involve the square of the fields, thus the reflectance is $R = |r|^2$. In the case of the CVe, the heat flux is already given by $|q(x, t)|$ and from Eq. (11) we have $R = |r|$.

2.2 Semi-infinite system

If we consider a periodic structure as in Fig. 1(b). Each unit cell is of period p and described by a total transfer matrix M . Applying the Floquet-Bloch theorem we obtain^{9,31}

$$\begin{pmatrix} T(Np) \\ q(Np) \end{pmatrix} = e^{iNpQ} \begin{pmatrix} T(0) \\ q(0) \end{pmatrix}, \quad (13)$$

and with helps of the transfer matrix in Eq. (9), we get

$$(e^{ipQ} \mathbb{I} - M) \begin{pmatrix} T(0) \\ q(0) \end{pmatrix} = 0, \quad (14)$$

that has a solution only if $\det(e^{ipQ} \mathbb{I} - M) = 0$. We transform this into a second degree equation for e^{ipQ}

$$e^{2ipQ} - e^{ipQ} \text{Tr}(M) + \det(M) = 0, \quad (15)$$

where $\det M = 1$. We note that *Floquet's thermal wave vector* is complex, so it is decomposed into its real and imaginary parts, $Q = Q' + iQ''$, where both parts must satisfy the following equation

$$\cos(p(Q' + iQ'')) = \frac{1}{2} \text{Tr}(M). \quad (16)$$

Since we have a wave propagating for $x > 0$, the meaningful solutions are those that satisfy $|e^{iQp}| < 1$. We point out that the values of Q that satisfy the two resulting implicit equations, define the *thermal dispersion relation*.

The reflection of thermal waves can also be calculated from Eq. (14) and Eq. (11) with the admittance of the periodic structure being

$$Y = \frac{i(e^{iQp} - M_{11})}{M_{12}}. \quad (17)$$

3 Results

3.1 Thermal Bragg Mirrors

Optical Bragg mirrors are made of alternate layers of high and low dielectric function materials. To extend the definition to thermal waves we consider three specific materials: Aluminum³² (Al) and two materials with thermal properties of biological tissue^{16,24,33}. From the experimental point of view, materials with biological-like responses can be design with specific thermal properties using gel-phantoms³⁴. In Table (1) the thermal properties of these materials are listed.

To illustrate the individual reflection properties of Al and Material 2, consider a half space made of each material in contact with a substrate made of Material 1. In Fig. 2 we show the reflectance R as a function of frequency of each half-space system. The green line corresponds to Al, that has a very small relaxation time, and there is very little dependence with the frequency. For the material 2 (red line), R shows a larger variation at small frequencies. As the frequency increases, the reflectance becomes almost constant.

In optics Bragg mirrors are characterized by having a combination of high and low index of refraction materials. The thermal Bragg mirrors we consider are made of alternate layers of two materials with incident medium and substrate made of material 1. As a first case we consider a thermal mirror made of alternate layers of material 2 and material 1. For example, a

Material	Thermal conductivity κ [W/m/K]	Heat capacity c_V [J/Kg /]	Mass density ρ [Kg/m ³]	Response time τ [s]
material 1	0.235	3600	1500	1
material 2	0.445	3300	1116	20
Al	237	921	2707	2×10^{-10}

Table 1. Thermal properties of the materials used in the numerical example of a layered system taken from^{16,24}.

Figure 2. Reflectance R between the medium labeled material 1 and a half space made of Al (a), material 2 (b). In all cases, as the frequency increases the reflectance becomes independent of frequency. The properties of the different materials are given in Table (1). As explained in the text, the reflectance is $R = |r|$, rather than $R = |r|^2$ as in other wave phenomena.

system with three bilayers, not including the incident and substrate layers, $n = 3$ is 2-1-2-1-2-1. The thickness of each layer is $d = 100 \mu\text{m}$. In Fig. 3(a) we show the reflectance $|r|$ as a function of frequency. The different lines are for different number of bilayers (unit cells): $n = 1$ (blue line) $n = 2$ (orange) $n = 3$ (green) and $n = 15$ (red). The purple marks correspond to the semi-infinite periodic system as the one depicted in Fig. 1(b). We see that even with a few bilayers the rejection-band expected in the periodic crystal is obtained. The rejection-band can be clearly seen in Fig. 3(b). The contour plot shows the heat flux $\vec{q} \cdot \hat{n}$ into the laminated system, normalized to the incident heat flux of magnitude q_0 . The vertical axis is the frequency and the horizontal axis the number of bilayers. The region where $q/q_0 \sim 0$ shows the heat-rejection band. As a reference, in panel (c) the dispersion relation for the semi-infinite system is shown, where the first rejection-band is shown (Eq. (16)). A similar situation occurs if we change material 1 by Al. The use of a metal is two-fold: it is easy to fabricate well defined metallic layers and the response time is very short. The different lines in Fig. 4(a) correspond to the same number of bilayers as in Fig. 3(a). Although the rejection-band is narrower in frequency, the heat flux into the system vanishes even with a few bilayers. Again, the dispersion relation is shown for the periodic semi-infinite case to show the frequency window of the first stop or rejection-band. For this system the thickness of the Al layers is of $d=1 \mu\text{m}$, the thickness of material 2 is $d = 100 \mu\text{m}$.

3.2 Defects and Asymmetric structures

Having the stop or rejection band in a frequency window opens the possibility of further tuning the heat flux by the introduction of defects. We will use the same materials as those of Fig. 3. In every other unit cell the thickness of the layer of material 1 varies by 10%. This is $1 - 2 - 1' - 2$, where the prime indicates the defective layer. As expected new defect states appear. This is shown in Fig. 5. Two defect states appear as indicated by the arrows in Fig. 5(a). We only plot a system of 15 bilayers (blue line) and the orange line is the case of a semi-infinite system. The consequences of these states are shown in Fig. 5(b) where the contour plot is the heat flux transmitted into the layered system. The arrows in Fig. 5(b) also indicate where the defects will change the heat-flux.

Finally, we consider a system where pass bands can be introduced by changing the order of the layers of the layers alternating the cell. This is 1-2-2-1-1-2-2-1 (inset of Fig. 6). The materials and the thickness of the layers is the same as Fig. 3. The reflectivity for 15 bilayers and the semi-infinite case is shown in Fig. 6(a). The arrows show the defect states or pass-bands that appear (compared to Fig. 3). In this case, these new defect-bands open new transmission channels for the heat flux into the system. The new bands are indicated by the arrows.

Figure 3. For a system with unit cells made of alternative layers of material 1 and material 2 (see Table 1) and both of thickness $d = 100 \mu\text{m}$, we show in (a) The reflectance $R = |r|$ for different number of bilayers n . For $n = 1$ (blue line) $n = 2$ (orange) $n = 3$ (green) and $n = 15$ (red). The crosses (purple) correspond to the semi-infinite case. The stop-band is recovered for a small number of bilayers. (b) The heat flux into the system at $x = 0$ is shown as function of frequency and n . The flux is normalized to the incident flux q_0 . The stop or rejection band is clearly seen even for a few bilayers. The dotted lines indicate the position of the first stop-band in the semi-infinite crystal. In (c), for comparison, the dispersion relation is shown. The first stop-band is shown.

4 Conclusions

In this paper, we demonstrate the possibility of Bragg mirrors for thermal waves that are a solution to the Cattaneo-Vernotte equation. The solution of the CVe has differences with another wave phenomenon. The mirrors are made of alternate layers of two different materials. Even for mirrors made of a few bilayers, a high reflection of the thermal waves is achieved. Reflectivities higher than 90% are possible. Combining materials with sizeable thermal response times or with very short response times, as is the case of materials, exhibits the expected behavior. The behavior of the Bragg mirrors is changed by introducing defects. In one case, very coherent stop bands are obtained. At the frequencies of these bands, no heat flows into the mirror. Another type defect can be made to generate coherent pass-bands where a large heat flux into the mirror is possible. Thus, effective thermal shields are possible by a judicious design of Bragg mirrors.

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Author contributions statement

A.CdR conceived the original idea, D.B. conducted the calculations, G. G. F. and R. E-S. analyzed the results. All authors reviewed the manuscript.

Additional information

Competing interests The authors declare this work is original, has not been published before and that there are no competing interests.

Figure 4. Same as in Fig. 3 but the layers of material 1 are replaced by an Al layer of thickness $d = 1 \mu\text{m}$. The thickness of material 2 remains at $d = 100 \mu\text{m}$. Even for thin metallic layers the regions of zero-heat flux is present.

Figure 5. The introduction of defects in the system opens new stop bands. In this case each bilayer is made of material 1 and material 2 however every other bilayer or unit cell the second layer has a different thickness (10% increase), as shown in the inset. (a) Reflectance $|r|$ for a system with $n = 15$ layers (blue line). The semi-infinite system is shown by the orange line. (b) Heat flux into the system as a function of frequency and number of bilayers. The new defect bands or states are indicated by the arrows.

Figure 6. By inverting the order of the layers every-other unit-cell . (a) We plot the reflectance as a function of frequency for a system with 15 bilayers and for the semi-infinite case(orange line). Compared to the reflectance shown in Fig. (3), e observe defect states with a low reflectance as indicated bu the arrows. (b) Normal heat flux into the layered structure at $x = 0$. In this case the defect states imply allowed bands where a large heat flux into the system is observed.

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Figures

Figure 1

(a) Finite layered system made of consecutive layers with different thermal properties. Each layer is characterized by its thickness d , thermal speed v and the thermal diffusivity α . The system is bounded by a substrate and outer medium. (b) Semi-infinite periodic system. The substrate is removed and the layered system extends indefinitely.

Figure 2

Reflectance R between the medium labeled material 1 and a half space made of Al (a), material 2 (b) . In all cases, as the frequency increases the reflectance becomes independent of frequency. The properties of the different materials are given in Table (1). As explained in the text, the reflectance is $R = |r|$, rather than $R = |r|^2$ as in other wave phenomena.

Figure 3

For a system with unit cells made of alternative layers of material 1 and material 2 (see Table 1) and both of thickness $d = 100 \mu\text{m}$, we show in (a) The reflectance $R = |r|$ for different number of bilayers n . For $n = 1$ (blue line) $n = 2$ (orange) $n = 3$ (green) and $n = 15$ (red). The crosses (purple) correspond to the semi-infinite case. The stop-band is recovered for a small number of bilayers. (b) The heat flux into the system at $x = 0$ is shown as function of frequency and n . The flux is normalized to the incident flux q_0 . The stop or rejection band is clearly seen even for a few bilayers. The dotted lines indicate the position of the first stop-band in the semi-infinite crystal. In (c), for comparison, the dispersion relation is shown. The first stop-band is shown.

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Same as in Fig. 3 but the layers of material 1 are replaced by an Al layer of thickness $d = 1 \mu\text{m}$. The thickness of material 2 remains at $d = 100 \mu\text{m}$. Even for thin metallic layers the regions of zero-heat flux is present.

Figure 5

The introduction of defects in the system opens new stop bands. In this case each bilayer is made of material 1 and material 2 however every other bilayer or unit cell the second layer has a different thickness (10% increase), as shown in the inset. (a) Reflectance $|r|$ for a system with $n = 15$ layers (blue line). The semi-infinite system is shown by the orange line. (b) Heat flux into the system as a function of frequency and number of bilayers. The new defect bands or states are indicated by the arrows.

Figure 6

By inverting the order of the layers every-other unit-cell . (a) We plot the reflectance as a function of frequency for a system with 15 bilayers and for the semi-infinite case(orange line). Compared to the reflectance shown in Fig. (3), we observe defect states with a low reflectance as indicated by the arrows. (b) Normal heat flux into the layered structure at $x = 0$. In this case the defect states imply allowed bands where a large heat flux into the system is observed.