Nonreciprocal Thermal Material by Spatiotemporal Modulation

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Non-Reciprocal Thermal Material by Spatio-Temporal Modulation

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The thermal properties of a material with a spatio-temporal modulation, in the form of a traveling wave, in both the thermal conductivity and the specific heat capacity are studied. It is found that these materials behave as materials with an internal convection-like term that provides them with non-reciprocal properties, in the sense that the heat flux has different properties when it propagates in the same direction or in the opposite one to the modulation of the parameters. An effective medium description is presented which accurately describes the modulated material, and numerical simulations support this description and verifies the non-reciprocal properties of the material. It is found that these materials are promising candidates for the design of thermal diodes and other advanced devices for the control of the heat flow at all scales.

The research on materials with non-reciprocal thermal properties has received a great attention in recent years. These materials have different propagation properties of the thermal energy along two opposite directions. With the so-called thermal diode being the most immediate application of these structures[1], other devices and applications are easily envisioned, like thermal transistors and even logic circuits[2].

Non-reciprocal materials have been properly studied theoretically and experimentally at different scales [3–6], and it has been demonstrated that the realization of a non-reciprocal material requires the use of a combination of non-linear and asymmetric structures[7]. However, the realization of non-reciprocal materials based on non-linear elements limits their applicability, since nonlinearity does not occurs at all temperatures and scales, so that we can find that the rectification properties of the materials are efficient in only a short range of temperature.

In this context, metamaterials, which are artificially structured materials with *a priori*-designed properties, have overcome one of the major drawbacks of common materials, since their properties depend on the internal artificial structure and not on intrinsic properties of the constituent materials, which in turns allow us to decide at which scale, frequency or temperature range we want to operate[8]. Here, a special type of metamaterial is employed presenting non-reciprocal properties, which consists in a material where the thermal properties are functions of both space and time in a wave-like fashion. This special type of modulation has been studied in elastic and acoustic materials[9–12], whose non-reciprocal properties for the propagation of waves have been widely demonstrated. We will apply these ideas to the diffusion equation describing thermal waves in solids, and non-reciprocal thermal transport will be found.

We present therefore an alternative mechanism for the realization of non-reciprocal thermal materials which can be applied to any scale, as long as the thermal transport be dominated by diffusion. It is demonstrated that, when the spatio-temporal modulation of the thermal properties of a material is of the form of a traveling wave, the material presents non-reciprocal thermal transport. Moreover, it is demonstrated that an effective medium description is possible for such a material, in which it is described as a homogeneous solid with constant constitutive parameters (in both space and time) but in which the temperature field satisfies a convection-diffusion equation. In other words, it is demonstrated that, although there is no transport of matter in the solid material, in an effective way an internal convective term appears, which is responsible of providing non-reciprocal properties to the solid even in the stationary regime. Analytical expressions are given for the effective parameters and time-domain numerical simulations show a perfect agreement with the effective medium description.

Figure 1 shows an example of realization of a material with a spatio-temporal modulation in its constitutive parameters. Panel *a)* shows a homogeneous material B with a thermal conductivity σ_B. Let us assume that the material's conductivity is sensitive to the application of some external field E, which can be the electric, magnetic or acoustic fields, for instance. Then, when the external field is applied, the conductivity changes to $\sigma_A = \sigma_B + \chi E$, with χ being some coupling constant. Panel *a)* shows the situation when the external field is turned off, and panel *b)* shows a situation in which we have turned on the external field but only in the regions marked by the arrows, so that it changes the material from σ_B to σ_A only in the neighborhood of the arrows. We have therefore induced a layered material by means of the external field $E(x)$, so that the conductivity of the material is now $\sigma(x) = \sigma_B + (\sigma_A - \sigma_B)\mathrm{rect}(2\pi x/d)$. Since the external field is induced artificially, we can set up the origin of the modulation, as shown in panel *c)*, where it has been displaced a quantity Δ, so that the conductivity is now $\sigma(x) = \sigma_B + (\sigma_A - \sigma_B)\mathrm{rect}(2\pi(x-\Delta)/d)$. Finally, if the external field is synchronized so that the spatial modulation is traveling along the x direction at a speed v_0, as represented in the panel *d)*, the induced conductivity will be a function of both space and time of the form $\sigma(x) = \sigma_B + (\sigma_A - \sigma_B)\mathrm{rect}(2\pi(x - v_0 t)/d)$. The reader interested in a possible mechanical realization of these materials can find a proposal through the supplementary movie "chaincylinders.gif", and its brief discussion in the Supplementary Material.

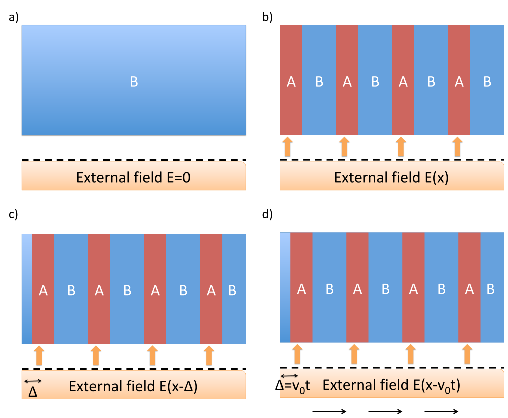

FIG. 1. Schematic representation of a possible realization of a material with a spatio-temporal modulation in the conductivity and the mass density.

The procedure described before shows that in order to have a spatio-temporal modulation in the thermal properties of a material we need essentially a tunable material whose control parameter could be modulated in both space and time. The domain of tunable metamaterials is broad enough to allow us to consider this modulation feasible, so that in the most general case we can postulate that we can obtain a materials whose thermal properties modulated in a wave-like fashion, $\sigma = \sigma(x - v_0 t)$ and $\rho = \rho(x - v_0 t)$, with σ and ρ being periodic functions of $n = x - v_0 t$ with period d. In a material with these properties, the energy balance is described by means of the local diffusion equation

$$\frac{\partial}{\partial x}\left(\sigma(x - v_0 t)\frac{\partial T}{\partial x}\right) = \rho(x - v_0 t)\frac{\partial T}{\partial t}, \tag{1}$$

where the heat capacity has been set to 1, in order to simplify the notation, however it is evident that in the above equation ρ means the specific heat capacity. It has to be pointed out that equation (1) is a particular case of a more general problem in which a term containing the temporal derivative of ρ should be added, however this term is canceled by the external field inducing the modulation, as explained in the Supplementary Material, which include reference [13].

In the so-called homogenization limit the spatio-temporal variation of the constitutive parameters is not "visible", and the material is perceived as a homogeneous material with some effective properties. In the following lines it will be shown that the homogeneous version of equation (1), which defines these effective parameters, contains additional constitutive parameters that induces non-reciprocity in the effective material.

The homogenization of equation (1) can be done more efficiently under the change of variables $n = x - v_0 t$ and $\tau = t$, so that the diffusion equation takes the form

$$\frac{\partial}{\partial n}\left(\sigma(n)\frac{\partial T}{\partial n}\right) = \rho(n)\frac{\partial T}{\partial \tau} - v_0\frac{\partial}{\partial n}(\rho(n)T), \tag{2}$$

which is a differential equation in which the coefficients depend only on the variable n. Equation 2 is a partial differential equation in the variables n and τ in which the coefficients are periodic functions of n with period d, so that Bloch theorem applies and the solutions for the temperature field are linear combinations of eigenfunctions of the form

$$T(n, \tau) = e^{-iKn}e^{i\Omega\tau}\phi(n), \tag{3}$$

with $\phi(n)$ being a d-periodic function of the variable n with the same periodicity of σ and ρ.

The spatio-temporal behavior of the temperature field is therefore composed of the "macroscopic" function $e^{-iKn}e^{i\Omega\tau}$ modulated by a "microscopic" function $\phi(n)$ over the period d. When the spatial variations of the field are larger than the typical period d equation (2) can be replaced by a "homogenized" version with constant coefficients with the same solution $\Omega = \Omega(K)$. Once the equation in the traveling frame is homogenized, we can return to the frame at rest to study its properties however, when we return to the system at rest, we don't recover a Fourier-type differential equation (like equation (1)) with constant coefficients, as should be expected, but we obtain a more complicated equation, in which additional constitutive parameters appear (see the Supplementary Material for further details),

$$\sigma^*\frac{\partial^2\langle T\rangle}{\partial x^2} = \rho^*\frac{\partial\langle T\rangle}{\partial t} + C\frac{\partial\langle T\rangle}{\partial x} - i(S + S')\frac{\partial^2\langle T\rangle}{\partial x\partial t}. \tag{4}$$

Therefore, the homogenized equation is the convection-diffusion equation with two additional coefficients, S and S', which are the thermal equivalent of the Willis coefficients found in the elastodynamics of inhomogeneous media[14–16]. These coefficients are coupling terms related with the non-symmetry of the unit cell, and although they are null for symmetric periodic materials[17], the non-reciprocity induced by the special modulation of the materials considered here makes them different than zero. These terms are relevant especially in the dynamic or transient regime, however in this work we are more interested in the non-reciprocal properties of the material in the nearly stationary regime, for which a further discussion about these terms is beyond the objective of the present work.

The responsible of the non-reciprocal properties of the material in the stationary regime is the convective term $C\partial_x T$ appearing in equation (4). It is interesting the relationship between the convective term C and the effective mass density ρ^*. It could be thought that, since v_0 is constant through the material, the effective convective term in the homogenized version of equation (2) would be simply $v_0\rho^*$. The consequence of this property would be that, when returning to the reference frame at rest, the convective term would disappear and then we would recover the diffusion equation with constant coefficients (plus the Willis terms). However, as it is demonstrated in the Supplementary Material, the effective convective term does not satisfy this condition, since although the variation of $v_0\rho$ is the same as of ρ, they appear multiplying a different operator in the equation, the temporal derivative and the spatial derivate, so that their role is completely different in the equation and, therefore, in the frame at rest we find that the diffusion equation (1) has become the diffusion-convection equation (4), which is known to be non-reciprocal due to the convective term C.

Therefore, the spatio-temporally modulated material behaves, in the homogenization limit, as a homogeneous material in which a convective term appears, so that the diffusion of heat will have non-reciprocal properties. It must be pointed out that the convective term is not induced by any transport of matter, as for sound propagation in moving fluids and similar processes, but it is induced by means of some external stimulus that modulates the properties of the material in a wave-like fashion, so that we can have not only a solid material with an internal effective convection, but we can have a finite structure with convection without the need of letting the flow of matter leave the structure.

For the analytical and numerical examples we propose a sinusoidal modulation of the form

$$\sigma(x - v_0 t) = \sigma_0\left[1 + \Delta_\sigma \cos\frac{2\pi}{d}(x - v_0 t)\right], \tag{5a}$$

$$\rho(x - v_0 t) = \rho_0\left[1 + \Delta_\rho \cos\frac{2\pi}{d}(x - v_0 t)\right], \tag{5b}$$

where the mass density and conductivity changes periodically from $\rho_b = \rho_0(1-\Delta_\rho)$ to $\rho_a = \rho_0(1+\Delta_\rho)$ and from $\sigma_b = \sigma_0(1-\Delta_\sigma)$ to $\sigma_a = \sigma_0(1+\Delta_\sigma)$, respectively. The effective parameters for this modulation can be approximated by (see equations 25 in the Supplementary Material)

$$\sigma^* \approx \sigma_0\left[1 - \frac{1}{2}\frac{\Delta_\sigma^2}{1+\Gamma^2}\right], \tag{6a}$$

$$\rho^* \approx \rho_0\left[1 - \frac{\Gamma^2}{2}\frac{\Delta_\rho^2}{1+\Gamma^2}\right], \tag{6b}$$

$$S = S' \approx -\frac{\rho_0 d}{2\pi}\frac{\Delta_\rho\Delta_\sigma}{2}\frac{i\Gamma}{1+\Gamma^2}, \tag{6c}$$

$$C \approx \frac{2\pi\sigma_0}{d}\frac{\Delta_\rho\Delta_\sigma}{2}\frac{\Gamma}{1+\Gamma^2}, \tag{6d}$$

where $\Gamma = \frac{v_0 d \rho_0}{2\pi\sigma_0}$.

Equations (6) show that the effective conductivity and mass density are both even functions of Γ, which means that reversing the direction of the modulation has no effect on their values. Contrarily, both S and C are odd functions, which is obvious since these parameters are the responsible of the non-reciprocal properties of the material. When there is no traveling modulation ($\Gamma = 0$), both S and C are zero, the mass density is just the average mass density $\rho^* = \rho_0$ and effective conductivity $\sigma^* = \sigma_0(1 - \Delta_\sigma^2/2)$, so that we recover reciprocity as expected. Interestingly, when $v_0 \to \pm\infty$ the non-reciprocal properties of the material also disappear, since S and C both tend to zero, and now the effective mass density is $\rho^* = \rho_0(1 - \Delta_\rho^2/2)$ and the effective conductivity is $\sigma^* = \sigma_0$. In this case the oscillations of the material's properties are so fast that the spatial variation almost disappear, therefore we can see an averaged material in time, which in turns means that the non-reciprocal properties disappears. It is interesting to note how the expressions for the effective parameters exchange their roles in the limiting situation $\Gamma = \pm\infty$ or $\Gamma = 0$, due to the exchange of them in front of the space and time derivatives in the diffusion equation. This simple analysis, which will be verified later, shows that the larger "non-reciprocity" is not obtained with the larger modulation velocity, but that there is an optimum velocity for the design of non-reciprocal materials.

Another interesting feature of equations (6) is that we need a modulation of both the mass density and the thermal conductivity to have non-reciprocity. This is indeed a general result, as shown in the Supplementary Material, where the effective convective term is shown to be

$$C = v_0 \sum_{G', G\neq 0} \rho_{-G'} G' \chi_{G'G} \sigma_G G \tag{7}$$

where the summation has to be performed for all the reciprocal lattice points $G = 2\pi m/d$, with m being an integer. $\chi_{G'G}$ is an interaction matrix, and ρ_G and σ_G are the Fourier components of the functions $\rho(n)$ and $\sigma(n)$, respectively. Given that in the above equation the summation excludes the term $G = 0$, it will be zero unless we have at least one pair (ρ_G, σ_G) for $G \neq 0$ different than zero, that is, we need a simultaneous variation of both σ and ρ.

This result shows that the origin of the convective term in the effective material is due to a coupling between the variation of the mass density and the conductivity, and enforces its analogy with the Willis term and chirality in electromagnetism.

In the stationary regime the macroscopic temperature $\langle T\rangle$ is independent of time, and equation (4) reduces to

$$\sigma^* \frac{\partial^2\langle T\rangle}{\partial x^2} = C\frac{\partial\langle T\rangle}{\partial x} \tag{8}$$

whose general solution is given by

$$\langle T\rangle = A + Be^{\alpha x}, \tag{9}$$

with $\alpha = C/\sigma^*$ being the convection-diffusion parameter that quantifies the non-reciprocity of the material, as will be demonstrated later on. For the harmonic perturbation studied in the present example, we can approximate α by

$$\alpha \approx \frac{2\pi}{d}\Delta_\sigma\Delta_\rho\frac{\Gamma}{1+2\Gamma^2}. \tag{10}$$

Figure 2 shows the dependence of this parameter as a function $2\pi\Gamma$. In these examples $\rho_a/\rho_b = 0.5$ and $\sigma_a/\sigma_b = 0, 0.01, 0.1, 0.5$ and 1, as indicated in the legends of the plot. We see that there is an optimum value of Γ for which we obtain the maximum value of α and, as before for C, when $\Gamma\to\infty$, α tends to zero and the material becomes reciprocal.

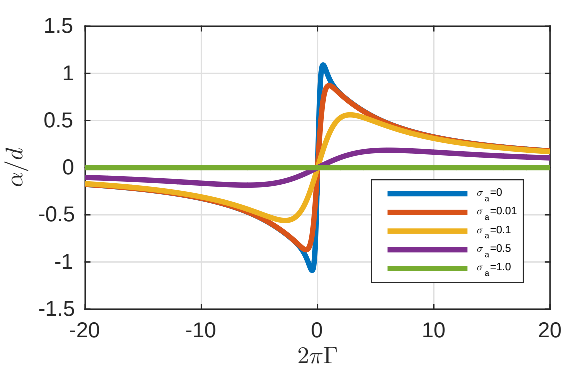

FIG. 2. Effective convection-diffusion coefficient as a function of the non-dimensional modulation velocity Γ.

Numerical simulations by the Finite Element Method (FEM) in time-domain have been performed. We have assumed a one dimensional domain (a solid bar, for instance) of length $L = 10d$, in which the initial temperature is set to 0. In the "forwards" (F) configuration, the temperature at the extreme $x = L$ is fixed to 0 and, for $t > 0$, the temperature at $x = 0$ is set to T_0. In the "backwards" configuration we have reversed the temperatures, so that at $x = 0$ the temperature is fixed to 0 and for $t > 0$ the temperature is fixed to T_0 at $x = L$. We have selected the same parameters for ρ_a and ρ_b as in the previous calculations, and the value of $\sigma_a = 0.01\sigma_b$. The simulations have been performed for $2\pi\Gamma = 0, 0.3, 1$ and 10, whose corresponding values for α/d are 0, 0.52, 0.87 and 0.32, respectively. According to equation (9) and the previously defined boundary conditions, the temperature distribution in the bar in the stationary regime for the forwards and backwards configuration is, respectively,

$$\langle T_F\rangle = T_0\frac{e^{\alpha L}-e^{\alpha x}}{e^{\alpha L}-1} \tag{11a}$$

$$\langle T_B\rangle = T_0\frac{e^{\alpha x}-1}{e^{\alpha L}-1} \tag{11b}$$

showing a non-symmetric profile in the forwards and backwards configurations, as expected. The total heat flux is composed of the diffusive plus the convective flux, so that $\Phi_T = -\sigma^*\partial_x\langle T\rangle + C\langle T\rangle$, and it is clearly different in the forwards and backwards configuration, since we have $\Phi_F = CT_0e^{\alpha L}/(1-e^{\alpha L})$ and $\Phi_B = -CT_0/(1-e^{\alpha L})$. Indeed, the ratio $|\Phi_B/\Phi_F| = e^{-\alpha L}\approx 0$ is the definition of a nearly perfect thermal diode, showing a very promissing application of these materials.

Figure 3 shows the numerical simulations performed by the comercial software COMSOL Multiphysics[18] (blue dots) at $t = t_f = 300d\rho_b/\sigma_b$, together with the corresponding analytical solution given by (11). A space element of size $\Delta x = 0.1d$ and a time step of $\Delta t = 0.01d\rho_b/\sigma_b$ was enough to ensure a good convergence, as it is demonstrated due to the perfect agreement with the numerical and analytical solution, although an additional modulation appears in the numerical simulation. This modulation is due to the fact that in the homogenized model we ignore the modulation function $\phi(n) = \phi(x - v_0t)$, which is obviously included in the numerical solution. Since the time is fixed to $t = t_f$ in figure 3, only the spatial variation of ϕ is detected, however the transient period and the time evolution of the system can be seen in the Supplementary Movies temperatureF.gif and temperatureB.gif, where the effect of $\phi(n)$ is more evident, although the relevant information is given by the analytical model shown in equation (11). It is obvious the diode-like behavior of the material, whose non-reciprocal nature is manifested not only in the static but also in the dynamic regime. The accuracy of the analytical solution provides also a very powerful tool to design more advanced devices based on these materials.

In summary, we have presented a structured solid material with non-reciprocal effective thermal properties, where the mechanism of non-reciprocity is due to an artificial convective term that appears in its effective behavior. The structured material consists of a modulated solid in which the local thermal properties depend not only on the position, but also on time, in such a way that these parameters have a wave-like behavior. It is shown that in the nearly-stationary regime the material presents non-reciprocity in the diffusion of heat, and it is shown how such a material can work as a thermal diode.

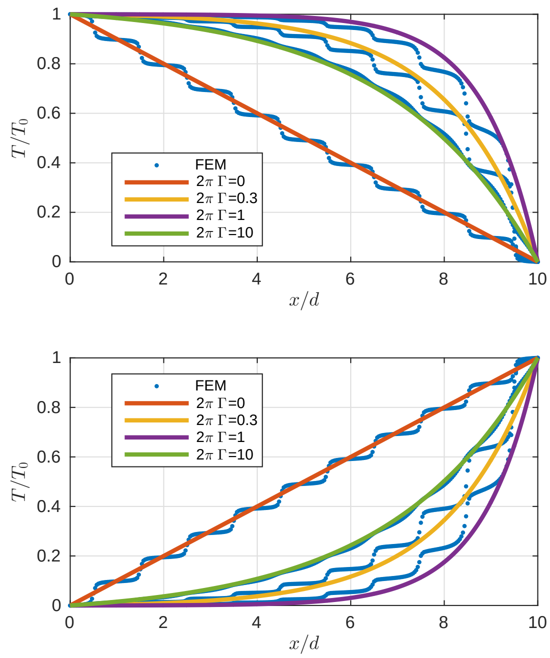

FIG. 3. Temperature distribution of the spatio-temporally modulated bar in the forward (upper panel) and backward (lower panel) configurations.

Several properties of the effective parameters are deduced and an effective medium theory is developed. The expression derived for the convective term shows that it is required a modulation in both the mass density and thermal conductivity, since this term appears as a coupling between the relative variations of both parameters. Coupling terms equivalent to the so-called Willis terms in elasticity or chiral coefficients in electromagnetism also appear, although their contribution is relevant only in the transitory or time-dependent regime. It is remarkable the fact that the non-reciprocal thermal effect presented here is the result of the artificial internal structure of the materials, what makes that effect be scalable and therefore useful in a wide variety of thermal problems and scales where the heat transport be dominated by diffusion.

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