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Anomalous refraction of heat flux in thermal metamaterials

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We discuss the possibility of bending of heat flux in a multilayered composite typical to abnormal negative refraction, according to which the horizontal and the vertical components of the incident and refracted heat flux vectors point in the opposite direction. The engineered anisotropy of the thermal conductivity tensor is integral to such effects. We propose practical designs where such anomalous refraction phenomena may be observed and be used for heat flux redirection. © 2014 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4867027]

In the interest of gaining greater control over the passage of heat in a solid medium, the concept of a metamaterial with an engineered sub-structure or arrangement of materials has gained much popularity. Much of the recent related work originates from a surge in theoretical ideas in the electromagnetics (EM) literature with fascinating implications ranging from higher efficiency antennae to invisibility cloaks. Subsequent work on the extension of similar principles to thermal phenomena was focused on long wavelength/near-infrared regimes. However, a major breakthrough—using principles not directly related with the electromagnetic counterparts—with an aim of controlling heat flux propagation was achieved through ingenious materials arrangements, seemingly following principles related to the tensorial characteristics of the thermal conductivity of the materials are ignored, i.e., the materials are isotropic with \( \kappa_{ij} = \kappa_i \) for medium \( i \), (ii) \( \phi_i \) and \( \phi_j \) are positive, with the angles considered positive in the counter-clockwise direction, and (iii) there is no total reflection of the heat. For isotropic materials, which are the norm in thermal conductivity, the heat flux density vector \( q_i \) follows the collinear temperature gradient with its magnitude determined only by the temperature gradient in that direction. We then define, in correspondence to the normal/positive refraction of EM waves, positive heat flux refraction to occur when the horizontal \((x)\) and the vertical \((y)\) components of the incident and refracted heat flux vector points in the same direction and have the same sign as indicated, for example, in Figure 1.

However, what has not been examined to date is the behavior of heat flux as it traverses thermally anisotropic media (i.e., with off-diagonal components of \( \kappa_{ij} \)). Such composites may be synthesized through alternately stacking materials with nominally isotropic thermal conductivities. We have previously shown that interesting phenomena may occur in such thermal metamaterials, e.g., wherein cross-coupling and concomitant bending of the heat flux were indicated, due to which the heat flux in the \( x \)-direction would be determined by the temperature gradient in both the \( x \) - and an orthogonal \((y/z)\) direction. In this paper, we further consider phenomena related to heat flux bending, corresponding to thermal refraction, in such metamaterials.

Generally, \( \kappa_{ij} \)—a second order thermal conductivity tensor with respect to an orthogonal \((x/y/z)\) coordinate system—is represented through, e.g.,

\[
\tan \phi_i / \kappa_1 = \tan \phi_j / \kappa_2, \tag{1}
\]

The relation in (1) could be written, as \( \rho_i \tan \phi_i = \rho_j \tan \phi_j \), where \( \rho_i \) and \( \rho_j \) represent the thermal resistivity (the inverse of the thermal conductivity) of the medium of incidence and the medium where refraction occurs, respectively. The implicit assumptions thus far are (i) that the tensorial characteristics of the thermal conductivity of the materials are ignored, i.e., the materials are isotropic with \( \kappa_{ij} = \kappa_i \) for medium \( i \), (ii) \( \phi_i \) and \( \phi_j \) are positive, with the angles considered positive in the counter-clockwise direction, and (iii) there is no total reflection of the heat. For isotropic materials, which are the norm in thermal conductivity, the heat flux density vector \( q_i \) follows the collinear temperature gradient with its magnitude determined only by the temperature gradient in that direction. We then define, in correspondence to the normal/positive refraction of EM waves, positive heat flux refraction to occur when the horizontal \((x)\) and the vertical \((y)\) components of the incident and refracted heat flux vector points in the same direction and have the same sign as indicated, for example, in Figure 1.

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\]
For demonstration of the fundamental phenomena as well as mathematical simplicity, we consider a reduced two-dimensional representation of the form: \( \begin{pmatrix} \kappa_{xx} & \kappa_{xy} \\ \kappa_{yx} & \kappa_{yy} \end{pmatrix} \), i.e., implying that there is no heat flux variation perpendicular to the \( xy \) plane (along the \( z \) axis) inside the anisotropic material. Consequently, with \( z \) as the angle made by the temperature gradient, \( \nabla T \) with the \( x \)-axis (see Figure 1(b)); \( \nabla T = (\nabla T \cos z) \hat{x} + (\nabla T \sin z) \hat{y} \), the flux is given by

\[
\vec{q} = -[(\kappa_{xx} \cos z + \kappa_{xy} \sin z) \hat{x} + (\kappa_{yx} \cos z + \kappa_{yy} \sin z) \hat{y}] \nabla T.
\]

The corresponding angle of heat flux orientation, \( \phi \), is related to the \( z \), by

\[
\phi = \tan^{-1} \left[ \frac{\kappa_{xx} \cos z + \kappa_{xy} \sin z}{\kappa_{yx} \cos z + \kappa_{yy} \sin z} \right] = \tan^{-1} \left[ \frac{\kappa_{xx} \cot z + \kappa_{yy}}{\kappa_{yx} \cot z + \kappa_{yy}} \right].
\]

We then consider the refraction of heat flux at the interface of two anisotropic media, designated through \( \kappa_{ij} \) = \( \begin{pmatrix} \kappa_{xx} & \kappa_{xy} \\ \kappa_{yx} & \kappa_{yy} \end{pmatrix} \) and \( \kappa'_{ij} = \begin{pmatrix} \kappa'_{xx} & \kappa'_{xy} \\ \kappa'_{yx} & \kappa'_{yy} \end{pmatrix} \), with \( (i,j=x,y) \), respectively, as indicated by the top and the bottom media, in Figure 1(b). The following two boundary conditions, assuming steady state conditions to be prevalent, are assumed:

(a) The continuity of heat flux along the \( x \)-axis, assuming no heat sources/sinks in the media, implies \( q \cdot \hat{x} = q' \cdot \hat{x} \) which then yields from Eq. (3)

\[
(\kappa_{xx} \cos z + \kappa_{xy} \sin z) \nabla T = (\kappa'_{xx} \cos z' + \kappa'_{xy} \sin z') \nabla T'.
\]

(b) The continuity of temperature gradient along the interface, assuming no interfacial resistance with, \( \nabla T \cdot \hat{y} = \nabla T' \cdot \hat{y} \), and implying

\[
\nabla T \sin z = \nabla T' \sin z'.
\]

Dividing (5a)/(5b) and using (4), we get

\[
\left( \frac{\kappa_{xx} - \kappa_{xy} \cot \phi}{\kappa_{xx} \kappa_{yy} - \kappa_{xy} \kappa_{yx}} \right) \tan \phi_i = \left( \frac{\kappa'_{xx} - \kappa'_{xy} \cot \phi_j}{\kappa'_{xx} \kappa'_{yy} - \kappa'_{xy} \kappa'_{yx}} \right) \tan \phi_j.
\]

For algebraic simplicity, Eq. (6) can be recast in terms of thermal resistivity (\( \rho \)) as

\[
\phi = \tan^{-1} \left[ \frac{\rho_{xx} \tan \phi_i + \rho_{xy} \rho_{yx} \rho_{yy} \rho_{xx}^{-1}}{\rho_{xx}^{-1}} \right].
\]

The \( \rho \) components can be derived using

\[
\rho_{ij} = \left( \begin{array}{cc} \rho_{xx} & \rho_{xy} \\ \rho_{yx} & \rho_{yy} \end{array} \right) = \kappa_{ij}^{-1} \text{ and } \rho'_{ij} = \left( \begin{array}{cc} \rho'_{xx} & \rho'_{xy} \\ \rho'_{yx} & \rho'_{yy} \end{array} \right) = \kappa'_{ij}^{-1}.
\]

It can then be deduced—from Eq. (7)—that the angle of refraction (\( \phi_j \)) may be positive/negative, according to whether: \( \tan \phi_j \geq \frac{\rho'_{xx} \rho_{yy} - \rho'_{xy} \rho_{yx}}{\rho'_{xx}} \), respectively. We illustrate positive (\( \phi_j > 0 \)) and negative refractions (\( \phi_j < 0 \)) through considering two isotropic and commonly available materials, e.g., with \( \kappa_1 = 20 \text{ W/mK} \) (e.g., carbon steel) and \( \kappa_2 = 0.1 \text{ W/mK} \) (e.g., polystyrene) of equal thickness stacked alternately as shown in Figure 2. It was generally observed that the extent of bending or refraction was proportional to the thermal conductivity contrast. The effective thermal conductivity of the composite in Figure 2(a) can then be derived to be (see supplementary material in Ref. 7)

\[
\kappa = \left( \begin{array}{ccc} \frac{2\kappa_1 \kappa_2}{\kappa_1 + \kappa_2} & 0 & 0 \\ 0 & \frac{2\kappa_1 \kappa_2}{\kappa_1 + \kappa_2} & 0 \\ 0 & 0 & 0 \end{array} \right) = \left( \begin{array}{ccc} 0.20 & 0 & 0 \\ 0 & 10.05 & 0 \\ 0 & 0 & 10.05 \end{array} \right).
\]

It was previously shown\(^7\) that when the composite in Fig. 2(a) was rotated in the \( xy \) plane by \( \theta \) (with \(-\pi/2 < \theta < \pi/2\), and \( \theta \) considered positive in the counterclockwise direction), the modified thermal conductivity (\( \kappa''_i \)) in the rotated system of coordinates is given by, \( \kappa''_i = \frac{J_{ij} \kappa''_j}{\det(J)} \), where \( J \) is the Jacobian for the rotation. We consider...
representative degrees of rotation of the multi-layered composite, of Figure 2(a), by \( \theta = \pi/4, \pi/3 \) and \(-\pi/6\), yielding the following thermal conductivity matrices in the three cases, with obvious anisotropy

\[
\begin{align*}
\kappa'_{ij,\theta=\pi/4} &= \begin{pmatrix} 5.12 & 4.93 \\ 4.93 & 5.12 \end{pmatrix}, \\
\kappa'_{ij,\theta=\pi/3} &= \begin{pmatrix} 7.58 & 4.27 \\ 4.27 & 2.67 \end{pmatrix}, \\
\kappa'_{ij,\theta=-\pi/6} &= \begin{pmatrix} 2.67 & -4.27 \\ -4.27 & 7.58 \end{pmatrix}.
\end{align*}
\]

We see straight away, e.g., in (C) above that some of the elements in the matrix are negative. It should be cautioned that the signs (positive or negative) of the off-diagonal components are due to the operation of rotation and choice of coordinate system and do not have physical significance. However, metamaterials fabricated through stacking various combinations of the above cases yield diverse phenomena corresponding to the positive or negative bending of the thermal flux. For instance, the passage of heat through the metamaterial structures corresponding to stacking of combinations (A)/(B) and (A)/(C), and (B)/(C), are illustrated in Figure 3. The values of \( \phi_r \) were calculated from Eq. (7). We have chosen these particular combinations as we found that \( \phi_r > 0 \) in the first case (representative of positive/normal refraction) while \( \phi_r < 0 \) (indicative of negative/anomalous refraction) in the latter two cases. Such conclusions were validated through simulations conducted using COMSOL\textsuperscript{10} Multiphysics software. For the simulations, the surfaces on the top and the bottom of a semi-infinite composite (of total height = 10 cm) were maintained at 350 K and 300 K, respectively. Additionally, the material interfaces were assumed to be smooth without interfacial resistance and end effects, along with heat loss due to convection and radiation has been ignored. We justify the assumption of negligible thermal interfacial resistance assuming that (a) the interface is sufficiently thin, and (b) that no heat is stored or dissipated in the interfacial layer. Additionally, for such a two-dimensional composite which is thin (i.e., where the height/width ratio tends to zero), boundary conditions, described through Eqs. (5a) and (5b) would still hold as the temperature gradient in the transverse direction tends to zero. It was also observed that the transmission at the interfaces is reciprocal, i.e., reversing the direction of temperature gradients reverses the direction of the heat flux vectors preserving the incident and transmission angles. However, when considered through the traditional optics viewpoint where ray propagation follows Snell’s law, negative refraction (with \( \theta_r < 0 \)) occurs for all incident angles (\( \theta_i \))—from \( \theta_r = \sin^{-1} \left( \frac{n_i}{n_r} \sin \theta_i \right) \) if \( n_r < 0 \) or \( n_i/n_r < 0 \), where \( n_i \) and \( n_r \) are the respective optical refractive indices of the incident and refracted media. As such effects are not always observed in our investigations, e.g., negative refraction (\( \phi_r < 0 \)) only occurs for negative arguments of the \( \tan^{-1} \) function in Eq. (7) when \( \phi_i > 0 \), the reverse bending may be termed as anomalous refraction. Our formulations can also be related to theoretical\textsuperscript{12} and experimental\textsuperscript{13} efforts in literature invoking “transformation thermodynamics,”\textsuperscript{12} which in essence relate to geometric transformations\textsuperscript{2} for modulating the isotropic thermal conductivity in polar coordinate systems for obtaining circular thermal cloaks. We have employed a rectangular coordinate system as pertinent to considering the refraction of a heat flux at a given point of the ambient/metamaterial composite interface. A rotation of the thermal flux\textsuperscript{14} would occur through a continuous change of the \( \phi_r \). Incidentally, when \( \phi_r = \phi_i - \pi \), a backwards refracted/propagating heat flux could be obtained.

\[
\begin{align*}
\text{(i) } &A/B \ (\phi_r = 44^\circ, \phi_i = 58^\circ), \\
\text{(ii) } &A/C \ (\phi_r = 44^\circ, \phi_i = -29^\circ), \\
\text{(iii) } &B/C \ (\phi_r = 58^\circ, \phi_i = -29^\circ) \text{ configurations.}
\end{align*}
\]
Our work is interesting in that the observations of reverse bending/anomalous refraction of heat flux—as seen in Figs. 3(b) and 3(c) is not possible at the interface of isotropic media, where a tangent law—per Eq. (1), governs the refraction. We have formulated a definitive criterion, through Eq. (7), to indicate whether such anomalous refraction is possible with a given combination of materials possessing isotropic values of thermal conductivity. Generally, manipulation of heat flux would be advantageous for control and channeling of the thermal energy and reduce heat wastage.

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