

Article

Defect-Induced Localization in One-Dimensional Thermal Wave Crystals

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Abstract

We investigate the existence and properties of defect-induced localized modes in one-dimensional thermal wave crystals governed by the Cattaneo–Vernotte (CV) hyperbolic heat equation. When a single defect layer is introduced into a periodic bilayer of biological tissues, translational symmetry is broken, and a localized thermal excitation emerges within the band gap, characterized by a discrete frequency at which the imaginary part of the Bloch wave vector exhibits a sharp minimum, indicating maximal penetration depth and energy confinement at the defect layer. Using the transfer matrix method, we show that the resonance frequency of this defect mode is determined by the properties of the defect material and its thickness, and is essentially independent of the number of mirror periods surrounding it. The spatial confinement of the mode, by contrast, is governed by the number of mirror periods: increasing this number dramatically sharpens the localization, in direct analogy with a high-quality-factor optical microcavity. We further demonstrate that the defect-mode frequency is continuously tunable across the entire band gap by varying the defect-layer thickness, for three biologically relevant candidate materials. These results establish the CV thermal wave crystal as a platform for engineering localized thermal excitations at the microscale, using materials and layer thicknesses that are experimentally accessible today, and provide a theoretical framework that may motivate future experimental studies on narrowband thermal filtering and biological-tissue characterization.

Keywords: thermal wave crystal; Cattaneo–Vernotte model; hyperbolic heat equation; transfer matrix method; band gap; defect mode; photonic crystal analogy; biological tissue; localized thermal mode; thermal microcavity



Academic Editors: YoungPak Lee and Luis M. Garcia-Raffi

Received: 17 April 2026

Revised: 3 July 2026

Accepted: 4 July 2026

Published: 8 July 2026

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1. Introduction

The control of heat flow using periodic structures has emerged as a rich direction in heat-transport engineering, driven by the analogy between thermal wave propagation and the behavior of electromagnetic and acoustic waves in photonic and phononic crystals [1–3]. When heat transport is governed by the Cattaneo–Vernotte (CV) model [4,5] rather than Fourier’s diffusion law, the parabolic diffusion equation is replaced by a damped wave equation—the thermal analogue of the telegrapher’s equation, whose solutions admit

interference effects and band-gap formation in periodic structures. A material relaxation time τ_q governs the transition from diffusive to wave-like behavior, and the resulting finite propagation speed sets the length and frequency scales of the periodic structure. This wave-like character enables band-gap formation in periodic multilayers—the so-called thermal wave crystals (TWCs) [6,7]—and opens the possibility of engineering the thermal band structure through unit-cell design [8].

The broader goal of guiding and localizing heat at specific frequencies draws direct inspiration from photonic and phononic crystal physics [9,10]. In photonic crystals, a structural defect within the periodic arrangement breaks translational symmetry and introduces a localized resonance within the band gap [11–13]. These defect modes underpin a wide range of devices, from narrowband filters [14] and biosensors [15,16] to microcavity-enhanced emitters [17]. In phononic crystals, analogous defect states have been exploited for acoustic filters, waveguides, and tunable sensors [18–20]. In both cases, within the band gap, the Bloch wave vector is purely imaginary, leading to exponential attenuation of waves away from the defect. The defect layer introduces a resonant condition where this attenuation is locally suppressed, producing a confined mode with exponentially decaying tails into the surrounding periodic medium.

Maldovan identified point-defect heat localization—“Thermal lattices”—as one of the six outstanding opportunities offered by thermocrystals [21], alongside heat waveguides, heat imaging, thermo-optics, thermal diodes, and thermal cloaking [10]. Realizing these phenomena requires engineering the phonon spectrum within a narrow hypersonic window around 100–300 GHz through nanostructured Si/Ge alloy films with periodicities of ~ 10 –20 nm. As Maldovan himself noted, this represents a formidable fabrication challenge, and experimental demonstrations of phonon-based heat localization at defect sites remain outstanding [10,21]. The omnidirectional mirror—another key target identified by Maldovan—has been demonstrated in a one-dimensional porous silicon thermocrystal [22], confirming that band-gap engineering in periodic thermal structures is physically realizable, while also highlighting the stringent nanofabrication requirements of the phononic approach. The present work addresses precisely this challenge, realizing the “Thermal lattices” phenomenology (Maldovan’s Figure 3b in [21]) in the alternative CV framework, where the nanofabrication bottleneck is replaced by length and frequency scales accessible to current experimental techniques.

The CV thermal wave crystal operates on a qualitatively different physical basis and provides access to the same wave phenomena at readily available scales. In CV materials, wave-like heat transport is encoded directly in the material relaxation time τ_q , without any requirement for phonon-spectrum engineering. Band gaps consequently form at layer thicknesses of ~ 10 μm —three orders of magnitude larger than in thermocrystals—and the relevant frequency scale of $1/\tau_q \sim 0.05$ –1 Hz is naturally matched by biological-tissue multilayers [6,7]. The two platforms are thus complementary: thermocrystals target hypersonic phonon control at the nanoscale, while CV-TWC systems access the same band-gap physics at the microscale with materials that are experimentally available today. Recent work on CV-TWC systems has addressed topics ranging from Bragg reflection [7] and heterostructure design [8] to omnidirectional band gaps [23] and plane-wave analysis [24,25]. In all of these studies, however, the crystal is perfect and periodic. The effect of a defect layer—and the possibility of energy localization at a specific site—has not been addressed.

The objective of the present work may be viewed in the broader context of wave-crystal physics. Historically, concepts first developed for electronic Bloch waves were later extended to photonic and phononic crystals. Once a new wave equation is shown to support periodic media and band-gap formation, a natural next question is whether the canonical phenomena of wave crystals, such as defect states, cavity modes, localization,

coupled cavities, and tunable resonances, also exist within that framework. The present study addresses this question for thermal wave crystals governed by the Cattaneo–Vernotte equation, an intrinsically dissipative wave system describing non-Fourier heat transport.

Here we investigate defect-induced localized modes in a one-dimensional CV thermal wave crystal formed by a stratum corneum/dermis bilayer superlattice. Using the transfer matrix method (TMM), we construct the defect supercell, compute the complex band structure, and identify the localized state through a sharp minimum of the imaginary Bloch wave vector. We show that the defect-mode frequency is continuously tunable across the gap by varying the defect-layer thickness, and that spatial confinement increases with the number of mirror periods, in direct analogy with a photonic crystal microcavity. The results are validated through zone folding of the supercell band structure.

2. Theory

The basis of this work is the Maxwell–Cattaneo constitutive relation, which is obtained by introducing a finite relaxation time τ_q between the establishment of a temperature gradient and the resulting heat flux [26,27]. Unlike Fourier’s law, which implies instantaneous propagation of thermal disturbances, the Maxwell–Cattaneo equation accounts for finite thermal propagation speeds and serves as the simplest hyperbolic extension of classical heat conduction. In the CV model, an empirical delay τ_q is introduced in the heat flux q to account for causality, leading to the modified Fourier-law relation [4,5,26]

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

where T is the temperature and κ is the thermal conductivity. Combined with energy conservation

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

where ρ and c_p are the density and specific heat, one obtains the hyperbolic heat equation

$$\frac{\tau_q}{D} \frac{\partial^2 T(x, t)}{\partial t^2} + \frac{1}{D} \frac{\partial T(x, t)}{\partial t} = \frac{\partial^2 T(x, t)}{\partial x^2}, \quad (3)$$

where $D = \kappa/(\rho c_p)$ is the thermal diffusivity. This is the thermal analogue of the telegrapher’s equation. The coexistence of the first- and second-order time derivatives is a direct consequence of combining the Maxwell–Cattaneo constitutive relation with energy conservation. The first-order term represents irreversible thermal dissipation and guarantees recovery of Fourier’s diffusion equation in the limit $\tau_q \rightarrow 0$, whereas the second-order term introduces finite propagation speed and wave-like behavior [27,28].

2.1. Solution in the Frequency Domain

For harmonic solutions $T(x, t) = \hat{T}(x, \omega) e^{-i\omega t}$, the spatial amplitude satisfies the Helmholtz equation

$$\frac{\partial^2 \hat{T}}{\partial x^2}(x, \omega) = -\gamma^2 \hat{T}(x, \omega), \quad (4)$$

with complex wave vector

$$\gamma^2 = \frac{\omega^2}{v^2} \left(1 + \frac{i}{\omega \tau_q} \right), \quad (5)$$

with wave speed

$$v = \sqrt{\frac{\kappa}{\rho c_p \tau_q}}. \quad (6)$$

The choice of branch $\text{Im}(\gamma) \geq 0$ ensures that the term $e^{+i\gamma x}$ decays as $x \rightarrow +\infty$ while $e^{-i\gamma x}$ decays as $x \rightarrow -\infty$, so that both forward and backward components remain physically bounded within each layer and can interfere coherently. The general solution in each layer is a superposition of forward and backward wave components:

$$\hat{T}(x, \omega) = T^+ e^{+i\gamma x} + T^- e^{-i\gamma x}, \quad (7)$$

$$\hat{q}(x, \omega) = Z \left(T^+ e^{+i\gamma x} - T^- e^{-i\gamma x} \right), \quad (8)$$

where T^+ and T^- are the forward and backward temperature-wave amplitudes, and

$$Z = \frac{-i\gamma\kappa}{1 - i\omega\tau_q} \quad (9)$$

is the thermal impedance of the medium, defined as the ratio of heat flux to temperature in a single progressive wave.

2.2. The Supercell

The supercell consists of N binary cells of period $d = d_a + d_b$ flanking a central defect cell on each side (Figure 1). The defect cell shares layer a with the mirror bilayer, followed by a defect material c of thickness d_c , giving defect-cell thickness $d' = d_a + d_c$ and total supercell period $D = 2Nd + d'$.

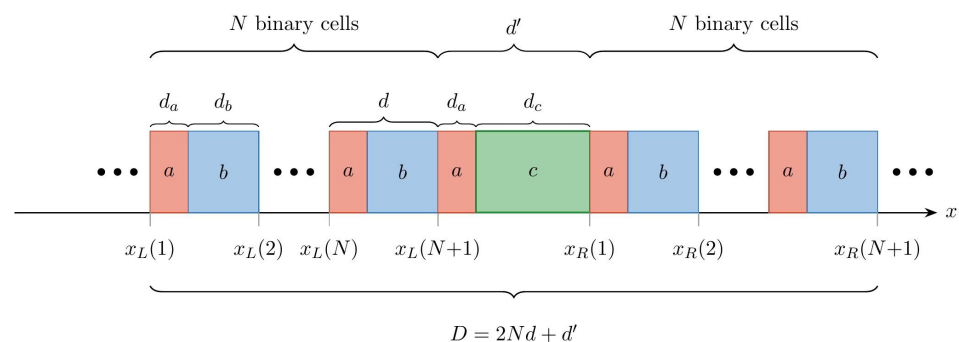


Figure 1. Schematic of the defect supercell $(ab)^N \cdot ac \cdot (ab)^N$. Each binary cell ab has period $d = d_a + d_b$; the defect cell ac has thickness $d' = d_a + d_c$, where d_c is the defect-layer thickness. The total supercell length is $D = 2Nd + d'$.

2.2.1. Fields in the Binary Cells

For each of the N binary cells to the left of the defect ($n = 1, \dots, N$), the temperature and heat-flux amplitudes are

$$\begin{bmatrix} \hat{T}_{a,n}(x, \omega) \\ \hat{q}_{a,n}(x, \omega) \end{bmatrix} = \mathbf{M}_a \mathbf{F}_{a,n}^L(x) \begin{bmatrix} t_{a,n}^+ \\ t_{a,n}^- \end{bmatrix}, \quad (10)$$

$$\begin{bmatrix} \hat{T}_{b,n}(x, \omega) \\ \hat{q}_{b,n}(x, \omega) \end{bmatrix} = \mathbf{M}_b \mathbf{F}_{b,n}^L(x) \begin{bmatrix} t_{b,n}^+ \\ t_{b,n}^- \end{bmatrix}, \quad (11)$$

where the interface matrices are

$$\mathbf{M}_\alpha = \begin{bmatrix} 1 & 1 \\ Z_\alpha & -Z_\alpha \end{bmatrix}, \quad (12)$$

with Z_α the thermal impedance of layer α , given by Equation (9) with the corresponding material parameters $\gamma_\alpha, \kappa_\alpha, \tau_{q,\alpha}$. The propagation matrices on the left side of the defect take the explicit form

$$\mathbf{F}_{a,n}^L(x) = \begin{pmatrix} e^{+i\gamma_a[x-x_L(n)]} & 0 \\ 0 & e^{-i\gamma_a[x-x_L(n)]} \end{pmatrix}, \quad (13)$$

with

$$x_L(n) = (n-1)d \quad (14)$$

the position of the left edge of cell n . The extremal value $x_L(N+1) = Nd$, shown in Figure 1, marks the right boundary of the left mirror stack and coincides with the left edge of the defect cell. The matrix $\mathbf{F}_{b,n}^L(x)$ has the same diagonal structure with γ_a replaced by γ_b and the reference point shifted by d_a (to the left edge of layer b within the cell).

For each of the N binary cells to the right of the defect, the propagation matrices have the same diagonal structure but are referenced to

$$x_R(n) = Nd + d' + (n-1)d, \quad (15)$$

that is, $\mathbf{F}_{a,n}^R(x)$ and $\mathbf{F}_{b,n}^R(x)$ are obtained from Equation (13) by replacing $x_L(n)$ with $x_R(n)$ (and, for layer b , adding the offset d_a). The corresponding extremal value $x_R(N+1) = 2Nd + d' = D$ marks the right boundary of the supercell. The interface matrices $\mathbf{M}_a$ and $\mathbf{M}_b$ are identical on both sides.

2.2.2. Cell-to-Cell Recurrence and Unit-Cell Matrix

Let $\mathbf{t}_{\alpha,n} = (t_{\alpha,n}^+, t_{\alpha,n}^-)^T$ denote the vector of forward and backward amplitudes in layer α of cell n . Imposing continuity of $\hat{T}$ and $\hat{q}$ at the $a|b$ interface at $x = x_L(n) + d_a$ gives

$$\mathbf{M}_a \mathbf{F}_a \mathbf{t}_{a,n} = \mathbf{M}_b \mathbf{t}_{b,n}, \quad (16)$$

where $\mathbf{F}_\alpha = \text{diag}(e^{\pm i\gamma_\alpha d_\alpha})$ is the propagation matrix evaluated over the thickness d_α of layer α . Similarly, continuity at the $b|a$ interface at $x = x_L(n+1)$ gives

$$\mathbf{M}_b \mathbf{F}_b \mathbf{t}_{b,n} = \mathbf{M}_a \mathbf{t}_{a,n+1}. \quad (17)$$

Note that $\mathbf{F}_a$ and $\mathbf{F}_b$ are independent of n and identical on both sides of the defect. Eliminating $\mathbf{t}_{b,n}$ between Equations (16) and (17) yields the cell-to-cell recurrence:

$$\mathbf{M}_a \begin{bmatrix} t_{a,n+1}^+ \\ t_{a,n+1}^- \end{bmatrix} = \mathbf{M}_{ab} \mathbf{M}_a \begin{bmatrix} t_{a,n}^+ \\ t_{a,n}^- \end{bmatrix}, \quad \mathbf{M}_{ab} = \mathbf{M}_a^{-1} \mathbf{M}_b \mathbf{F}_b \mathbf{M}_b^{-1} \mathbf{M}_a \mathbf{F}_a. \quad (18)$$

The unit-cell transfer matrix $\mathbf{M}_{ab}$ satisfies $\det(\mathbf{M}_{ab}) = 1$, and the Bloch dispersion relation of the perfect crystal is

$$\cos(kd) = \frac{1}{2} \text{tr}(\mathbf{M}_{ab}), \quad (19)$$

where $k = k_r + ik_i$ is the Bloch wave vector of the binary unit cell.

The order of matrix multiplication is determined by the physical sequence of layers and interfaces. As in photonic-crystal transfer-matrix theory, the matrices do not generally commute.

2.2.3. Defect Block and Supercell Transfer Matrix

Applying the same two-step procedure (continuity at the $a|c$ and $c|a$ interfaces, with propagation matrix $\mathbf{F}_c = \text{diag}(e^{\pm i\gamma_c d_c})$) gives the defect block

$$\mathbf{M}_a \mathbf{t}_{a,N+1} = \mathbf{M}_{ac} \mathbf{M}_a \mathbf{t}_{a,N}, \quad \mathbf{M}_{ac} = \mathbf{M}_a^{-1} \mathbf{M}_c \mathbf{F}_c \mathbf{M}_c^{-1} \mathbf{M}_a \mathbf{F}_a. \quad (20)$$

Applying the recurrence (Equation (18)) N times on each side and combining with Equation (20), the relation between $\mathbf{t}_{a,2N+1}$ and $\mathbf{t}_{a,1}$ defines the supercell transfer matrix

$$\mathbf{M}_{\text{super}} = (\mathbf{M}_{ab})^N \cdot \mathbf{M}_{ac} \cdot (\mathbf{M}_{ab})^N, \quad D = 2Nd + d'. \quad (21)$$

2.2.4. Perfect-Crystal Limit and Numerical Validation

Setting $d_c = d_b$ and $c = b$ (defect layer identical to mirror material b) gives $\mathbf{M}_{ac} \rightarrow \mathbf{M}_{ab}$, so

$$\mathbf{M}_{\text{super}}|_{d_c=d_b, c=b} = (\mathbf{M}_{ab})^{2N+1}, \quad (22)$$

corresponding to $2N + 1$ defect-free bilayers with period $D = (2N + 1)d$. This identity provides a stringent numerical check: K_i extracted from $\mathbf{M}_{\text{super}}$ with period $(2N + 1)d$ must agree with k_i from $\mathbf{M}_{ab}$ with period d (after the appropriate rescaling) to within floating-point precision.

2.2.5. Bloch Dispersion Relation of the Supercell

Imposing the Bloch condition $\mathbf{t}_{a,2N+1} = e^{iKD} \mathbf{t}_{a,1}$ leads to an eigenvalue problem for $\mathbf{M}_{\text{super}}$. Since $\det(\mathbf{M}_{\text{super}}) = 1$, the supercell dispersion relation is

$$\cos(KD) = \frac{1}{2} \text{tr}(\mathbf{M}_{\text{super}}), \quad (23)$$

where $K = K_r + iK_i$ is the complex Bloch wave vector of the supercell, extracted from the eigenvalues of $\mathbf{M}_{\text{super}}$. The defect mode corresponds to a frequency at which $|K_i(f)|$ exhibits a sharp local minimum within the band gap of the perfect crystal. We denote this defect-mode frequency by f^* ; at f^* , the mode is maximally localized at the defect site.

3. Material Selection and Single-Layer Dispersion

The CV dispersion relation for a homogeneous medium follows from Equation (4) with γ defined in Equation (5). The real part $\text{Re}(\gamma)$ determines the spatial oscillation (phase velocity) of the temperature wave, while $\text{Im}(\gamma)$ governs its intrinsic attenuation within each layer. Here the subscript α labels the constituent material; in particular, $\tau_{q,\alpha}$ denotes the relaxation time of material α , whereas τ_q (Section 2) denotes the generic relaxation time of the CV model. From Equation (5), we obtain:

$$\gamma_\alpha^2 = \frac{\omega^2}{v_\alpha^2} + i \frac{\omega}{v_\alpha^2 \tau_{q,\alpha}}, \quad (24)$$

with $|\gamma_\alpha^2| = (\omega^2/v_\alpha^2) \sqrt{1 + 1/(\omega^2 \tau_{q,\alpha}^2)}$. Taking the branch $\text{Im}(\gamma) \geq 0$, the real and imaginary parts of γ_α admit the closed form

$$\text{Re}(\gamma_\alpha) = \frac{\omega}{v_\alpha} \left[\frac{1}{2} \left(\sqrt{1 + \frac{1}{\omega^2 \tau_{q,\alpha}^2}} + 1 \right) \right]^{1/2}, \quad (25)$$

$$\text{Im}(\gamma_\alpha) = \frac{\omega}{v_\alpha} \left[\frac{1}{2} \left(\sqrt{1 + \frac{1}{\omega^2 \tau_{q,\alpha}^2}} - 1 \right) \right]^{1/2}. \quad (26)$$

These expressions make explicit how the CV model interpolates between two well-separated transport regimes. In the wave-like regime $\omega\tau_{q,\alpha} \gg 1$, Equations (25) and (26) reduce to $\text{Re}(\gamma_\alpha) \simeq \omega/v_\alpha$ and $\text{Im}(\gamma_\alpha) \simeq 1/(2v_\alpha\tau_{q,\alpha})$: the real part grows linearly with frequency and the imaginary part saturates at a frequency-independent attenuation, recovering standard wave propagation with finite speed v_α and weak damping. In the diffusive regime $\omega\tau_{q,\alpha} \ll 1$, both parts collapse to $\text{Re}(\gamma_\alpha) \simeq \text{Im}(\gamma_\alpha) \simeq \sqrt{\omega/(2D_\alpha)}$, with $D_\alpha = \kappa_\alpha/(\rho_\alpha c_{p,\alpha}) = v_\alpha^2\tau_{q,\alpha}$ denoting the thermal diffusivity, which is the characteristic dispersion of the Fourier diffusion equation. The crossover between the two regimes occurs at $\omega_\alpha^* = 1/\tau_{q,\alpha}$, i.e., $f_\alpha^* = 1/(2\pi\tau_{q,\alpha})$, and sets the natural frequency scale of each material. For the five materials in Table 1, f_α^* ranges from 8 mHz (dermis, $\tau_{q,\alpha} = 20$ s) to 0.16 Hz (stratum corneum, $\tau_{q,\alpha} = 1$ s). The defect-mode frequency $f^* \approx 2.6$ Hz identified in the Section 4 therefore sits well within the wave-like regime ($\omega\tau_{q,\alpha} \gg 1$) for every material considered, where interference effects and band-gap formation are physically meaningful.

Table 1 lists the thermophysical parameters for all materials considered. The thermal relaxation time $\tau_{q,\alpha}$ is the most uncertain parameter. Since no direct measurement of $\tau_{q,\alpha}$ has been reported for intact biological tissue [29], the values adopted here are representative estimates within the range reported in the literature: for the stratum corneum and dermis we follow the skin-tissue parametrization of Xu et al. [29], and for subcutaneous tissue and processed meat we adopt values consistent with [30] and [31], respectively, the latter resting on a measurement that has been questioned [32]. The skeletal-muscle relaxation time is taken as a representative value within the same physiological range.

Table 1. Thermophysical parameters for the CV thermal wave crystal materials. $v = \sqrt{\kappa/(\rho c_p \tau_{q,\alpha})}$. Sources: [†] Xu et al. [29]; [‡] representative value within the reported tissue range [29,31]; [§] Kaminski [30]; ^{||} Mitra et al. [31]; κ, ρ, c_p from Duck (1990) via Xu et al. [29].

Material	κ (W m ^{−1} K ^{−1})	ρ (kg m ^{−3})	c_p (J kg ^{−1} K ^{−1})	$\tau_{q,\alpha}$ (s)	v (mm s ^{−1})	Ref.
Stratum corneum	0.235	1500	3600	1.0	0.209	[†]
Dermis	0.445	1116	3300	20.0	0.078	[†]
Skeletal muscle	0.490	1090	3420	6.9	0.138	[‡]
Subcutaneous	0.185	971	2700	5.0	0.119	[§]
Processed meat	0.500	1050	3500	15.5	0.094	

Figure 2 shows the CV dispersion relation for all five materials. Dermis has the largest $\text{Re}(\gamma)$ at every frequency, confirming its role as the high-index (slow) mirror component with $v = 0.078$ mm/s, while stratum corneum forms the low-index (fast) component with $v = 0.209$ mm/s. The velocity contrast $v(\text{Stratum})/v(\text{Dermis}) \approx 2.7$ produces wide band gaps comparable to high-contrast photonic crystals. A material suitable as a defect layer must have v intermediate between the two mirror materials, so that its resonance frequency falls inside the gap. All three candidate materials in Table 1 satisfy this criterion: their dispersion curves in panel (a) lie between the two solid mirror lines. Among them, skeletal muscle is adopted as the primary defect material, with $\tau_{q,\alpha}$ taken as a representative value within the physiological range.

The thermal waves considered here are assumed to be generated by an external harmonically modulated heat source. Examples include frequency-domain thermoreflectance (FDTR) [33], photothermal excitation [34], and periodically driven resistive heaters [35]. In such experiments, the deposited heat power is modulated at frequency f , producing temperature oscillations that propagate through the medium according to the Cattaneo–Vernotte equation. The frequency range investigated in this work (~ 1 –4 Hz) is readily accessible using existing modulated-heating techniques and serves as the excitation fre-

quency for the thermal wave crystal. In this sense, the thermal wave crystal plays a role analogous to that of a photonic or phononic crystal, acting as a filter for externally generated waves rather than as their source.

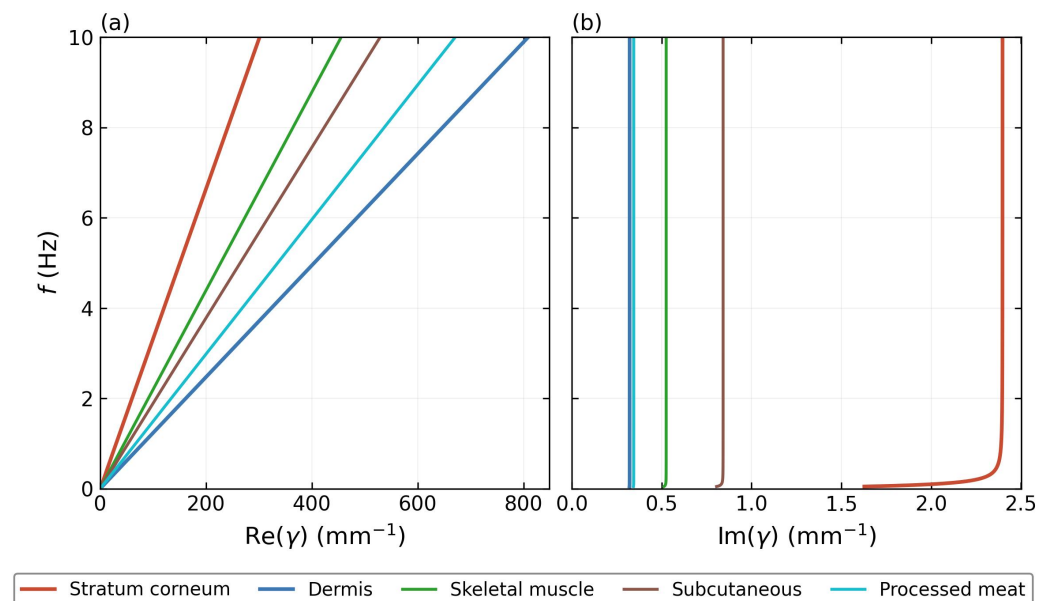


Figure 2. CV dispersion relation for the five materials in Table 1. (a) Real part $\text{Re}(\gamma)$ (mm^{-1}), proportional to the phase accumulation per unit length. (b) Imaginary part $\text{Im}(\gamma)$ (mm^{-1}), governing the intrinsic attenuation of thermal waves within each layer. Solid lines: stratum corneum (red) and dermis (blue), forming the mirror bilayer. Thinner solid lines: skeletal muscle (green), subcutaneous tissue (brown), and processed meat (teal), used as candidate defect materials whose wave speeds are intermediate between those of the mirror materials. For materials with sufficiently large relaxation times $\tau_{q,\alpha}$, the condition $\omega\tau_{q,\alpha} \gg 1$ is satisfied throughout most of the plotted frequency range, causing $\text{Im}(\gamma)$ to approach the asymptotic limit $1/(2v\tau_{q,\alpha})$ predicted by Equation (26) and become nearly frequency independent. Stratum corneum ($\tau_{q,\alpha} = 1\text{ s}$) reaches this regime only at higher frequencies, resulting in the residual frequency dependence visible in panel (b).

It should be emphasized that the periodic multilayer considered here is an engineered structure rather than a naturally occurring biological tissue. The biological materials are employed because experimentally reported values of the thermal relaxation time are available, enabling realistic estimates of the thermal wave band structure.

4. Results

4.1. Band Structure and Zone-Folding Validation

Before presenting defect-mode results, we validate the supercell method in the perfect-crystal limit (where $d_c = d_b$ and $c = b$), for which the Bloch wave vector extracted from $\mathbf{M}_{\text{super}}$ must coincide with that obtained directly from the unit-cell matrix $\mathbf{M}_{ab}$. This validation establishes the numerical reliability of the supercell approach before the defect layer is introduced and, at the same time, characterizes the band structure of the perfect stratum corneum/dermis crystal that will serve as the reference throughout the remainder of the paper.

We further validate the supercell transfer matrix against the analytical formula of Chen et al. [6]:

$$\cos(kd) = \cos(\gamma_a d_a) \cos(\gamma_b d_b) - \frac{1}{2} \left(\frac{Z_a}{Z_b} + \frac{Z_b}{Z_a} \right) \sin(\gamma_a d_a) \sin(\gamma_b d_b), \quad (27)$$

with Z_a and Z_b the thermal impedances of the two layers as defined in Equation (9). Our TMM computes the same quantity by direct matrix multiplication, extracting k via Equation (19).

Agreement between both routes is within the floating-point rounding error ($\sim 10^{-15}$), confirming the correctness of the interface and propagation matrices. The mathematical structure of Equation (27) is identical to that encountered in one-dimensional photonic and phononic crystals. This reflects the fact that all three systems can be described by transfer matrices and Bloch theory. The specific form used here was derived by Chen et al. [6] for thermal wave crystals governed by the Cattaneo–Vernotte equation, where the electromagnetic impedance [36] is replaced by the thermal impedance defined in Equation (9).

Figure 3 presents the zone-folding validation using the perfect-crystal limit of the supercell (Equation (22)) with $N = 6$, giving $\mathbf{M}_{\text{super}} = (\mathbf{M}_{ab})^{13}$ and supercell period $D = 13d$. The layer thicknesses used throughout this work are $d_a = d_b = 10 \mu\text{m}$, giving a unit-cell period $d = 20 \mu\text{m}$. At the frequencies of interest ($f \approx 2\text{--}3\text{Hz}$), the corresponding thermal wave wavelengths, estimated from the wave-regime relation $\lambda = v/f$, range from approximately $30 \mu\text{m}$ (dermis) to $80 \mu\text{m}$ (stratum corneum). The wavelength is therefore comparable to the periodicity of the structure, with $\lambda \approx 1.5d\text{--}4d$, placing the system in the Bragg-scattering regime required for thermal wave band-gap formation. This relationship between wavelength and periodicity is analogous to that encountered in photonic and phononic crystals, where interference effects become significant when the wavelength is of the same order as the lattice period.

Panel (a) shows the band structure of the perfect crystal: three band gaps are visible within the displayed range, with the first centered near $f_2 = 2.68 \text{ Hz}$ with edges at $f_3 = 1.83 \text{ Hz}$ and $f_1 = 3.53 \text{ Hz}$. The large velocity contrast $v(\text{Stratum})/v(\text{Dermis}) \approx 2.7$ produces wide gaps comparable to high-contrast photonic crystals. Panel (b) shows the supercell result: the band structure is folded 13 times into the reduced Brillouin zone $[0, \pi/D]$, in direct analogy with zone folding in phononic and semiconductor superlattices [37,38]; to our knowledge, this is its first explicit demonstration within the Cattaneo–Vernotte thermal wave crystal framework. Panel (c) provides the critical numerical check: $k_i(f)$ from the unit cell and $K_i(f)$ from the supercell coincide to within 10^{-7} mm^{-1} , seven orders of magnitude smaller than the physical gap values ($\sim 10\text{--}50 \text{ mm}^{-1}$), confirming that Equation (22) holds to full double-precision accuracy. This three-way validation—analytical formula, matrix multiplication, and zone folding—establishes the numerical reliability of the supercell method before the defect layer is introduced.

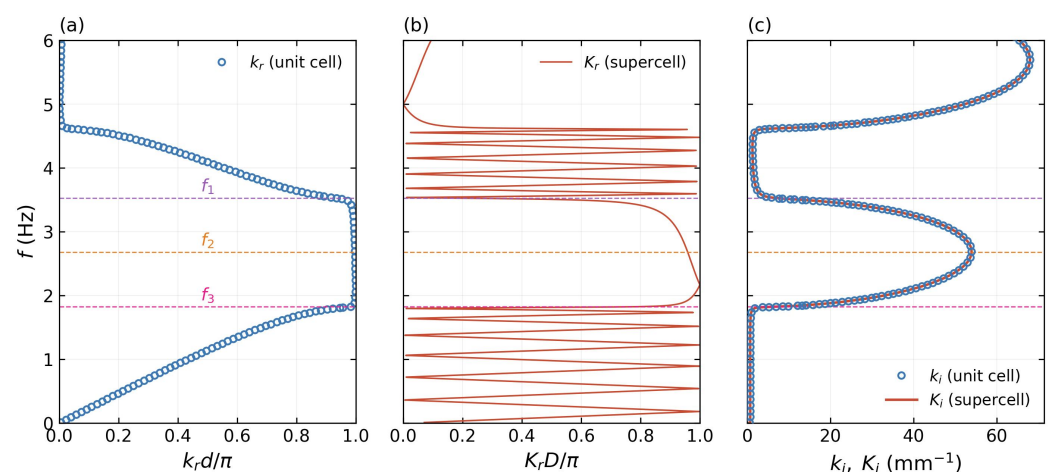


Figure 3. Zone-folding validation ($N = 6$, perfect-crystal limit $d_c = d_b$, $c = b$, $D = 13d$, $d_a = d_b = 10 \mu\text{m}$). (a) Perfect-crystal band structure $k_r d / \pi$ from $\mathbf{M}_{ab}$ (Equation (19)). (b) Supercell band structure $K_r D / \pi$ from $(\mathbf{M}_{ab})^{13}$: the $\times 13$ zone folding is clearly visible. (c) Imaginary Bloch wave vector: k_i from the unit cell (blue open circles) and K_i from the supercell (red solid) coincide to within 10^{-7} mm^{-1} , confirming exact numerical equivalence. Dashed horizontal lines mark gap edges $f_3 = 1.83 \text{ Hz}$ (pink), gap center $f_2 = 2.68 \text{ Hz}$ (orange), and $f_1 = 3.53 \text{ Hz}$ (purple).

4.2. Mode Profiles of the Perfect Crystal

Figure 4 shows the heat-flux amplitude $|\hat{q}(x, \omega)|$ for three representative frequencies within gap 1, reconstructed from the eigenvector of $\mathbf{M}_{ab}$ via the Bloch relation and Equation (8).

Panel (a), at the upper gap edge $f_1 = 3.53$ Hz, shows the heat-flux amplitude concentrated within the stratum corneum (a) layers. This is the thermal analogue of the dielectric band rule in photonic crystals [11]: at the upper band edge, the mode concentrates in the low-index (fast) material, here stratum corneum with $v = 0.209$ mm/s. The nearly flat Bloch envelope ($k_i \approx 0$) confirms that this frequency lies at the band edge where propagation just becomes allowed. Panel (b), at the gap center $f_2 = 2.68$ Hz, shows purely evanescent character: the amplitude decays as $e^{-k_i x}$ with k_i at its maximum, meaning wave propagation is most strongly suppressed at this frequency. Panel (c), at the lower gap edge $f_3 = 1.83$ Hz, shows the complementary situation: the mode concentrates in the dermis (b) layers, the high-index (slow) material with $v = 0.078$ mm/s. The three panels together establish the mode character of the perfect crystal and provide the reference against which the defect state is identified.

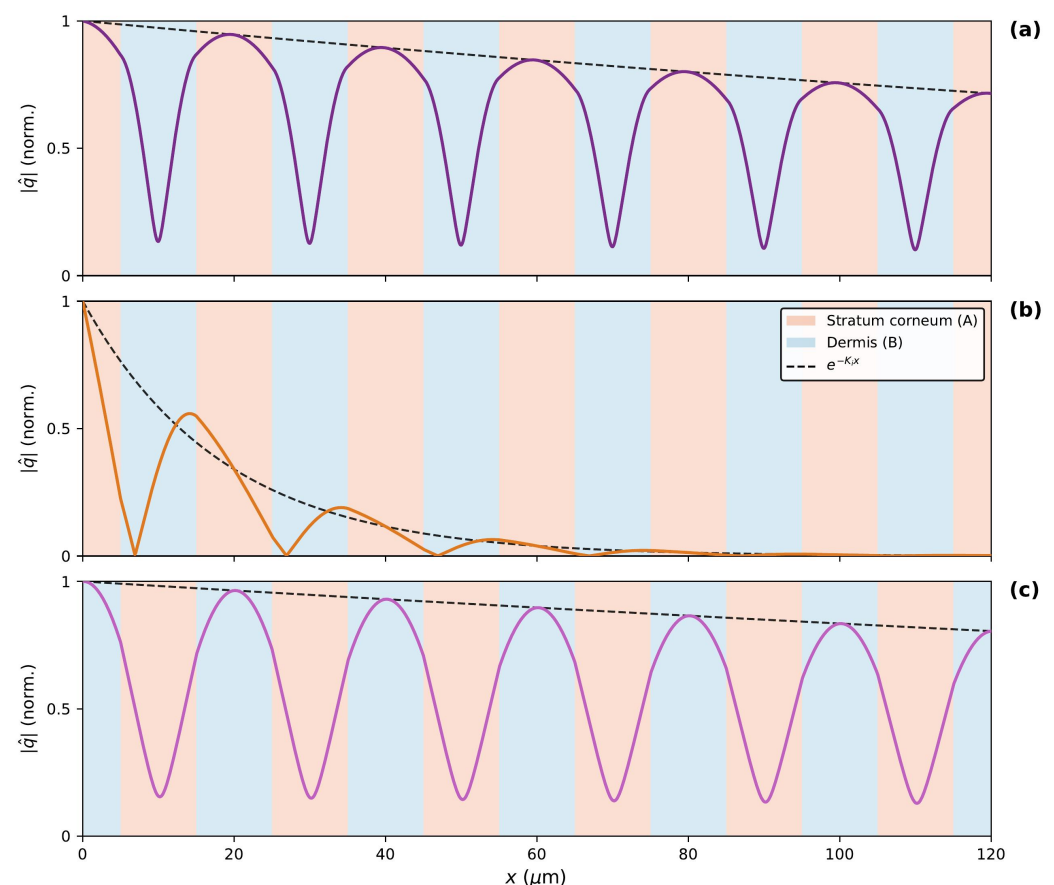


Figure 4. Heat-flux amplitude $|\hat{q}(x, \omega)|$ for gap 1 ($d_a = d_b = 10 \mu\text{m}$, $x \geq 0$). Black dashed line: Bloch envelope $e^{-k_i x}$. Solid line: heat-flux amplitude $|\hat{q}(x, \omega)|$, colored to match the corresponding frequency marker in Figure 3 (f_1 purple, f_2 orange, f_3 pink). Background: stratum corneum (A, salmon) and dermis (B, blue). (a) Upper gap edge ($f_1 = 3.53$ Hz): mode concentrated in stratum corneum, the low-index material at the upper band edge. (b) Gap center ($f_2 = 2.68$ Hz): purely evanescent decay, k_i at maximum—strongest thermal reflection. (c) Lower gap edge ($f_3 = 1.83$ Hz): mode concentrated in dermis, the high-index material at the lower band edge.

4.3. Effect of N on the Defect Mode

Figure 5 shows $K_i(f)$ for the perfect crystal and for defect supercells with $N = 2, 3, 4$ mirror periods (per side), at fixed skeletal-muscle defect thickness $d_c = 0.319d = 6.4\ \mu\text{m}$. This value is chosen so that the defect mode lies deep inside the band gap, well separated from both edges; it does not coincide with the thickness that maximizes the confinement, $d_c/d \approx 0.15$, identified in the tunability study of Section 4.5. The shaded region indicates the band gap $[1.83, 3.53]\ \text{Hz}$ of the perfect crystal.

Each supercell curve develops a sharp downward spike at a defect-mode frequency $f^* \approx 2.586\ \text{Hz}$, located well inside the gap. The frequency f^* is essentially independent of N , determined mainly by the thermal impedance of the defect material and its thickness d_c . By contrast, the depth of the minimum— $K_i^* = 13.2, 24.5$, and $31.1\ \text{mm}^{-1}$ for $N = 2, 3, 4$, respectively—grows strongly with N . Increasing the number of surrounding periods deepens the minimum of K_i at the defect-mode frequency, resulting in stronger exponential suppression of the mode amplitude away from the defect layer. This is the direct thermal analogue of increasing the number of mirror pairs in a photonic crystal microcavity: more mirrors reflect more strongly, pushing the resonance deeper into the gap and increasing the spatial confinement of the mode. The pass-band oscillations visible above and below the gap correspond to Fabry–Pérot resonances of the finite supercell and are not numerical artifacts.

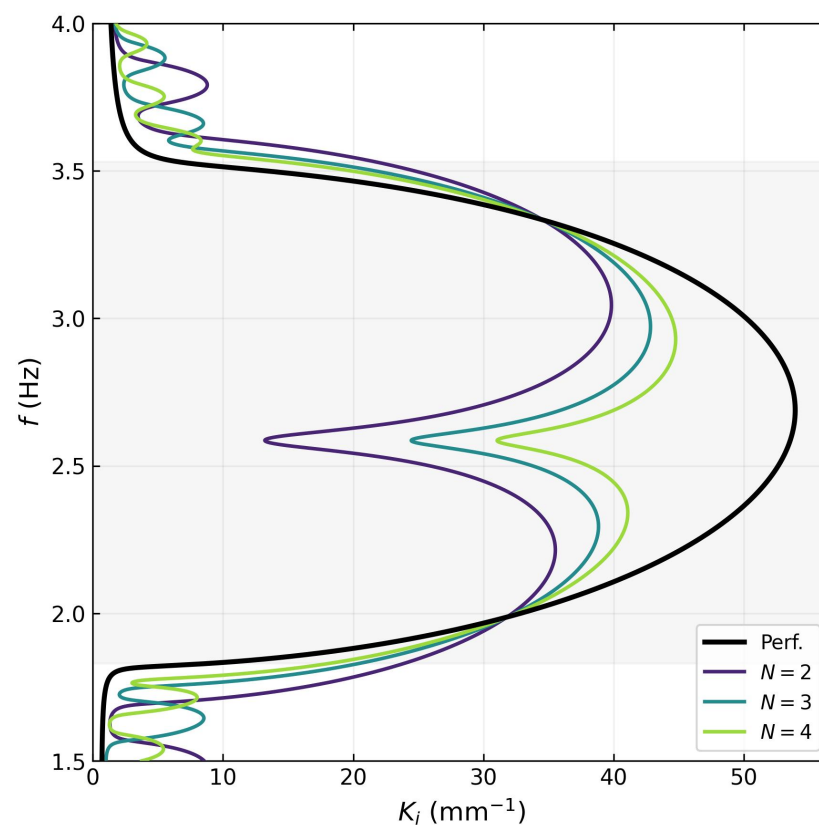


Figure 5. Imaginary Bloch wave vector $K_i(f)$ across the full frequency range (1.5–4.0 Hz) for the perfect crystal (black) and defect supercells with $N = 2, 3, 4$ mirror periods (per side) (color, viridis scale), at fixed defect thickness $d_c = 0.319d = 6.4\ \mu\text{m}$ (skeletal muscle). The shaded region marks the band gap $[1.83, 3.53]\ \text{Hz}$. The sharp minimum at $f^* \approx 2.586\ \text{Hz}$ is the defect mode; its frequency is independent of N while its depth K_i^* increases markedly, reflecting stronger spatial confinement for larger N . Pass-band oscillations outside the gap are Fabry–Pérot resonances of the finite supercell.

Figure 6 examines this trend over an extended range, $N = 1\text{--}16$. K_i^* increases monotonically with N , with a growth that is fast (up to $N \approx 4$) and progressively slows thereafter,

approaching the mid-gap attenuation of the unperturbed mirror crystal. Over the same range, the defect-mode frequency remains essentially constant, $f^* \simeq 2.586$ Hz, confirming that the resonance condition is fixed by the defect cell alone.

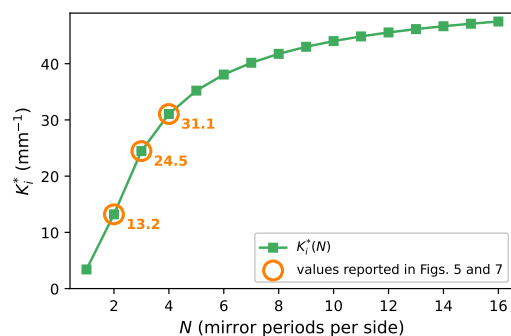


Figure 6. Localization K_i^* as a function of the number of mirror periods N (per side), at fixed $d_c = 0.319$ d (skeletal muscle), for $N = 1$ –16. The growth is monotonic but not linear: fast up to $N \approx 4$ and progressively slower thereafter. Open squares mark the cases shown in Figures 5 and 7, namely the three defect configurations $N = 2, 3, 4$ whose spectra (Figure 5) and spatial profiles (Figure 7) are reported there; this is what the legend label “values reported in Figures 5 and 7” denotes. The exact values are $K_i^* = 13.2, 24.5$, and 31.1 mm^{−1} for $N = 2, 3, 4$, respectively, corresponding to $\ell_{\text{loc}} = 1/K_i^* = 76, 41$, and 32 μm.

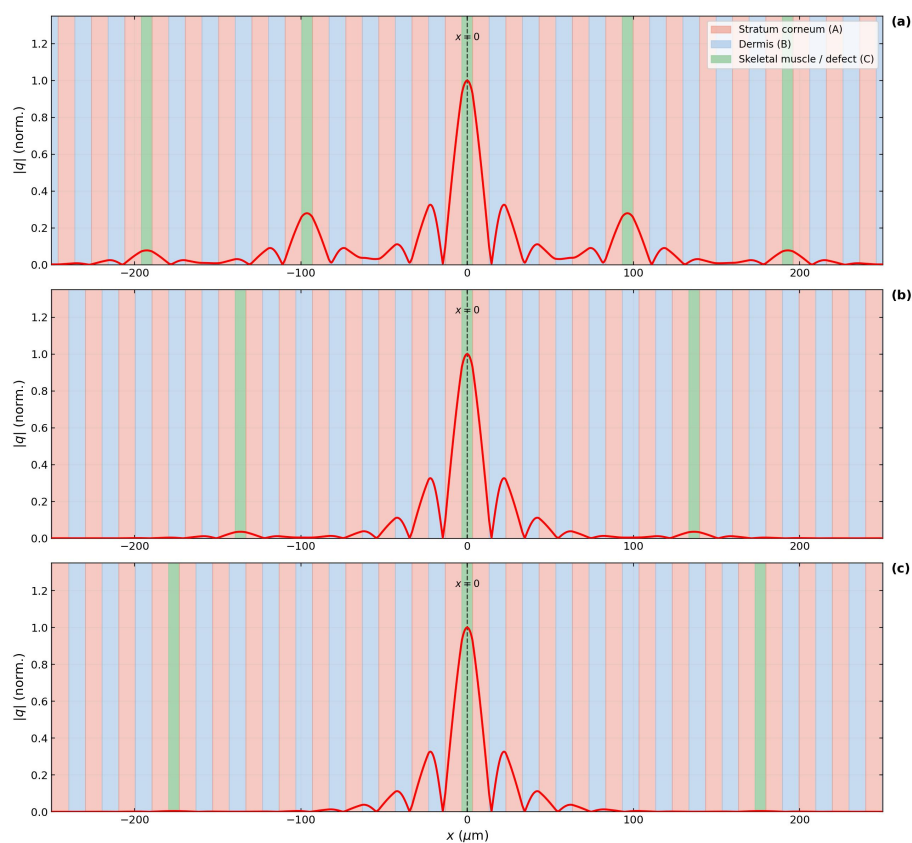


Figure 7. Normalized heat-flux amplitude $|\dot{q}(x)|$ of the defect mode (red line), evaluated at the defect-mode frequency f^* for each case. (a) $N = 2$, $f^* = 2.5863$ Hz; (b) $N = 3$, $f^* = 2.5858$ Hz; (c) $N = 4$, $f^* = 2.5858$ Hz. Background: stratum corneum (A, salmon), dermis (B, blue), defect layer (C, green). The mode is sharply peaked at the defect center ($x = 0$, dashed line) and decays exponentially into the mirror crystal, with the decay length $\ell_{\text{loc}} = 1/K_i^*$ decreasing from 76 μm to 32 μm as N increases from 2 to 4 (mirror periods per side). Additional green bands outside the central defect layer are periodic images of the supercell, a consequence of the Bloch periodicity underlying the transfer-matrix formulation, and are not additional physical defects.

4.4. Spatial Profile of the Defect Mode

While Figure 5 characterizes the defect mode in the spectral domain, Figure 7 presents the complementary real-space picture: the spatial profile of the mode, whose decay length $\ell_{\text{loc}} = 1/K_i^*$ is the direct real-space expression of the spectral minimum. The figure shows the normalized heat-flux amplitude $|\hat{q}(x)|$ of the defect mode for $N = 2, 3, 4$, evaluated at the respective f^* . In all panels, the profile is sharply peaked at $x = 0$ (the center of the defect layer) and decays exponentially into the mirror crystal on both sides, with a decay length ℓ_{loc} that decreases from $76 \mu\text{m}$ ($N = 2$) to $41 \mu\text{m}$ ($N = 3$) and $32 \mu\text{m}$ ($N = 4$). This spatial confinement is the defining signature of a localized cavity mode. The mode envelope follows the exponential predicted by Bloch theory, with no evidence of reflections from the supercell boundaries. The defect layer (green) is clearly visible at the center of each panel, flanked by the alternating stratum corneum (salmon) and dermis (blue) layers of the mirror crystal.

4.5. Tunability of the Defect Mode

Figure 8 demonstrates that the defect mode is continuously tunable across the entire band gap by varying the defect-layer thickness d_c . As d_c/d increases from 0 to ~ 0.6 , $f^*(d_c)$ decreases monotonically for all three candidate materials, sweeping from near the upper gap edge ($\sim 3.3 \text{ Hz}$) down toward the lower edge ($\sim 2.0 \text{ Hz}$). Physically, varying d_c modifies the phase accumulation $\text{Re}(\gamma_c)d_c$ within the defect layer and the impedance mismatch at the $a|c$ and $c|a$ interfaces, thereby shifting the resonance condition that selects f^* within the gap. The dashed horizontal line at the gap center ($f = 2.68 \text{ Hz}$) indicates the crossing point accessible to each material.

The bottom panel shows that the localization $K_i^*(d_c)$ peaks at $d_c/d \approx 0.1\text{--}0.2$ for all materials before decreasing as the mode approaches the gap edges, where $K_i \rightarrow 0$. The optimal confinement is achieved near $d_c/d \approx 0.15$, where K_i^* reaches $13\text{--}15 \text{ mm}^{-1}$ for $N = 2$ mirror periods (per side). Among the three materials, subcutaneous tissue (brown) and processed meat (teal) allow the mode to reach lower frequencies within the gap for the same d_c , due to their lower v values. Skeletal muscle (green), adopted as the reference defect material, provides a representative and conservative tuning curve.

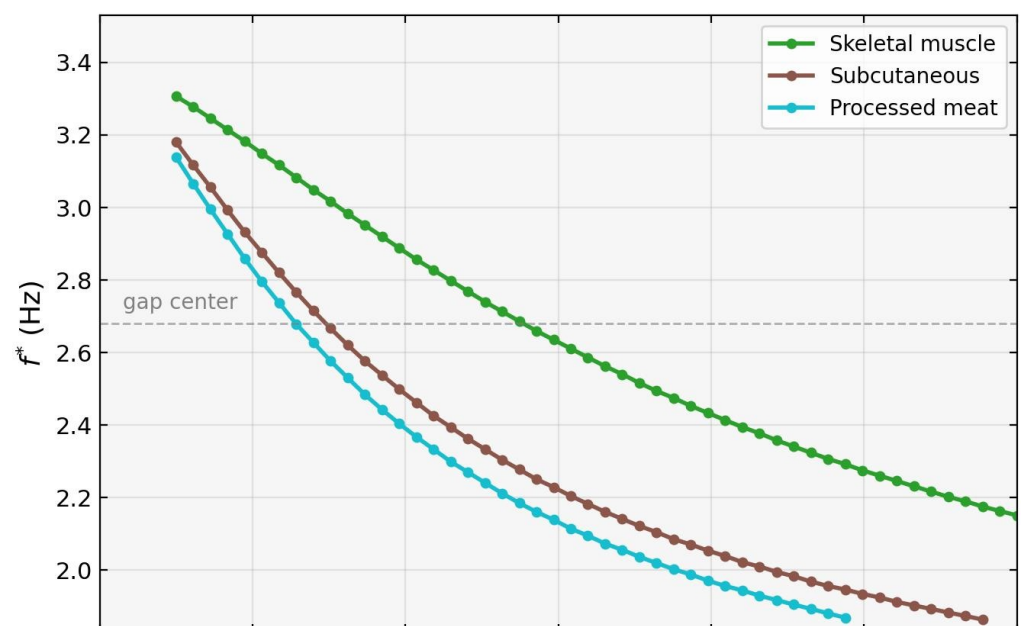


Figure 8. Cont.

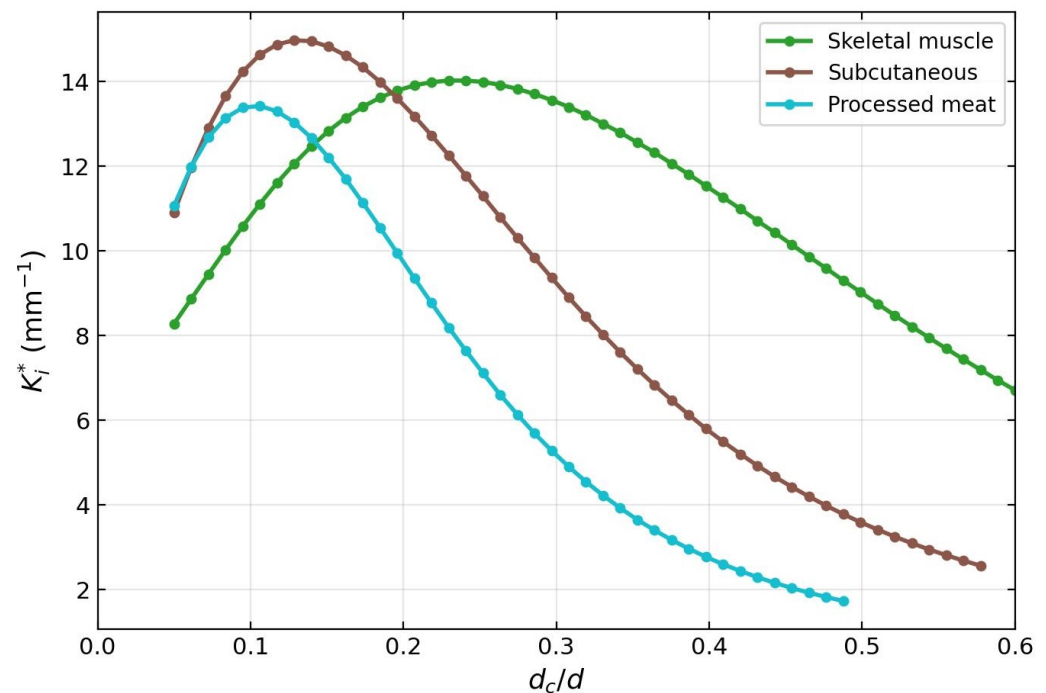


Figure 8. Tunability of the defect mode for $N = 2$ mirror periods (per side). **(Top)** defect-mode frequency $f^*(d_c/d)$ as a function of normalized defect thickness, for skeletal muscle (green), subcutaneous tissue (brown), and processed meat (teal), matching the color convention of Figure 2 (skeletal muscle: $\kappa = 0.490 \text{ W m}^{-1} \text{ K}^{-1}$, $\tau_{q,\kappa} = 6.9 \text{ s}$; subcutaneous: $\kappa = 0.185$, $\tau_{q,\kappa} = 5.0 \text{ s}$; processed meat: $\kappa = 0.500$, $\tau_{q,\kappa} = 15.5 \text{ s}$; see Table 1). The dashed horizontal line marks the gap center at $f = 2.68 \text{ Hz}$. f^* decreases monotonically as d_c increases, sweeping the defect mode continuously from near the upper gap edge toward the lower edge. **(Bottom)** Localization $K_i^*(d_c/d)$. The maximum confinement is achieved at $d_c/d \approx 0.15\text{--}0.2$ for all three materials, reaching $K_i^* \approx 13\text{--}15 \text{ mm}^{-1}$; beyond this range, K_i^* decreases as the mode approaches the gap edges where $K_i \rightarrow 0$. Together, the two panels establish that defect material and thickness act as coarse and fine tuning controls of the defect-mode operating point.

5. Discussion

The results presented in Section 4 establish a close phenomenological correspondence between the defect modes of a CV thermal wave crystal and those of a photonic crystal microcavity. Unlike photonic and phononic crystals, the CV thermal wave crystal constitutes an intrinsically dissipative Bloch medium in which the wave vector remains complex even in homogeneous materials. The existence of localized defect states is therefore not guaranteed a priori and represents a nontrivial extension of defect-state physics to non-Fourier heat transport. Three aspects of this correspondence deserve emphasis.

First, the decoupling of frequency and confinement— f^* essentially independent of N , while K_i^* increases monotonically (though not linearly) with N (Figure 6)—is the hallmark of a high-quality-factor cavity mode [11]. The defect material and its thickness fix the resonance condition, whereas the mirror crystal sets the rate of energy leakage out of the cavity. This clean separation enables an independent design of operating frequency and mode confinement, a feature that has been exploited extensively in photonic [14,17] and phononic [19,20] devices, and which our calculations show to carry over quantitatively to the thermal wave regime.

Second, the continuous tunability of f^* across the whole band gap by varying d_c (Figure 8) provides a design lever that could be exploited for narrowband thermal filtering if the predicted modes are experimentally confirmed. Varying the defect-layer thickness modifies the phase accumulation $\text{Re}(\gamma_c) d_c$ and the effective impedance mismatch at the in-

interfaces, thereby shifting the resonance condition that defines the localized mode frequency within the band gap. Because all three candidate defect materials yield monotonically decreasing $f^*(d_c/d)$ curves—but with distinct slopes set by their v values—the platform allows both coarse (material choice) and fine (thickness) tuning, analogously to multilayer optical filters.

Third, the length scales involved are accessible to existing microfabrication and tissue-engineering techniques. Layer thicknesses of order 10 μm are three orders of magnitude larger than those required by phononic thermocrystals [10,21], eliminating the need for nanoscale patterning of Si/Ge alloys. The predicted operating window of $\sim 2\text{--}3$ Hz is also directly compatible with modulated-heating characterization methods used on biological multilayers [29,39]. Combined with the omnidirectional band gap previously demonstrated in porous-silicon thermocrystals [22] and in finite CV multilayers [23], the present results outline a viable route toward experimental realization of such cavity resonances in the CV regime.

Several limitations of the present analysis deserve explicit discussion. First, the results rest on the assumption that heat transport in the layered biological medium is adequately described by the CV model within the frequency range considered. The applicability of the CV model to biological tissue remains a subject of active investigation: no direct measurement of $\tau_{q,\alpha}$ for intact tissue is available [29], and the values used here are representative estimates within the range reported in the literature [29,31]; alternative formulations such as the dual-phase-lag [40] or fractional-derivative [2] models have been proposed to capture non-Fourier transport in heterogeneous tissues. The values of $\tau_{q,\alpha}$ for subcutaneous tissue [30] and processed meat [31] rest on measurements that have been questioned in the literature [32]; our Figure 8 therefore serves primarily to illustrate the tuning mechanism, with skeletal muscle as the reference candidate material. Accordingly, the numerical values of f^* and K_i^* reported here should be interpreted as predictions contingent on the CV parametrization rather than as definitive quantitative claims about real tissue.

Second, the present analysis is strictly one-dimensional and assumes homogeneous, non-dispersive CV parameters within each layer. Real biological tissues exhibit anisotropy, perfusion effects, and frequency-dependent $\tau_{q,\alpha}$, all of which would broaden the sharp $K_i(f)$ minimum reported here. A two-dimensional treatment incorporating lateral heterogeneity and the vascular contribution to heat transport is a natural next step. Finally, the present work is purely theoretical and numerical; experimental demonstration of the predicted modes—and thereby validation of the underlying CV description over the relevant frequency range—remains an open challenge, which we address in the paragraph that follows.

The experimental requirements that follow from the present calculations are concrete. The predicted defect mode lies at $f^* \approx 2.6$ Hz with a spectral width set by $1/K_i^* \sim 30\text{--}80$ μm , implying that a measurement must resolve sub-Hertz spectral features while probing depth variations on the 10 μm scale. Two experimental modalities are naturally suited to this regime. Frequency-domain thermoreflectance (FDTR) with modulation frequencies in the sub-Hz to tens-of-Hz range has been used to observe non-Fourier thermal transport in solids [39], and its extension to layered biological samples would require mainly an appropriate probe geometry and the preparation of stacked tissue layers of controlled thickness. Photothermal and photoacoustic techniques operating in the same frequency window are other candidates, with the practical advantage that the thermal response of skin and near-surface tissue is already routinely measured by these methods. In either case, the experimental signature of the defect mode would be a narrow minimum in the apparent thermal attenuation as a function of modulation frequency, evaluated for a sample prepared with a well-defined defect layer of thickness d_c between N mirror

bilayers. The sensitivity of f^* to d_c predicted in Figure 8 provides an internal consistency check: a correctly realized sample should display the linear dependence $f^*(d_c/d)$ across the range of defect thicknesses explored here. Such a measurement would constitute both a confirmation of the defect-mode physics and an independent test of the CV description of heat transport in layered biological media.

6. Conclusions

We have demonstrated the existence and properties of defect-induced localized modes in a one-dimensional CV thermal wave crystal. A single defect layer inserted into a periodic stratum corneum/dermis bilayer creates a localized resonance—a cavity mode—whose frequency lies within the band gap of the perfect crystal. The mode is identified unambiguously through a sharp minimum of the imaginary Bloch wave vector $K_i(f)$ in the supercell band structure, in direct analogy with defect modes in photonic and phononic crystals. The spatial profile of the mode is a sharply peaked, exponentially decaying function centered at the defect layer, with a localization length $\ell_{\text{loc}} = 1/K_i^*$ ranging from 76 μm at $N = 2$ to 32 μm at $N = 4$ mirror periods per side.

Two key design parameters control the mode independently. First, the number of mirror periods N controls the degree of spatial confinement: K_i^* increases from 13.2 to 31.1 mm^{-1} as N goes from 2 to 4, while f^* remains essentially constant at ≈ 2.586 Hz. This decoupling of frequency and confinement is precisely the behavior of a photonic crystal microcavity, where adding mirror pairs increases the quality factor without shifting the resonance frequency. Second, the defect-mode frequency is fully tunable across the gap by varying the defect-layer thickness d_c : for all three candidate biological materials (skeletal muscle, subcutaneous tissue, and processed meat), f^* decreases monotonically as d_c increases, sweeping continuously from near the upper gap edge to near the lower edge.

The method is validated at three levels: analytical agreement with the Chen et al. [6] dispersion formula, matrix multiplication consistency, and exact zone-folding recovery of the perfect-crystal band structure from the supercell limit (Equation (22)), with numerical agreement to within 10^{-7}mm^{-1} .

From a broader perspective, these results establish that the phenomenology of photonic crystal microcavities—localized resonance, exponential confinement, mirror-controlled quality factor, continuous frequency tuning—is fully reproduced in the CV thermal wave crystal at the microscale, using biologically available materials and layer thicknesses of order 10 μm . The CV platform is thus a viable route to engineered heat localization, complementary to phononic thermocrystals but accessible at far larger scales and without nanofabrication.

Several directions for future work are suggested by these results. The extension to heterostructures with multiple defects could realize coupled-cavity arrays and tight-binding bands in this thermal setting. The sensitivity of f^* to the defect material parameters—particularly $\tau_{q,\alpha}$ —suggests that defect-mode spectroscopy could, in principle, serve as a probe of thermal relaxation times in layered structures. Application to biological tissue would require independent validation of CV-type transport at the relevant frequencies. Finally, the experimental realization of the CV thermal wave crystal via frequency-domain thermorefectance [39] remains an important open challenge, and the present calculations provide the quantitative predictions required to guide such experiments.

Author Contributions: Conceptualization, J.M.-M. and R.E.-S.; methodology, J.M.-M. and B.M.-M.; software, J.M.-M. and D.S.-P.; validation, J.M.-M., B.M.-M. and D.S.-P.; formal analysis, J.M.-M. and R.E.-S.; investigation, J.M.-M., B.M.-M., R.E.-S. and D.S.-P.; writing—original draft preparation, J.M.-M.; writing—review and editing, B.M.-M., R.E.-S. and D.S.-P.; visualization, J.M.-M.; supervision, J.M.-M.; project administration, J.M.-M. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding author.

Acknowledgments: J.M.-M. and R.E.-S. would like to acknowledge the UNISON–UNAM collaboration program for its support.

Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

CV	Cattaneo–Vernotte
TWC	Thermal wave crystal
TMM	Transfer matrix method
PhC	Photonic crystal
PnC	Phononic crystal

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