DOI: https://doi.org/10.36602/jsba.2025.20.74

Modeling the Impact of Lattice Vibrations on Thermal Transport: Energy Generation and Diffusivity Modulation Approaches

Tarek M. Fayez*, Rabia A. M. Alsakit
Department of Physics, Sebhau University, Libya
*Corresponding author: tar.ahmad@sebhau.edu.ly

Submission date: 05.10.2025 Acceptance date: 21.12.2025 Electronic publishing date: 23.12.2025

Abstract: Two supplementary modeling methods are introduced in this study to examine the impact of lattice vibrations (phonons) on one-dimensional heat transmission in solids. The initial approach in Program 1 uses a velocity-squared source term added to the traditional heat equation to depict the direct heat produced by atomic motion and incorporate a dynamic phonon-heat interaction. The second technique in Program 2 indirectly captures the impact of phonons by enabling the thermal diffusivity coefficient to change as a function of lattice displacement, both temporally and spatially. Both models were applied to two representative materials, silicon (a high-conductivity semiconductor) and alumina (a low-conductivity ceramic), using finite-difference simulation in MATLAB program. The results show that there are material-specific thresholds for phonon-induced instability. In the case of Program 1, thermal breakdown occurs at $\beta_{critical}=10^{-8}$ K.s/m^2 for silicon and $\beta_{critical}=10^{-11}$ K·s/m^2 for alumina. The highest possible stable values of the coupling parameter C (in m/s) in Program 2 are 2.23 for time-dependent diffusivity and 1.27 for space-dependent diffusivity across both materials. According to the findings, a thorough description of thermal transport in thermally sensitive or micro-structured materials requires consideration of both phonon-induced energy generation and phonon-modulated diffusivity.

Keywords: Heat conduction, phonon dynamics, thermal transport modeling, diffusivity modulation

Introduction

Classical Fourier theory, which posits a continuous medium with instantaneous energy transfer across infinitesimal distances, has long been the mainstay of the study of heat conduction in solid materials. Fourier's law, which is still valid for many macroscopic systems, does not account for important physical phenomena at the micro- and nanoscale, where lattice vibrations (phonons) are the primary heat carriers [1,2]. The non-classical effects of phonon interactions, such as finite heat propagation rates, ballistic transport, and temperature-dependent material properties, necessitate the use of more complex models to accurately describe them [3]. Recent developments have emphasized that including lattice dynamics into thermal models may lead to a greater understanding of energy transfer processes, especially in semiconductors and insulators, where phonon activity has a significant influence on performance [4-6].

To study the dependence of heat conductivity on temperature and lattice parameters, numerical simulations were conducted using discrete Frenkel-Kontorova (FK), φ–4, and sinh-Gordon models [7]. These simulations investigated heat conduction in 1D lattices with various on-site potentials, incorporating both nonlinearity and a quadratic potential for nearest-neighbor interactions. The results demonstrated that the anharmonicity of the on-site potential alone is insufficient to ensure normal heat conductivity in these systems. The nature of heat conduction is determined by the spectrum of nonlinear excitations specific to each model and, therefore, depends on the exact potential shape and the lattice temperature. In the sin-Gordon and φ–4 models, phonons are scattered by a thermalized lattice of topological solitons. In contrast, in the sinh-Gordon and φ–4 models, phonons are scattered by localized high-frequency breathers. In the φ–4 model, the scattering mechanism shifts as the temperature increases.

For nanoscale structures (such as nanowires and nanotubes), a study on heat conduction in a quasi-1D harmonic chain system with 3D vibrations (both longitudinal and transverse) demonstrated that for a finite-size system, heat conduction is anomalous and energy diffusion is superdiffusive. The study also showed that both the anomalous heat conduction exponent (β) and the anomalous diffusion exponent (α) depend on the dimensionless quantity a/√T, where α =A+B ln(a/√T), with *a* representing the lattice constant and *T* the temperature. It was also found that the lattice constant had no effect when atoms were considered to move around their equilibrium positions; however, in the 3D case, the situation is completely different, and the lattice constant significantly influences heat conduction [8]. For an equation describing anomalous heat conduction:

$$\ddot{T} + \frac{1}{t}\dot{T} = cT'' \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

(c is the speed of sound in a one-dimensional crystal), exact solutions with regard to localized initial perturbations (rectangular, triangular, and sawtooth initial impulses) were studied in a 1D infinite harmonic chain. The study results showed that the solutions to the previous equation are the opposite of the solutions for the classical heat equation:

$$\dot{T} = \beta T'' \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

(β is thermal diffusivity), as they have a very clear wavefront. For the rectangular case, it was shown that the decay of the solution near the wavefront is proportional to 1/√T. Near zero, the decay is proportional to 1/t. In the case of an initial triangular temperature perturbation, the solution exhibits a smooth onset at the wavefront and maintains smooth behavior at the peak. For a sawtooth initial perturbation, the solution is asymmetric: the left wavefront has a smooth onset but an infinite derivative and a vertical tangent at the peak, whereas the right wavefront starts with an infinite derivative and a vertical tangent, yet transitions smoothly at the peak, where it has a zero derivative and a horizontal tangent [9].

Extensive research has been done on heat transmission in low-dimensional systems, with a focus on harmonic and anharmonic lattices. Prior research has revealed that perfect harmonic chains exhibit ballistic heat transport, in which Fourier's law of diffusion is broken and the thermal conductivity varies with system size and time [10,11]. In the study [12] analyze the fundamental mechanisms governing energy transport along a harmonic chain and investigate the establishment of local thermodynamic equilibrium (LTE) in the absence of phonon-phonon scattering. The author consider a one-dimensional harmonic chain where atoms on the left side (n ≤ N) were initially maintained at a prescribed temperature T_0, while the right side (n > N) was at zero temperature at t = 0. This thermal excitation propagates through the lattice in the form of phonon waves, leading to the excitation of locally dominant phonon modes at different spatial positions. The local phonon excitation process follows:

$$k_{max}(x, t) = a \cos(x/c_1 t)(2/a)\ldots\ldots\ldots(3)$$

where $c_1 = a\sqrt{(\chi/m)}$, (where m, χ, a are the mass, spring constant and lattice constant), which describes the progressive activation of phonon modes from low-frequency (long-wavelength) modes to higher frequencies over time. However, because phonon-phonon scattering is absent in the harmonic chain, not all phonon modes are populated instantaneously, preventing the system from reaching full LTE. The energy density at position x and time t is determined by the available phonon modes and follows:

$$E(x,t) = II^* \frac{k_{max}}{\pi/a} = II^* a\cos(\frac{x}{c_1 t})\frac{2}{\pi} \ldots (4)$$

where $II^* = T_0 C_v$ is the energy density in the left part of the chain and C_v is the heat capacity. This expression indicates that energy is primarily concentrated at locations where lower-frequency phonons dominate, leading to an anisotropic energy distribution along the chain. A key result of this study was the confirmation that energy transport remains ballistic, characterized by a constant energy flux:

$$J = II^* \frac{2}{\pi} c_1 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (5)$$

To further investigate the nature of thermal transport, author compares his results to Fourier's law, which describes diffusive heat conduction in conventional materials. According to Fourier's law, the temperature distribution should satisfy:

$$T(x,t) = T_0[1 - \mathrm{erf}\left(\frac{x}{\sqrt{\frac{4kt}{C_v}}}\right)] \ldots\ldots\ldots (6)$$

where k is the thermal conductivity. By equating the energy flux obtained from the ballistic transport model to that derived from Fourier's equation, he extract an effective thermal conductivity:

$$k = 4c_1^2 C_v t/\pi \ldots\ldots\ldots\ldots\ldots (7)$$

Thermal conductivity, as shown by this finding, is not a material constant in a harmonic chain but rather rises indefinitely with time. Due to scattering mechanisms like impurity scattering and Umklapp processes [11,13], thermal conductivity in traditional materials stabilizes, which is very different from this behavior. These results offer significant insights into heat transport in low-dimensional and nanoscale systems, where phonon scattering is frequently reduced, causing deviations from Fourier's law.

From a different viewpoint, other theoretical analyses have proposed an alternative framework based on the Fokker-Planck Equation (FPE), which offers a stochastic representation of lattice vibrations. The study of lattice thermal conductivity κ_{Latt} is essential for comprehending heat transfer in crystalline and amorphous materials. The phonon Boltzmann transport equation (BTE), which is based on the phonon gas (PG) model, is used in conventional methods. This model, however, fails in systems with significant mode-mode interactions (strong phonon-phonon interactions) or disorder-induced localized modes. These interactions alter the phonon spectrum, resulting in what are known as effective phonons, which cannot be modeled using traditional BTE-based models [14,15].

Recent studies have challenged the conventional phonon gas model and Boltzmann Transport Equation (BTE) in phonon-mediated heat transport, highlighting its limitations in systems with strong anharmonicity or intense phonon–phonon interactions. Advanced theories that include higher-order scattering processes reveal that these interactions can significantly alter the phonon spectrum, resulting in deviations from the predictions of standard three-phonon BTE formulations [16]. Recent developments indicate that in regimes with strong interactions, the assumption of propagating phonons is insufficient, necessitating higher-order or alternative transport descriptions beyond classical Boltzmann transport equation (BTE) theory [17]. In parallel, alternative stochastic frameworks have been suggested to analyze lattice vibrations and diffusive heat transport in complex systems, leading to the emergence of effective phonon modes where traditional transport models are inadequate [18]. This progress encourages the creation of continuum-level models that can better represent lattice-induced changes in thermal transport, moving beyond conventional phonon gas theories.

We explore two alternative methods for simulating the impact of lattice vibrations on heat transmission in a one-dimensional domain in this study. By directly linking atomic velocity to thermal energy production, the initial strategy introduces a phonon-induced energy source into the heat equation. The second method allows the thermal diffusivity to change dynamically under the influence of lattice displacement. Under regulated starting and boundary circumstances, these models are used to two representative materials: silicon, a semiconductor with high thermal conductivity, and aluminum oxide (Al_2O_3), a ceramic with low thermal conductivity. The goal of this study is to comprehend the dual function of phonons as both energy carriers and heat conduction property modulators. By introducing a dual modeling approach that accounts for both direct and indirect impacts of lattice vibrations on thermal conduction in one-dimensional systems, this work tackles a key challenge in microscale heat transfer. By facilitating improved heat flow control at the nanoscale, its findings are crucial for improving the design of phononic devices, insulating materials, and semiconductors. The study lays the foundation for potential advances in phononic engineering and thermal management by identifying material-specific phonon-heat interaction parameters and aiding in the creation of realistic simulation tools.

Model Description

By combining the wave equation for lattice dynamics with the heat conduction equation, it is possible to simulate how lattice vibrations affect heat transfer. This connection occurs because lattice vibrations (phonons) contribute to energy transfer, which has an impact on the temperature field. We must establish a mathematical relationship between the heat transfer equation in one dimension and the lattice vibration equation in order to combine the two systems.

For monatomic solid, the Heat Equation in 1D follow:

$$\frac{\partial T(x,t)}{\partial t} = \propto \frac{\partial^2 T(x,t)}{\partial x^2} \dots\dots\dots\dots\dots\dots (8)$$

where T(x,t) is the temperature at position x, time t, and α is the thermal diffusivity of the matter. The thermal diffusivity coefficient is defined by:

$$\alpha = \frac{k}{\rho C_p} \dots\dots\dots\dots\dots\dots\dots\dots (9)$$

where k is the thermal Conductivity, ρ is the density, and C_p is the specific heat capacity at a constant pressure.

The behavior of phonons in a one-dimensional lattice can be described using an elastic wave equation:

$$m \frac{\partial^2 u(x,t)}{\partial t^2} = K \frac{\partial^2 u(x,t)}{\partial x^2} \dots\dots\dots\dots (10)$$

where u(x,t) is the displacement of atoms, m is the mass of the atom, and K (N/m) is the stiffness constant.

Heat transfer impacts lattice vibrations by affecting local stiffness, K(T), while lattice vibrations generate thermal energy, resulting in phonon scattering or dissipation, as described by the coupled system:

$$\frac{\partial T(x,t)}{\partial t} = \propto \frac{\partial^2 T(x,t)}{\partial x^2} + \beta \left(\frac{\partial u(x,t)}{\partial t} \right)^2 (11)$$

$$m \frac{\partial^2 u(x,t)}{\partial t^2} + \eta \frac{\partial u(x,t)}{\partial t} = K(T) \frac{\partial^2 u(x,t)}{\partial x^2} (12)$$

where β ($K.s/m^2$) is coupling constant indicating the strength of lattice vibration's influence on heat transfer, and η (kg/s) is damping coefficient (internal damping or phonon damping). The damped wave equation (Eq. 12) provides a robust foundation for studying the role of lattice vibrations in thermal transport. To account for physical energy dissipation within the lattice, a damping term proportional to the first time derivative of displacement is introduced. This term models phonon scattering and internal friction mechanisms, which are common in real materials and become significant during dynamic lattice vibrations. We'll assume a simple linear dependence of K(T)**:**

$$K(T) = K_0(1 - \gamma T(x,t)) \dots\dots\dots (13)$$

Where K_0 is the stiffness at room temperature, γ (1/K) is a temperature sensitivity coefficient (material-dependent), and T(x,t) is the local temperature at that point.

Equation (11) represents the heat equation, including the effect of lattice vibrations. Heat diffusion $\alpha.(\partial^2 T/\partial x^2)$ is combined with the effect of lattice vibration βv^2. The velocity that related to phonon energy is computed as $v(x,t)=\partial u(x,t)/\partial t$. Lattice vibrations can act as energy carriers. The kinetic energy from lattice vibrations (via displacement or velocity of atoms) dissipates into thermal energy, influencing the temperature field. This effect is proportional to the square of atomic velocity, as phonon energy dissipation scales with velocity.

On the other hand, lattice vibration mode (phonons) influences heat transfer by modifying thermal properties like thermal conductivity k and diffusivity α, which are dynamically updated based on these modes. We can express α as a function of u(x,t):

$$\alpha(x,t) = f(u(x,t)) \dots\dots\dots\dots (14)$$

$$\frac{\partial T(x,t)}{\partial t} = \propto (x,t)\frac{\partial^2 T(x,t)}{\partial x^2} \dots\dots\dots\dots (15)$$

We employ an analytical solution of equation (10) to prevent numerical instabilities and isolate the impact of phonons on heat conduction:

$$u(x,t) = A sin(\pi x)\cos(\omega t)$$

$$with\ \omega = \sqrt{\frac{K}{m}}\pi \dots\dots (16)$$

Two formulations are proposed for incorporating lattice vibrations' influence: Time-Dependent Diffusivity α(t) and Space-Dependent Diffusivity α(x). Case A updates thermal diffusivity based on lattice displacement at a fixed spatial location, typically the midpoint of the domain:

$$\alpha(t) = \alpha_0 + C|u(x_0,t)| \dots\dots\dots\dots (17)$$

This model suggests that vibrational activity at a specific location affects heat conduction rate and mimics the average phonon scattering effect over time. Case B involves calculating the space-dependent diffusivity α(x) from the initial spatial distribution of lattice displacement, which remains fixed during the simulation:

$$\alpha(x) = \alpha_0 + C|u(x,0)| \dots\dots\dots\dots (18)$$

The initial vibrational heterogeneity on the medium impacts the spatial distribution of heat from the outset.

Thus, the equation (15) becomes as follows:

$$\frac{\partial T(x,t)}{\partial t} = \propto (t)\frac{\partial^2 T(x,t)}{\partial x^2} \dots\dots\dots\dots\dots (19)$$

$$\frac{\partial T(x,t)}{\partial t} = \propto (x)\frac{\partial^2 T(x,t)}{\partial x^2} \dots\dots\dots\dots (20)$$

The baseline thermal diffusivity, α0, is absent from phonon effects, while C (in m/s) is a scaling parameter indicating the thermal diffusion's sensitivity to atomic vibration amplitude. This methodology isolates the impact of phonon-induced variation in thermal diffusivity without feedback mechanisms or nonlinear coupling, allowing clear identification of threshold values for C at which classical heat propagation behaviour significantly deviates.

Numerical Implementation

The model utilizes a coupled system of partial differential equations to explain the impact of dynamic lattice vibrations on heat transfer in a one-dimensional domain. The system consists of three key equations 11, 12, and 13 (Program 1), discretized using a finite difference method (FDM) with explicit time-stepping, and initial conditions applied. (1) Initial temperature: a normalized Gaussian profile centered at the domain midpoint, $T(x,0)=\exp(-100(x-0.5)^2)$. (2) Displacement: a localized Gaussian pulse, or sinusoidal profile, $u(x,0)=A\cdot\exp(-\delta(x-0.5)^2)$. (3) Velocity: set to zero at t=0, then updated dynamically.

A second-order central difference scheme was utilized for velocity computation, enhancing stability and accuracy by computing the phonon heat generation term $\left(\frac{\partial u(x,t)}{\partial t}\right)^2$ by:

$$v(x,t_n) = \frac{u(x,t_{n+1}) - u(x,t_{n-1})}{2\Delta t} \dots\dots (21)$$

The Stability Conditions were established using Dirichlet boundary conditions for temperature and displacement boundaries, with a small damping coefficient η introduced to stabilize lattice oscillations and prevent non-physical growth, using specific parameters for lattice response.

In a complementary numerical scheme (Program 2), a simplified formulation is implemented based on equations 10, 17, 18, 19, and 20, which exclude direct phonon energy terms and instead allow the thermal diffusivity α(x,t) to vary dynamically in response to lattice displacement. Program 2 introduces a basic formulation using equations 10, 17, 18, 19, and 20, allowing dynamic thermal diffusivity α(x,t) to vary based on lattice displacement. The formulation, unlike Program 1, does not include velocity or energy generation terms, instead focusing on temperature field modulation through changes in diffusivity caused by the lattice motion.

Results and Discussion

Case 1: Program 1 for Equations 11, 12 and 13

The heat equation is now being solved, taking into account the impact of lattice vibrations. As illustrated in Figure 1, the baseline heat conduction behavior for silicon is defined at β=0 and $\eta=10^{-7}$kg/. With no impact from phonon dynamics, the initial Gaussian heat pulse in this baseline solution progressively spreads and decays due to classical conductive transport, exhibiting smooth and symmetric thermal diffusion. The temperature surface stays constant and completely conforms to the baseline shape for $\beta \leq 10^{-8}$K.s/m^2 when β rises marginally above zero. This shows that the phonon-induced energy source term $\beta\left(\frac{\partial u}{\partial t}\right)^2$ is too weak to have a detectable effect on the thermal profile in this range. However, the temperature surface starts to diverge from the baseline when $\beta \geq 10^{-7}$ K.s/m^2, which results in a noticeable change in mean thermal diffusion and a distortion of the temperature front's symmetry. In general, when $\beta \geq 10^{-7}$K.s/m^2, the system becomes unstable and the temperature field shows nonphysical development, steep gradients, or thermal blow-up. This is caused by the classical diffusion mechanism being overpowered by excessive phonon-induced heating. These findings validate that $\beta_{critical}=10^{-8}$ K.s/m^2 is the crucial threshold for phonon impact in silicon. This threshold reflects the intrinsic balance between silicon's high thermal conductivity and its capacity to absorb vibrational energy without destabilizing the heat profile.

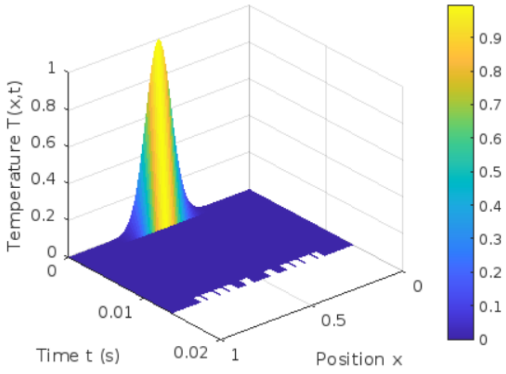

Fig.1. Temperature evolution in silicon at baseline condition with β=0 and η=10-7 kg/s

As illustrated in Figure 2, the baseline thermal behavior for alumina Al_2O_3, an electrical insulator with comparatively poor thermal conductivity, is also characterized at β=0 and $\eta=10^{-7}$kg/s. Because of alumina's poor heat conductivity, the temperature profile in this reference state changes gradually and stays spatially confined. The thermal field maintains its stable and symmetric configuration while the initial Gaussian pulse gradually dissipates without deformation. For all values up to $\beta \leq 10^{-11}$K.s/m^2, the surface form stays the same as β grows from zero. This demonstrates that the temperature field acts as predicted under simply diffusive transport and that phonon-induced heat production is minimal in this range. However, the temperature surface starts to exhibit noticeable departures from the baseline when $\beta \geq 10^{-10}$K.s/m^2. The symmetry is slightly disrupted and heat spreads faster, suggesting that the phonon-thermal coupling is getting strong enough to affect conduction. In general, the solution becomes unstable and unphysical with abrupt spikes, erratic thermal growth, or complete collapse of the heat profile when β grows further to $\beta \geq 10^{-10}$K.s/m^2. This illustrates how alumina is considerably more susceptible to phonon-induced heat input than silicon due to its low thermal conductivity and low thermal inertia. Therefore, $\beta_{critical}=10^{-11}$ K.s/m^2 is the critical phonon coupling threshold for alumina. This extreme sensitivity emphasizes how crucial it is to take into consideration even minute phonon effects in low-temperature-diffusive insulators.

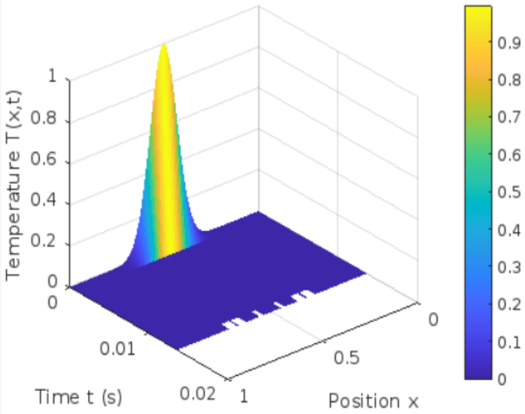

Fig.2. Temperature evolution in Alumina at baseline condition with β=0 and η=10-7 kg/s.

In order to reduce numerical instabilities and offer a minimal but physically plausible opposition to lattice acceleration, the damping coefficient η was developed. It was discovered that a little constant value, $\eta=10^{-7}$kg/s, was adequate to stabilize the displacement field without reducing the phonon-thermal interaction's dynamics. While smaller values run the danger of unphysical resonance or numerical instability, larger values of η unduly dampen the vibrational action and obscure the role of β.

Case 2: Program 2 for Equations 10, 17 and 19, and Equations 10, 18 and 20

The second simulation approach introduces a variable thermal diffusivity, α, that may be varied in space or time to investigate how lattice vibrations affect heat conduction. Simulations were performed using two different formulations for silicon and alumina: space-dependent diffusivity in equation 18 and time-dependent diffusivity in equation 17. In order to determine the point at which the system deviates from classical heat diffusion behavior, the coupling parameter C was gradually increased in both scenarios. The lattice displacement *u(x,t)* was analytically dictated using a sinusoidal standing wave solution.

Both materials demonstrated exceptional tolerance to increasing values of C in the α(t) formulation, where the diffusivity evolves uniformly over the spatial domain in time based on the displacement at a fixed location. As anticipated, the baseline heat surface for silicon (at C = 0, Figure 3a) was smooth and symmetrical. Up to C = 2.24m/s, this form essentially stayed the same, with the diffusion rate only slightly increasing. However, the temperature distribution showed obvious indications of instability, including steep gradients and excessive thermal development, at C > 2.24m/s (such as C=2.3m/s, Figure 4). Alumina (the baseline at C = 0, Figure 3b) showed a similar pattern, with the temperature field being constant and stable up to C=2.23m/s, and then showing signs of instability at C > 2.23m/s (such as C=2.3m/s, Figure 5). These results show that both materials can withstand the global modulation caused by time-varying α up to a threshold coupling value of roughly 2.23-2.24m/s. Given that the critical values for the two materials are similar, it can be concluded that time-based phonon effect is less susceptible to the material's inherent thermal characteristics.

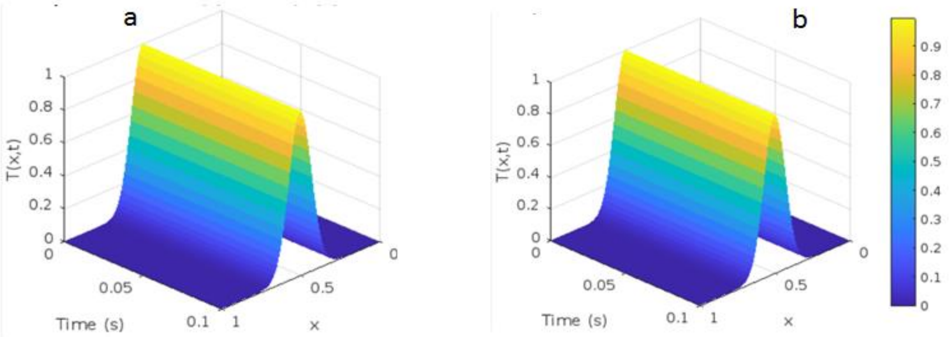

Fig.3. Temperature evolution in silicon (a) and Alumina (b) at baseline condition with C=0 in the α(t) formulation.

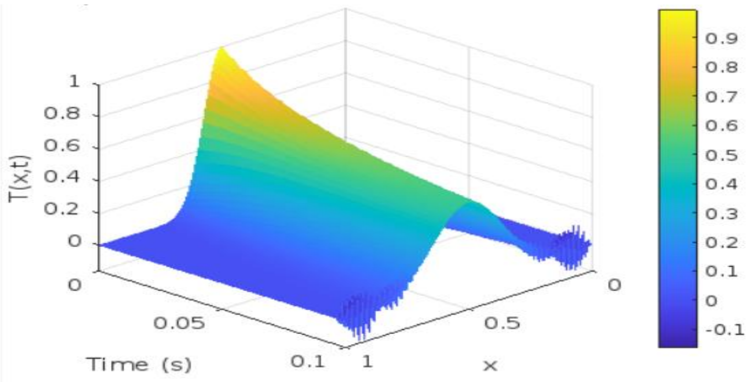

Fig.4. Temperature evolution in silicon C=2.3m/s in the α(t) formulation.

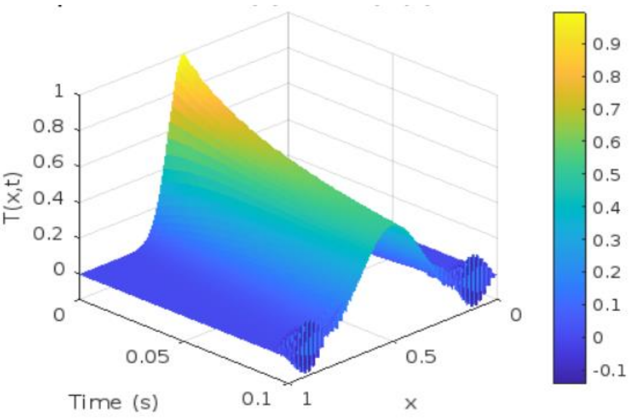

Fig.5. Temperature evolution in Alumina C=2.3m/s in the α(t) formulation.

The α(x) formulation, on the other hand, produced an earlier onset of instability by imposing a temporally stable but spatially changing diffusivity profile. The temperature surface in both silicon and alumina stayed physically acceptable until about C = 1.27m/s as shown in Figure 6, beyond which distortion and numerical breakdown were noticeable (i.e., at C >1.27m/s as shown in Figures 6c and 6g). Localized areas of enhanced or suppressed conductivity are probably caused by the spatial heterogeneity in α, and this leads to thermal amplification, abrupt gradients, and asymmetric heat spreading. This early instability, in contrast to the α(t) instance, emphasizes how spatial non-uniformity in thermal diffusivity can be more disruptive, especially in materials like alumina that have low thermal inertia.

Overall, these findings demonstrate that heat transport can be substantially changed by phonon-coupled modulation of thermal diffusivity; however, the stability and sensitivity to coupling strength are highly dependent on whether the modulation is temporal or spatial. While spatial modulation creates fixed heterogeneity that causes an earlier breakdown, temporal modulation evenly distributes the influence and maintains larger values of C. When phonon contributions start to dominate or disrupt classical conduction, the extracted critical thresholds C=2.24m/s for α(t) and C=1.27m/s for α(x) act as material-specific indicators. These numbers offer a helpful point of reference for choosing parameters in upcoming phonon-influenced heat transport models.

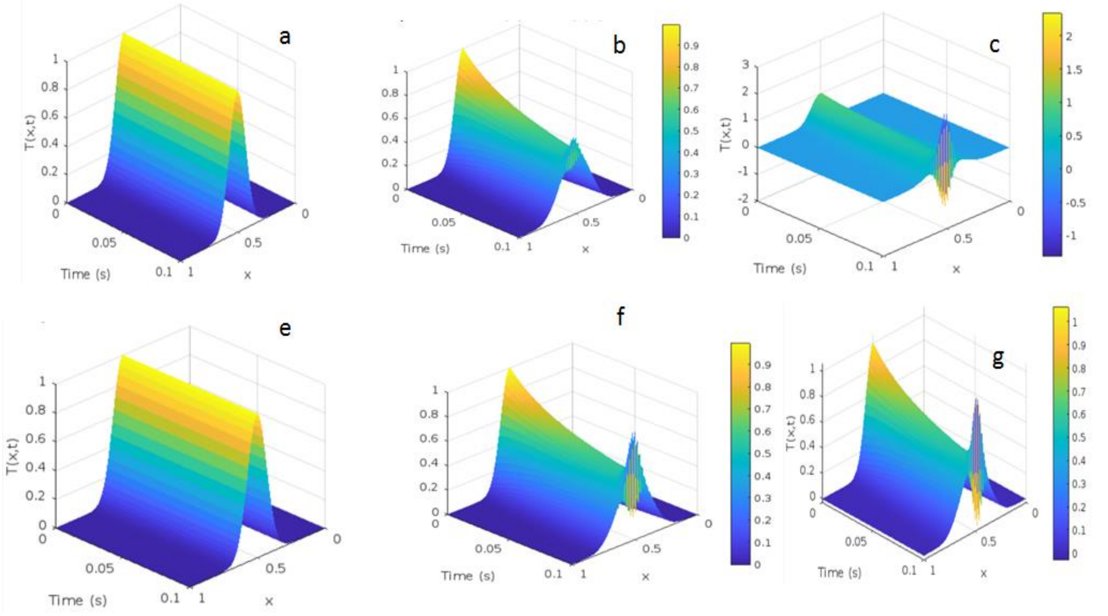

Fig.6. Temperature evolution in silicon (a) C=0 (b) C=1.27 (c) C=1.28m/s, and Alumina (e) C=0 (f) C=1.27 (g) C=1.28m/s C=2.3m/s, in the α(x) formulation.

Conclusion

In order to evaluate the impact of lattice vibrations on heat transmission in one-dimensional systems, this paper offers a dual-framework simulation experiment. The two modeling techniques that were investigated were: the first, phonon-induced heat generation via a direct velocity-dependent source term (Program 1), and the second, phonon-modulated thermal diffusivity through displacement-based variability in α (Program 2). The two methods are demonstrated to be complementary rather than sequential or substitutive, since each captures a different physical mechanism: Program 1 models how vibrational motion injects energy into the system, while Program 2 models how that motion affects the material's ability to conduct heat. Critical threshold values for the phonon-thermal coupling parameters (β and C) were identified, beyond which temperature fields destabilize or become nonphysical. Because of variations in thermal conductivity and lattice responsiveness, these thresholds vary between materials. The research provides parameter limits for the safe use of such coupling in simulations of heat transport in semiconductors and insulators, and it creates a strong modeling foundation for phonon-heat interaction. This framework could be applied to higher-dimensional models in the future or to experimentally validating the coupling variables found here.

References:

[1] Kittel, C. (2004). *Introduction to Solid State Physics*. Wiley.

[2] Cahill, D. G., Ford, W. K., Goodson, K. E., Mahan, G. D., Majumdar, A., Maris, H. J., Merlin, R., & Phillpot, S. R. (2003). Nanoscale thermal transport. *Journal of Applied Physics*, *93*(2), 793–818. https://doi.org/10.1063/1.1524305

[3] Chen, G. (2005). *Nanoscale Energy transport and conversion: A Parallel Treatment of Electrons, Molecules, Phonons, and Photons*. Oxford University Press.

[4] Volz, S. (2009). *Thermal nanosystems and nanomaterials*. Springer Science & Business Media.

[5] Majumdar, A. (1993). Microscale heat conduction in dielectric thin films. *Journal of Heat Transfer*, *115*(1), 7–16. https://doi.org/10.1115/1.2910673

[6] Neogi, S., Reparaz, J. S., Pereira, L. F. C., Graczykowski, B., Wagner, M. R., Sledzinska, M., Shchepetov, A., Prunnila, M., Ahopelto, J., Sotomayor-Torres, C. M., & Donadio, D. (2015). Tuning thermal transport in ultrathin silicon membranes by surface nanoscale engineering. *ACS Nano*, *9*(4), 3820–3828. https://doi.org/10.1021/nn506792d

[7] Savin, A. V., & Gendelman, O. V. (2003). Heat conduction in one-dimensional lattices with on-site potential. *Physical Review. E, Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics*, *67*(4). https://doi.org/10.1103/physreve.67.041205

[8] Liu, Z., & Li, B. (2008). Heat Conduction in a One-Dimensional Harmonic Chain with Three-Dimensional Vibrations. *Journal of the Physical Society of Japan*, *77*(7), 074003. https://doi.org/10.1143/jpsj.77.074003

[9] Sokolov, A. A., Krivtsov, A. M., & Müller, W. H. (2017). Localized heat perturbation in harmonic 1D crystals: Solutions for the equation of anomalous heat conduction. *Physical Mesomechanics*, *20*(3), 305–310. https://doi.org/10.1134/s1029959917030067

[10] Rieder, Z., Lebowitz, J. L., & Lieb, E. (1967). Properties of a harmonic crystal in a stationary nonequilibrium state. *Journal of Mathematical Physics*, *8*(5), 1073–1078. https://doi.org/10.1063/1.1705319

[11] Dhar, A. (2001). Heat conduction in the disordered harmonic chain revisited. *Physical Review Letters*, *86*(26), 5882–5885. https://doi.org/10.1103/physrevlett.86.5882

[12] Xu, Z. (2015). Phonon Excitation and Energy Redistribution in Phonon Space for Energy Dissipation and Transport in Lattice Structure with Nonlinear Dispersion. *Communications in Theoretical Physics*, *63*(1), 101–108. https://doi.org/10.1088/0253-6102/63/1/16

[13] Casher, A., & Lebowitz, J. L. (1971). Heat flow in regular and disordered harmonic chains. *Journal of Mathematical Physics*, *12*(8), 1701–1711. https://doi.org/10.1063/1.1665794

[14] Zeng, Y., & Dong, J. (2019). Fokker-Planck equation for lattice vibration: Stochastic dynamics and thermal conductivity. *Physical Review. B*, *99*(1). https://doi.org/10.1103/physrevb.99.014306

[15] Zhang, Y., Chen, S., Wang, J., & Zhao, H. (2013). Breakdown of effective phonon theory in one-dimensional chains with asymmetric interactions. *arXiv (Cornell University)*. https://doi.org/10.48550/arxiv.1301.2838

[16] Jain, A. (2024). Impact of four-phonon scattering on thermal transport in carbon nanotubes. *Physical Review. B./Physical Review. B*, *109*(15). https://doi.org/10.1103/physrevb.109.155413

[17] Jain, A., Srivastava, Y., Gokhale, A. G., Virakante, N., & Kagdada, H. L. (2025). Higher-Order Thermal Transport Theory for phonon thermal transport in semiconductors using lattice dynamics calculations and the Boltzmann Transport equation. *Journal of the Indian Institute of Science*. https://doi.org/10.1007/s41745-025-00487-3

[18] Saurav, S., & Mazumder, S. (2023). Extraction of thermal conductivity using phonon Boltzmann Transport Equation based simulation of frequency domain thermo-reflectance experiments. *International Journal of Heat and Mass Transfer*, *204*, 123871. https://doi.org/10.1016/j.ijheatmasstransfer.2023.123871