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Research Article

Keywords:

Posted Date: October 23rd, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-10335339/v1>

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Additional Declarations: No competing interests reported.

Experimental and Computational Investigation of Thermal Conductivity in Porous Silicon: Doping-Dependent Performance of Molecular Dynamics and Physics-Informed Neural Networks

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Abstract

Porous silicon (pSi) is a highly promising material for nanoscale thermal management, but predicting its thermal conductivity remains challenging due to complex structure-property dependencies. In this work, we present a comprehensive multiscale investigation of heat transport in pSi, combining experimental gas-microphone photoacoustic (PA) measurements with atomistic Molecular Dynamics (MD) simulations and continuum-level Physics-Informed Neural Networks (PINNs). Mesoporous pSi layers with porosities ranging from 48% to 75% were fabricated via electrochemical etching of highly doped p⁺-type silicon, and their effective thermal conductivity was experimentally determined. Our findings reveal that the thermal properties are fundamentally governed by the initial substrate doping, which dictates the formation of either isotropic sponge-like or anisotropic columnar morphologies. We demonstrate that MD simulations accurately capture the thermal behavior of heavily doped samples by explicitly accounting for phonon confinement, whereas the PINN approach excellently models percolation and macroscopic heat flux in stochastic networks typical of lightly and moderately doped silicon. By integrating these computational and experimental datasets with literature values, we utilized symbolic regression to derive a generalized analytical expression for the effective thermal conductivity of pSi as a function of porosity and temperature. This hybrid multiscale framework connects nanoscale phonon mechanics to macroscopic thermophysical properties, providing a predictive tool for the design of porous silicon-based thermoelectric and thermal-insulation devices.

1. Introduction

Porous silicon (pSi) is a versatile nanostructured material fully compatible with conventional silicon-based technologies [1]. Control over electrochemical etching

conditions enables deterministic tuning of porosity, pore size, and structural anisotropy [2, 3]. This morphological tunability directly enables the engineering of its thermophysical properties - most notably a significant reduction in thermal conductivity - making pSi an exceptional platform for controlling heat transport at the nanoscale [4, 5]. Consequently, this material has been extensively investigated for high-efficiency thermoelectric energy conversion and thermal insulation [6, 7], microelectronic thermal management [8], lithium-ion batteries [9], and advanced sensing and optoelectronic systems [10].

The substantial reduction of thermal conductivity in porous silicon (pSi) compared to bulk crystalline silicon is primarily driven by intense phonon scattering at pore boundaries, surfaces, and defects [3, 4]. Beyond total porosity, this reduction is strongly governed by the matrix morphology, including pore size distribution, tortuosity, anisotropy, and the connectivity of the silicon skeleton [5]. Furthermore, the doping level and conductivity type of the initial substrate directly predetermine both the intrinsic matrix properties and the resulting pore architecture during etching [11]. Consequently, heat transport in pSi is a multiscale phenomenon determined by the complex interplay of phonon confinement, percolation, and structural heterogeneity [5, 7].

Numerous experimental and theoretical studies have addressed thermal transport in pSi. Advanced experimental approaches, such as gas-microphone photoacoustic techniques, Raman thermometry, and transient methods, demonstrate that the effective thermal conductivity of pSi can decrease by orders of magnitude compared to bulk silicon [3]. However, significant discrepancies in reported thermal conductivity values are commonly observed even within identical porosity ranges [5]. These variations are inherently tied to structural sensitivity - namely, differences in pore morphology, fabrication regimes, and substrate doping profiles [7]. Consequently, establishing definitive structure-property relationships remains a critical challenge for the predictable integration of pSi into thermal management systems.

From a theoretical perspective, effective medium approximations (EMA) and percolation models provide analytical insights into porosity-dependent thermal conductivity. Yet they often oversimplify realistic porous morphologies and neglect nanoscale phonon transport effects, such as boundary scattering and coherent wave phenomena, which are critical in disordered systems [12]. Conversely, molecular dynamics (MD) simulations provide atomistic rigor by capturing phonon scattering and confinement, making them effective for small-scale geometric analysis [13, 14]. However, the high computational cost of MD limits its applicability to isolated unit cells or small domains, failing to capture the macroscopic heat flux behavior inherent to large-scale, stochastic porous media [14].

To bridge this gap, machine learning has emerged as a powerful alternative for modeling transport phenomena in heterogeneous media. Specifically, Physics-Informed Neural Networks (PINNs) integrate governing physical laws directly into the training process, enabling physically consistent, computationally efficient predictions of temperature and heat flux distributions. By bypassing the need for computationally expensive numerical solvers while maintaining partial differential equation constraints, PINNs offer a robust way to bridge the gap between atomistic insights and continuum-level predictions. Despite these advantages, the application of PINNs to heat transport in porous silicon (pSi) remains largely unexplored, particularly in their integration with experimental datasets and atomistic simulations.

In this work, we propose a comprehensive multiscale framework to investigate heat transport in pSi by combining gas-microphone photoacoustic experiments, MD simulations, and PINN modeling. Electrochemical etching was used to fabricate pSi layers at distinct porosity levels, and their effective thermal conductivity was determined via photoacoustic measurements. At the atomistic scale, MD simulations were deployed to isolate phonon-mediated transport and geometric scattering effects. Concurrently, PINN-based continuum modeling captured heat transfer in stochastic porous morphologies, enabling predictable mapping of thermal behavior across broad porosity and temperature ranges. Ultimately, these integrated datasets were used to derive a generalized analytical expression for the thermal conductivity of pSi. In addition, an extensive set of published data was reviewed and synthesized. This hybrid approach establishes a direct link between nanoscale phonon mechanics, stochastic morphology, and macroscopic thermophysical properties.

2. Materials and Methods

2.1. Sample Preparation

Porous silicon layers were fabricated by electrochemical etching of monocrystalline p^+ type silicon wafers with Si (100) surface orientation, a resistivity of 0.01-0.02 $\Omega \cdot \text{cm}$, and a thickness of 500 μm . The etching process was carried out in a Teflon electrochemical cell using an $\text{HF}:\text{C}_2\text{H}_5\text{OH}$ electrolyte mixture with a volume ratio of 1:1 (see Fig.1). A platinum (Pt) electrode was used as the cathode. The process was performed at room temperature under galvanostatic conditions. The active etching area was 2.7 cm^2 . After etching, the samples were rinsed with ethanol and dried at room temperature.

As illustrated in Fig. 2, the kinetic parameters of the process were systematically evaluated. Both the etching rate (v) and the resulting porosity (p) exhibit a pronounced linear dependence on the applied anodic current density (j). As a result, a set of pSi

samples with $\sim 20\ \mu\text{m}$ thickness and porosities ranging from 48% to 75% were obtained. The porosity of the fabricated layers was determined using the gravimetric method.

The thickness and structural morphology of the fabricated pSi layers was characterized using scanning electron microscopy (SEM). Fig. 3 presents cross-sectional SEM images of the samples prepared at different current densities, corresponding to porosities of 45% (A), 55% (B), and 65% (C). The micrographs reveal a highly interconnected mesoporous network with a distinct columnar anisotropy characteristic of heavily doped, etched p^+ -type silicon, in which pores propagate predominantly perpendicular to the substrate surface.

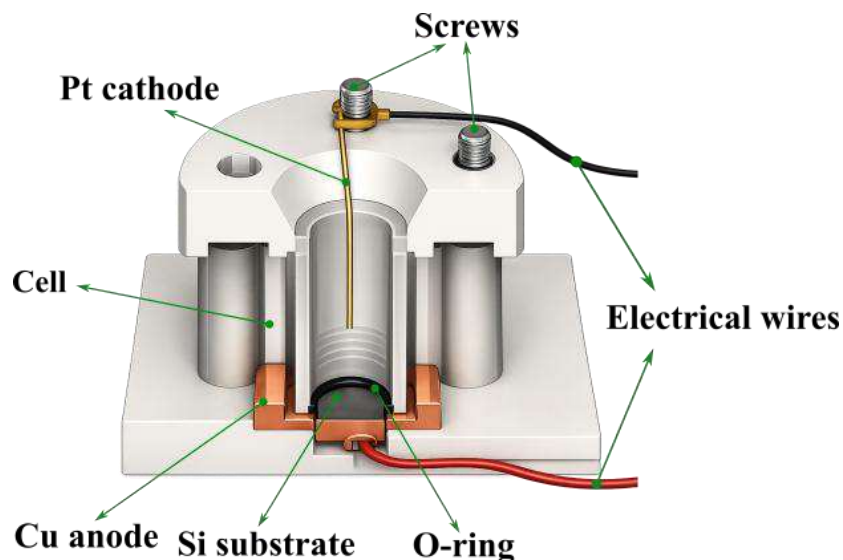


Fig.1. Schematic representation of the electrochemical cell used for porous silicon formation by electrochemical etching.

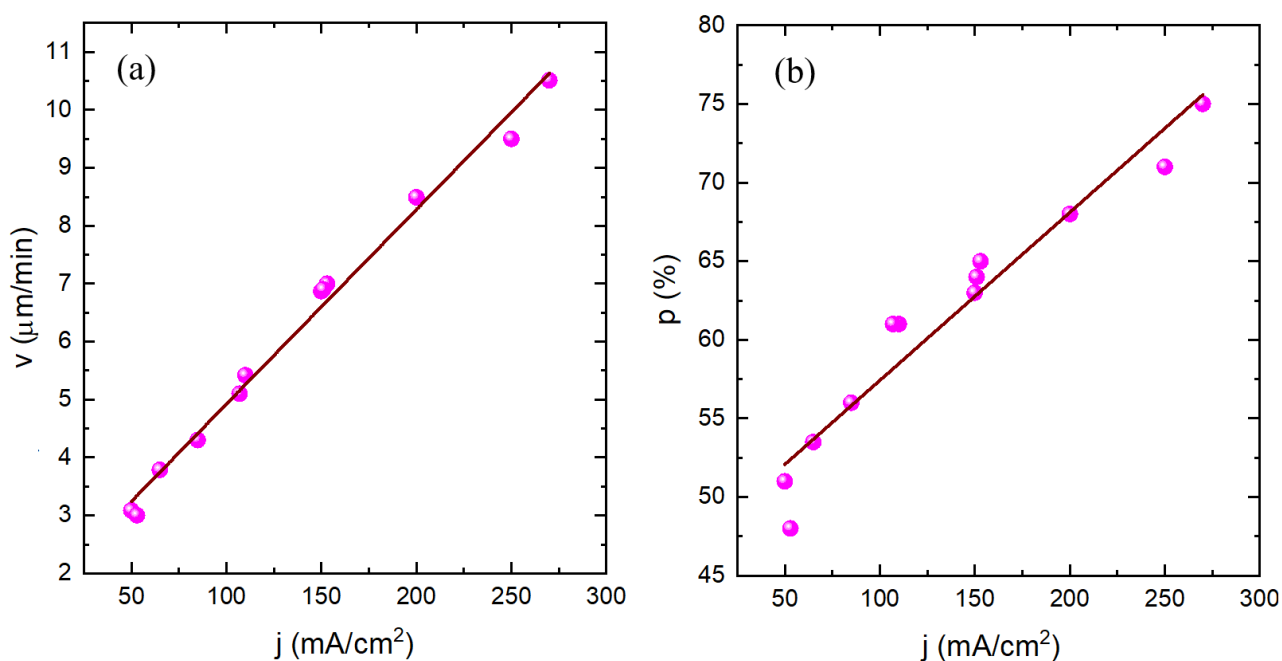


Fig.2. Dependence of the etching rate (v) and resulting porosity (p) on the applied anodic current density (j).

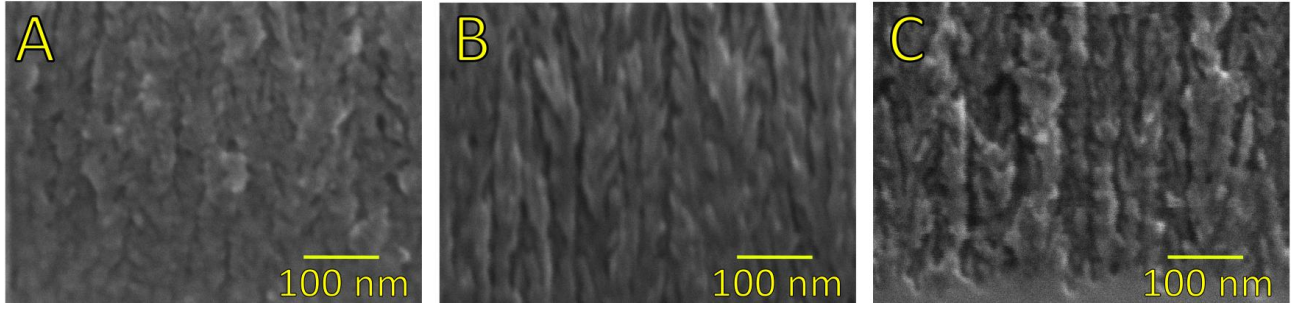


Fig.3. Cross-sectional scanning electron microscopy (SEM) images of the porous silicon structures with different porosities: (A) 48%, (B) 55%, and (C) 65%.

2.2. Photoacoustic Measurements

The photoacoustic setup is designed to generate and record acoustic signals arising from the absorption of modulated light radiation by the sample under study. The main components of the system are an optical excitation source, an optical path, a photoacoustic cell containing the sample, an acoustic detector, and a signal recording system (see Fig. 4). In this work, the thermophysical properties of sample were investigated using a gas-microphone configuration, which is one of the most sensitive methods for analyzing heat transfer in solids [7, 15].

A continuous wave diode laser with a wavelength of 405 nm and a power of 90 mW was used as the excitation source. The intensity of the laser radiation was harmonically modulated in the frequency range from 10 Hz to 2000 Hz, which allowed us to investigate the frequency dependence of the photoacoustic signal. The laser beam was focused onto the sample, forming a spot approximately 1-2 mm in diameter.

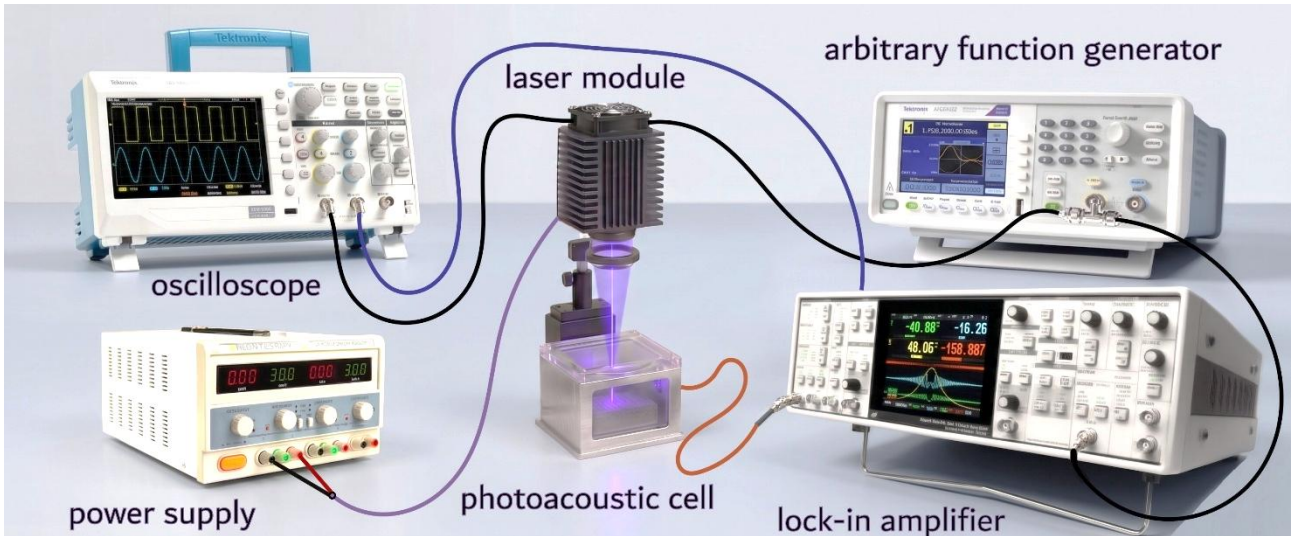


Fig.4. Schematic representation of the experimental setup for gas-microphone photoacoustic measurements.

The sample was placed in the input window of the photoacoustic (PA) cell, ensuring efficient transfer of thermal excitation into the gas layer directly above the

surface. The absorption of modulated light causes periodic heating of the sample and the generation of thermal waves that propagate into the surrounding gas, inducing corresponding pressure oscillations. These oscillations are recorded by an electret microphone and fed to a synchronous detector (lock-in amplifier), which allows for the precise determination of the amplitude-frequency characteristics of the photoacoustic signal.

To extract the effective thermal conductivity of the pSi layer, the experimental amplitude-frequency dependencies were fitted using a 1D thermal wave model based on the Rosencwaig-Gersho theory [16]. Specifically, the sample was modeled as a two-layer structure consisting of the porous silicon layer ($j = 1$) and the underlying bulk crystalline silicon substrate ($j = 2$). The spatial distribution of the complex temperature fluctuation amplitude, $\theta_j(z)$, was calculated by solving the 1D heat diffusion equation for each layer [17]:

$$\frac{d}{dz}(\chi_j \frac{d\theta_j(z)}{dz}) - i\omega\rho_j c_j \theta_j(z) = -Q_j(z) \quad (1)$$

where χ_j , ρ_j , and c_j are the thermal conductivity, density, and specific heat capacity of the j -th layer, respectively; $\omega = 2\pi f$ – is the angular modulation frequency; and $Q_j(z)$ denotes the volumetric heat-generation rate due to optical absorption of the modulated laser radiation. For the absorbing porous silicon layer, $Q_1(z) = \alpha I_0 e^{-\alpha z}$, whereas $Q_2(z) = 0$ in the crystalline silicon substrate.

The acoustic pressure oscillations δP in the cell are generated by the heat transfer from the sample surface into the adjacent gas layer, which can be expressed as:

$$\delta P \sim -\theta_1(0) \sqrt{\frac{\chi_g}{i\omega\rho_g c_g}} \quad (2)$$

where $\theta_1(0)$ is the temperature fluctuation at the sample-gas interface, and χ_g , ρ_g , and c_g – are the thermophysical properties of the surrounding gas inside the PA cell.

By applying the continuity conditions for temperature and heat flux at the solid-solid and solid-gas interfaces, the theoretical PA response was simulated. The effective thermal conductivity of the porous layer was then determined as a fitting parameter by matching the experimental amplitude-frequency curves, using the bending-frequency position and the curve slopes as primary fitting criteria, as described in detail elsewhere [17].

Fig. 5 presents a typical experimental amplitude-frequency dependence alongside theoretical curves simulated for a range of effective thermal conductivity

values for 19.1 μm pSi samples with 75% of porosity. As demonstrated, the theoretical PA response is highly sensitive to the thermal properties of the porous layer, particularly in the mid-frequency range. By minimizing the deviation between the experimental data points and the analytical model, the precise value of the effective thermal conductivity can be unambiguously determined (e.g., 0.6 $\text{W}/(\text{m}\cdot\text{K})$) for the sample shown in Fig. 5.

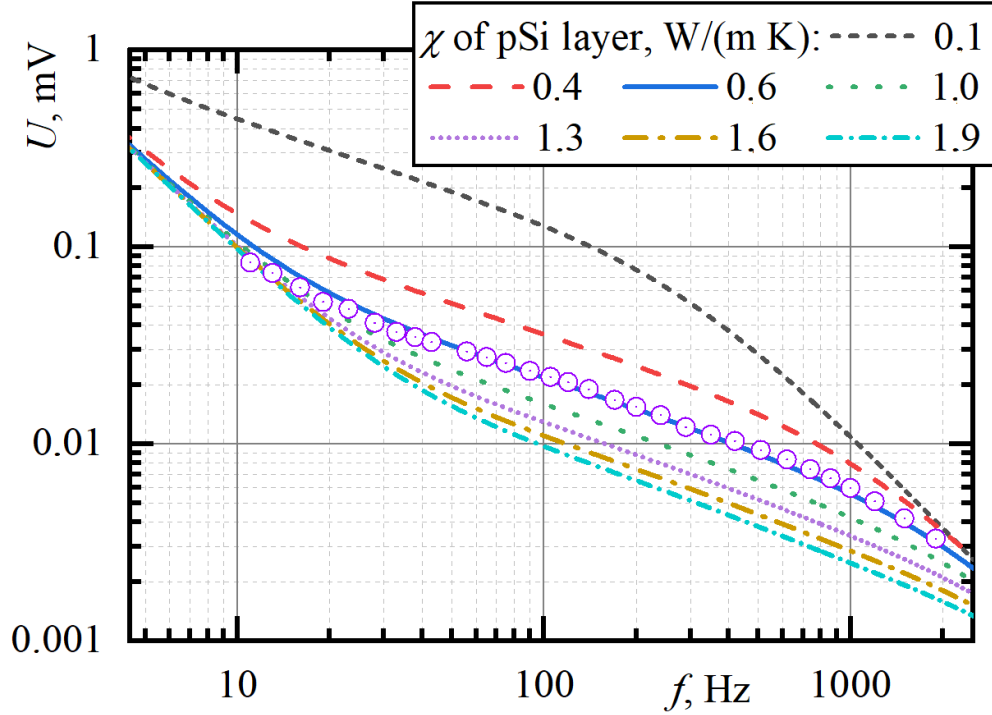


Fig.5. Experimental amplitude-frequency dependence of the photoacoustic signal (symbols) and theoretical curves (lines) simulated for various values of the effective thermal conductivity (χ) of the 19.1 μm 75% porous silicon layer.

2.3. Molecular Dynamics Simulations

All simulations were performed using the equilibrium molecular dynamics in LAMMPS package [18]. The initial model consisted of a single-crystalline silicon supercell containing $12 \times 12 \times 12$ unit cells, corresponding to 13824 atoms in the pristine configuration. Periodic boundary conditions were applied in all directions. Porosity was introduced by removing atoms within a single spherical region located at the center of the simulation box. The sphere's radius was adjusted to achieve the desired porosity. Interatomic interactions were described using a modified Stillinger-Weber potential [19]. The equations of motion were integrated using the velocity-Verlet algorithm with a time step of 1 fs.

Before dynamical simulations, all structures were subjected to energy minimization using the conjugate-gradient method to remove unfavorable atomic configurations. The modeled structures were then annealed at 1000 K for 100 ps within

the isothermal-isobaric (NPT) ensemble using a Nosé-Hoover thermostat and barostat. This annealing procedure was found to be essential for stabilizing the porous structures. In particular, annealing at lower temperatures led to unstable thermal behavior during subsequent thermal conductivity calculations, characterized by an uncontrolled increase in the system temperature. After annealing, the systems were cooled down to the target temperature and equilibrated for an additional 100 ps in the NPT ensemble.

Following equilibration, production runs were performed in the microcanonical (NVE) ensemble. Thermal conductivity was calculated using the Green-Kubo formalism [20], based on the time integration of the heat current autocorrelation function (HCACF). The heat flux was sampled every 50 timesteps, and the autocorrelation function was computed over a correlation length of 10000 steps. The total duration of each production run corresponded to $5 \cdot 10^5$ timesteps. To improve statistical accuracy, ten independent simulations with different initial velocity distributions (generated according to the Maxwell-Boltzmann distribution) were performed for each temperature. The reported thermal conductivity values were obtained by averaging these independent runs.

2.4. Physics-Informed Neural Networks Calculation

To compute the thermal conductivity of porous silicon structures using PINNs, we adopted the methodology proposed in [21, 22]. The input data consisted of a two-valued matrix $\chi(x, y)$ representing the two-dimensional spatial distribution of thermal conductivity within the porous medium. The convolutional encoder-decoder neural network was designed to predict the temperature field $T(x, y)$ and the heat flux components field $Q_x(x, y)$ i $Q_y(x, y)$. During training, a temperature gradient was imposed between the left and right boundaries along the x -direction. The optimization procedure minimized the physics-informed loss function:

$$\Omega = \lambda_1 \Omega_F + \lambda_1 \Omega_{PDE} + \lambda_3 \Omega_{DBC} + \lambda_4 \Omega_{NBC}, \quad (3)$$

where Ω_F corresponds to the residual of Fourier's law

$$\Omega_F = \frac{1}{n} \left\| \hat{\vec{Q}} + \hat{\chi} \vec{\nabla} \hat{T} \right\|_2^2, \quad (4)$$

Ω_{PDE} represents the steady-state heat equation residual in the absence of internal heat sources

$$\Omega_{PDE} = \frac{1}{n} \left\| \vec{\nabla} \hat{Q} \right\|_2^2, \quad (5)$$

Ω_{DBC} accounts for the Dirichlet boundary conditions applied to the boundaries normal to the x-direction

$$\Omega_{DBC} = \left(\frac{1}{n_l} \left\| \hat{T} \Big|_{x=x_{\min}} - T_1 \right\|_2^2 + \frac{1}{n_r} \left\| \hat{T} \Big|_{x=x_{\max}} - T_2 \right\|_2^2 \right), \quad (6)$$

and Ω_{NBC} accounts for the Neumann boundary conditions imposed on the boundaries normal to the y-direction.

$$\Omega_{NBC} = \left(\frac{1}{n_t + n_b} \left\| \hat{Q}_y \Big|_{y=y_{\min}, y_{\max}} \right\|_2^2 \right), \quad (7)$$

where, $\lambda_1, \lambda_2, \lambda_3$ and λ_4 denote the weighting coefficients associated with the physics-informed loss terms; n is the total number of uniform grid points; and n_l, n_r, n_t , and n_b represent the numbers of grid points located on the left, right, top, and bottom boundaries, respectively.

The computations were performed using 128×128 matrices, with the weighting coefficients set to $\lambda_1 = 1, \lambda_2 = 1, \lambda_3 = 10$ and $\lambda_4 = 10$.

The initial matrix χ obtained thermal conductivity values corresponding to the silicon matrix phase (χ_{Si}) and the air pore phase (χ_{Air}). The values of χ_{Si} at different temperatures were selected according to [23], whereas the values of χ_{Air} were taken from [24]. The spatial distribution of thermal conductivity for the porous medium was generated using a custom implementation of the Quartet Structure Generation Set (QSGS) algorithm [25, 26]. During structure generation, pore growth proceeded stochastically from randomly distributed seeds. The probability of transformation of a solid cell into a pore depended on the number of neighboring pores in both axial and diagonal directions.

In addition to the primary stochastic growth mechanism, the algorithm incorporated morphological stabilization procedures to ensure physically realistic structures. Small isolated regions of the solid phase were automatically removed, followed by compensatory adjustments to preserve the target porosity. The connectivity of the solid phase was treated separately. When multiple disconnected solid clusters

formed, they were iteratively merged into a single continuous network through local boundary expansion. This procedure preserved the sample's overall morphology while ensuring the formation of a continuous, load-bearing solid framework. Porosity was controlled throughout the generation process by continuously monitoring the number of pore elements and applying compensatory corrections after each structural modification to maintain agreement between the actual and target porosity values. All compensatory operations involving pore addition or removal were performed adaptively and locally to preserve morphological integrity. New pores were preferentially introduced adjacent to existing pores, whereas pore removal was applied in the most isolated regions. This approach prevented excessive structural uniformity while preserving the natural texture of the porous medium.

For each selected temperature and the corresponding $\chi_{\text{Si}}/\chi_{\text{Air}}$ ratio, a PINN was trained independently using a dataset of 16,384 samples generated for different porosity levels. The boundary temperatures, T_1 and T_2 , were set to 0.5 K above and below the temperature at which the material properties were defined, respectively. Fig. 6 illustrates a typical example of the initial structure together with the temperature and heat flux fields predicted by the trained networks.

For each sample (input χ matrix), the effective thermal conductivity is computed as an energy-weighted spatial average:

$$\chi_{\text{eff}} = \frac{\langle \hat{\chi} |\vec{\nabla} \hat{T}|^2 \rangle}{\langle |\vec{\nabla} \hat{T}|^2 \rangle}, \quad (8)$$

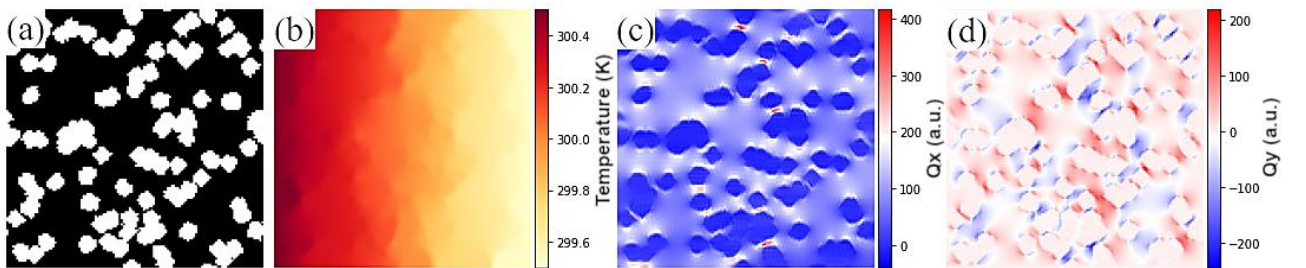


Fig.6. Initial thermal conductivity distribution matrix (a) and the corresponding PINN-predicted distribution of temperature (b) and heat flux components Q_x (c) and Q_y (d). The images correspond to a structure with a porosity of 0.3 at $T = 300$ K.

To determine thermal conductivity values at specific temperatures and porosities, a set of 1,024 matrices was generated. Each matrix was processed using a pre-trained model to estimate its corresponding parameters. The final value for a given medium configuration was obtained by averaging the individual results.

3. Results and Discussion

The thermal conductivity values of pSi layers obtained using different methodologies (experimental measurements, MD calculation, and PINN-based modeling) are summarized in Fig. 7. The figure also includes experimental data reported by various authors [4, 27, 36–45, 28, 46–50, 29–35], classified according to the conductivity type and carrier concentration of the bulk crystalline silicon used for pSi fabrication.

Notably, excellent agreement is observed between the experimental results obtained in this study, the PINN simulations, and literature data for p -type Si (with the sole exception of [28]), n -type Si, and part of the p^+ -Si dataset. In contrast, the MD simulation results yield slightly lower thermal conductivity values for $p < 0.5$, which are generally consistent with those reported for n^+ and certain p^+ samples. It should be noted that the thermal conductivity of the silicon matrix typically decreases upon transitioning from moderately to heavily doped regimes [51, 52], with the magnitude of this effect depending on the dopant species [51]. However, at a carrier concentration of approximately 10^{18} cm^{-3} (corresponding to p^+ -Si:B with a resistivity of $10 \text{ m}\Omega\cdot\text{cm}$), the reduction in matrix thermal conductivity is approximately 20%. This relatively small change cannot account for the several-fold decrease in thermal conductivity observed for p^+ -pSi at porosities of $p = 0.2\text{--}0.4$ (see Fig. 7).

According to the percolation model [4, 33, 49]:

$$\chi = (1 - p)g_0\chi_{\text{Si}}^{\text{eff}}, \quad (9)$$

where g_0 denotes the percolation strength, which characterizes the fraction of the solid phase that is continuously interconnected and directly contributes to heat transport. This parameter depends on the physical dimensions of the nanostructures, the chemical state of the surface, and the degree of structural order within the silicon matrix. In contrast, the Looyenga model, which is frequently used to describe porous silicon within the framework of the effective medium approximation [4, 28, 30, 34, 53], is given by:

$$g_0 = (1 - p)^2, \quad (10)$$

However, experimental studies have shown that the exponent for real samples may deviate from 2 and depend on the conductivity type [28]. Consequently, the generalized expression for the thermal conductivity of porous silicon can be written as:

$$\chi = \chi_{\text{Si}}^{\text{eff}} (1 - p)^{1+\alpha}, \quad (11)$$

where χ is determined, in particular, by phonon scattering processes, and α reflects the degree of interconnectivity of the silicon skeleton.

Table 1 summarizes the parameters obtained by fitting the data in Fig. 2, including both experimental results and various computational estimates, using Eq. (11). As the data indicate, the pSi thermal properties depend strongly on the carrier concentration of the initial crystal rather than on the conductivity type. In lightly doped samples, an isotropic sponge-like structure predominantly forms. The observed percolation exponent, which exceeds the value predicted by the Looyenga model, indicates a highly tortuous, labyrinth-like heat conduction pathway and a relatively rapid loss of skeletal connectivity. However, these structures often contain large crystallites (50 nm or larger), which do not induce strong phonon scattering; consequently, the thermal conductivity of the solid phase remains high, approaching that of crystalline silicon.

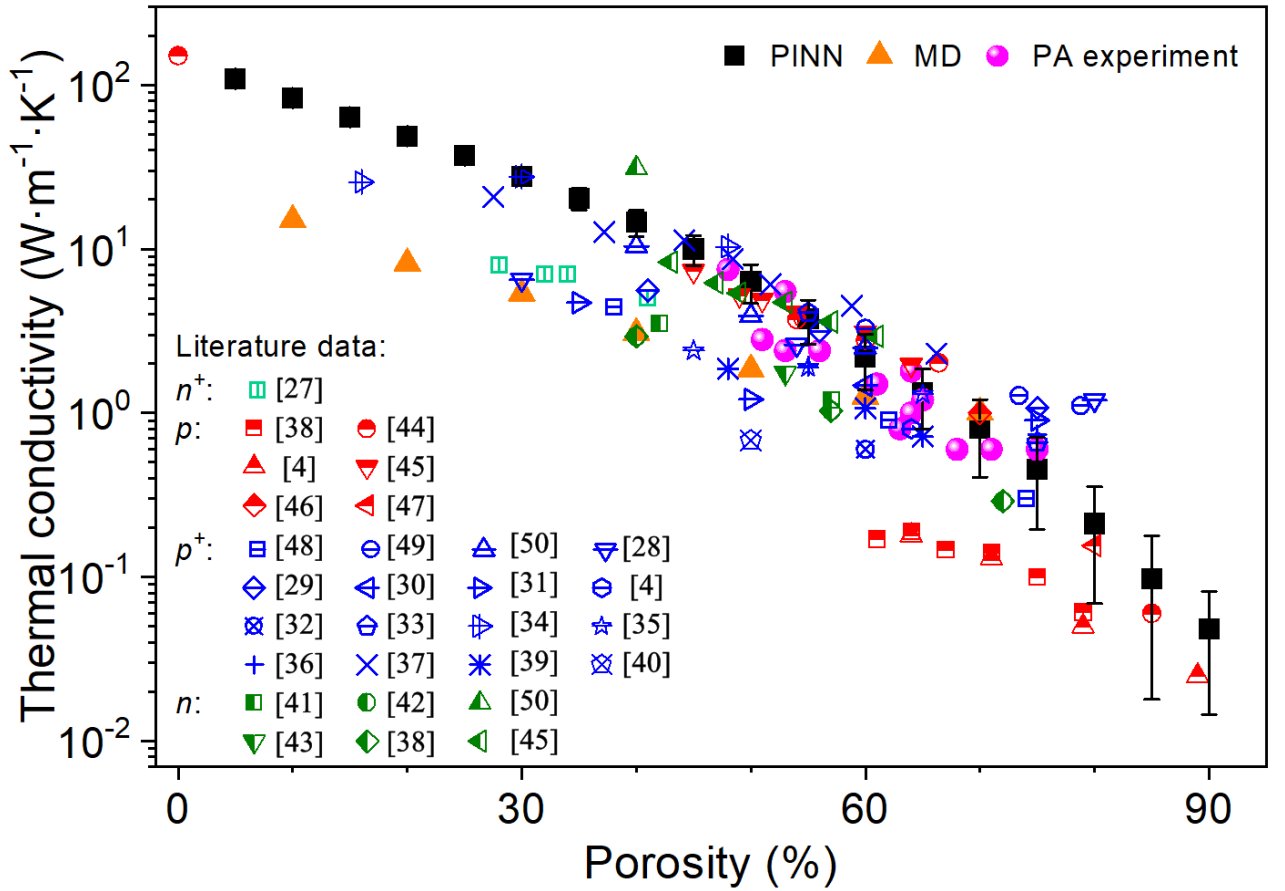


Fig.7. Effective thermal conductivity of pSi as a function of porosity. The data points represent both the results obtained in this work (filled symbols) and those reported in the literature by other authors.

Table 1. Fitting results for experimental and calculated thermal conductivity values of porous silicon according to Eq. (11).

Source of porous silicon	$\chi_{\text{Si}}^{\text{eff}}$, W/m K	α
p-Si	40±7	2.8±0.6
n-Si	70±15	3.2±1
p ⁺ -Si	22±4	1.6±0.3
n ⁺ -Si	18±2	1.4±0.3
PINN	109±2	2.9±0.1
MD	14±1	1.5±0.3

In contrast, heavily doped samples frequently exhibit a mesoporous structure with columnar anisotropy [4]. In particular, this morphology was clearly confirmed by SEM analysis of the investigated samples (see Fig. 3). These columns act as thermal highways with low tortuosity, ensuring high percolation strength even at substantial porosity levels. At the same time, the column wall dimensions are often smaller than the phonon mean free path in silicon (~43 nm), which significantly reduces the intrinsic thermal conductivity of the skeletal material. Notably, p^+ samples exhibit considerable scatter in the results (see Fig. 7), suggesting that isotropic structures similar to those observed in lightly doped systems can also form in heavily doped regimes.

Interestingly, the characteristics of the MD-derived results (see Table 1) closely resemble those of heavily doped samples, whereas the PINN results show greater similarity to moderately doped specimens. In the MD simulations, as noted previously, porosity was introduced by removing atoms within a single spherical region at the center of the simulation box. This geometric configuration enables relatively straight heat flux pathways and ensures high percolation strength. At the same time, the explicit treatment of atomic trajectories naturally captures phonon confinement effects.

In contrast, the neural networks were trained on images of porous structures exhibiting the stochastic morphology typical of lightly and moderately doped silicon. Furthermore, this approach accounts for phonon confinement in a less pronounced manner, resulting in thermal conductivity values that remain closer to those of the bulk material in n- and p-type samples.

Thermal conductivity distributions were also modeled for structures exhibiting columnar pore anisotropy, as shown in Fig. 8. For these structures,

the application of the PINN approach yielded a percolation exponent of $\alpha = 2.08 \pm 0.05$. This value is lower than that obtained for structures with stochastic pore distributions (see Table 1), thereby supporting the aforementioned assumptions.

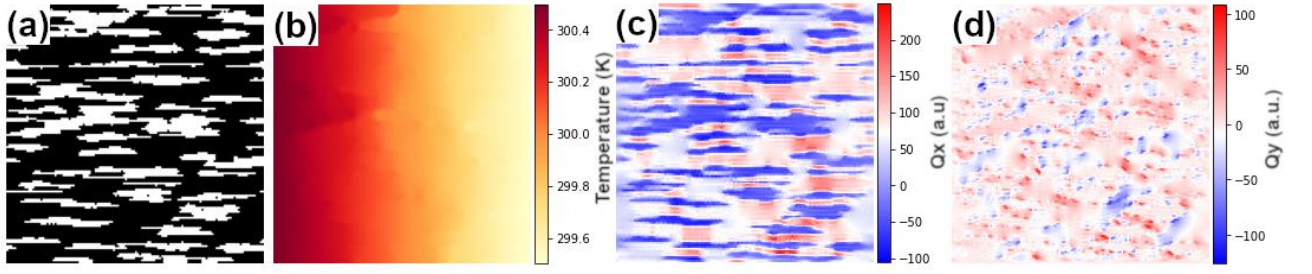


Fig.8. Initial thermal conductivity distribution matrices (a) and the corresponding PINN-predicted distributions of temperature (b) and heat flux components Q_x (c) and Q_y (d) for structure with columnar anisotropy and porosity of 0.3 at $T = 300$ K.

When porous silicon is employed as a thermal insulation material, knowledge of the temperature dependence of its thermal conductivity above room temperature is of critical importance. However, to the best of our knowledge, most existing studies have investigated $\chi(T)$ over substantially lower temperature ranges, typically up to 20 K [54], 300 K [4, 55], or, at most, 350 K [56, 57]. To date, only Kojda et al. [42] have reported thermal conductivity data for pSi over a temperature range extending to 800 K, which is particularly relevant for practical applications.

In the present work, PINNs were employed to estimate the thermal conductivity in the 300–900 K range. Fig. 9a presents the calculated temperature dependencies for two porosity values together with the experimental results. A high degree of agreement is observed, confirming the applicability of the PINN approach to this problem.

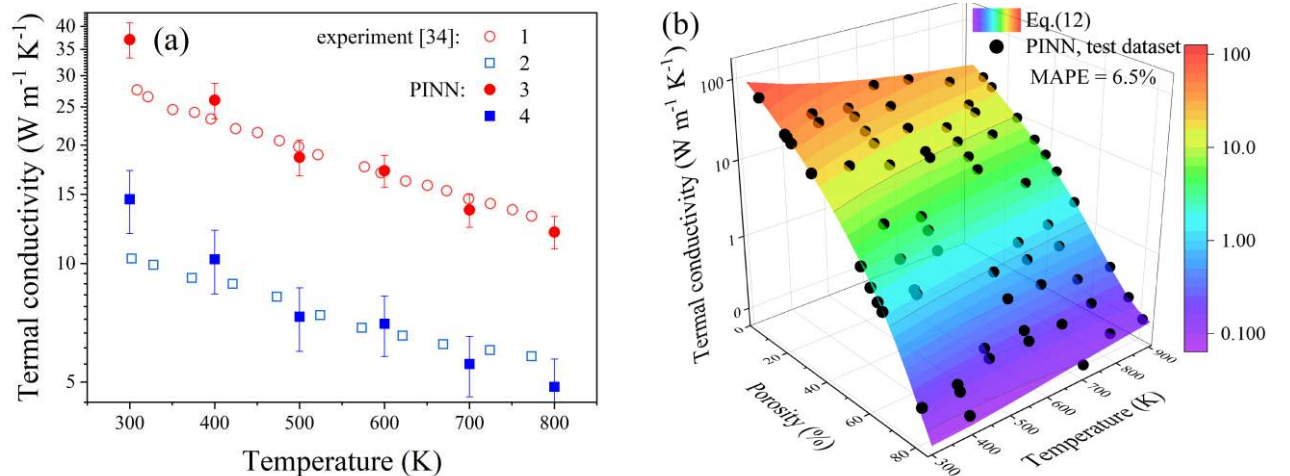


Fig.9. (a) Temperature dependence of the thermal conductivity of pSi, measured experimentally [42] (1, 2) and calculated using PINNs (3, 4). Porosity p (%): 30 (1, 3), 48 (2), and 40 (4). (b) Thermal conductivity of pSi as a function of temperature and

porosity, calculated according to Eq. (12) (surface), together with test dataset points obtained using PINNs.

The obtained thermal conductivity values were used to derive a generalized expression for the $\chi(p, T)$ dependence via symbolic regression [58, 59]. The PySR package [60] was employed for this purpose. The training dataset consisted of values evaluated on a two-dimensional p – T grid, where the porosity ranged from 5% to 85% with a step of 5%, and the temperature varied from 300 K to 900 K with a step of 100 K. The test dataset included 70 values corresponding to randomly selected porosity levels. As a result, the following expression was obtained, with its calculated multidimensional surface plotted in Fig. 9b alongside the PINN test dataset points:

$$\chi(p, T) = \frac{2.95 \cdot 10^4 (1 - p)^{4.33}}{T - 70.4} + 1.28 \cdot 10^{-4} T, \quad (12)$$

The Mean Absolute Percentage Error (MAPE) of the resulting expression on the training dataset is no more than 6.5%. As can be seen, the value of α in this case is 3.33, while the first term is inversely proportional to temperature, consistent with the behavior typically observed for semiconductors and dielectrics. Interestingly, the obtained value of 70.4, which appears in the denominator, is close to the temperature corresponding to the maximum in the experimentally observed temperature dependence of the pSi thermal conductivity reported by Song and Chen [55]. We believe that expression (12) can be applied to pSi with randomly distributed pores in the 300–900 K temperature range and within porosity regimes where phonon confinement effects are not yet dominant.

4. Conclusion

In this work, a comprehensive multiscale framework was developed to investigate the thermal conductivity of porous silicon by integrating experimental gas-microphone photoacoustic measurements, atomistic molecular dynamics simulations, and continuum modeling via Physics-Informed Neural Networks. This combined approach enabled a direct correlation between nanoscale phonon mechanics, stochastic morphological features, and macroscopic heat transport. Our findings demonstrate that the developed multiscale framework successfully captures and quantitatively rationalizes how heat transport features are governed by the substrate's carrier concentration rather than its conductivity type. While it is known that doping level predetermines the structural divergence (anisotropic columnar vs. stochastic sponge-like networks), this work provides a unified physical standard. By benchmarking the boundaries of atomistic phonon confinement via MD and macroscopic percolation

pathways via PINNs, we successfully interpret the long-standing discrepancies and scatter observed across various historical datasets in literature.

The implementation of the two distinct computational methodologies proved highly complementary in capturing these diverse structural regimes. MD simulations inherently accounted for atomistic phonon confinement and boundary scattering, yielding results that align closely with the thermal behavior observed in heavily doped, highly anisotropic samples. At the continuum level, the PINN framework successfully modeled the macroscopic heat flux and complex percolation pathways within stochastic media, demonstrating excellent agreement with experimental data for lightly doped structures over a wide temperature range.

Finally, by synthesizing the computational, experimental, and literature datasets, symbolic regression was employed to derive a generalized analytical expression for the effective thermal conductivity of pSi as a function of both porosity and temperature. This unified model provides reliable predictions across a broad porosity range (5%–85%) and at elevated temperatures (300 K–900 K), achieving a MAPE of less than 6.5%. Ultimately, this multiscale approach not only clarifies existing discrepancies in reported pSi thermal properties but also delivers a robust, computationally efficient predictive tool for the design and optimization of advanced porous silicon-based thermal insulation and thermoelectric devices.

Acknowledgements

During the preparation of this work, the authors used Gemini (Google) to assist with language editing and text refinement. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the published article.

Funding

The work was supported by the National Research Foundation of Ukraine (project No. 2023.03/0252).

Author Contributions

Conceptualization: all authors; sample preparation: P.L., L.C., and V.S.; investigation (general characterization and structural analysis): V.S. and M.B.; photoacoustic measurements, data curation, and interpretation: P.L. and L.C.; molecular dynamics simulations, software, and formal analysis: V.K.; PINN modeling, software, and formal analysis: O.O.; original draft preparation, review, and editing: O.O., V.K., L.C., and P.L. All authors have read and agreed to the published version of the manuscript.

Data Availability

All data generated or analyzed during this study are included in this published article.

Declarations

Ethical approval not applicable.

Competing Interests

The authors declare no competing interests

References

1. Canham L (2015) Handbook of Porous Silicon | Leigh Canham | Springer
2. Cullis AG, Canham LT, Calcott PDJ (1997) The structural and luminescence properties of porous silicon. *J Appl Phys* 82:909–965. <https://doi.org/10.1063/1.366536>
3. Dubyk K, Chepela L, Lishchuk P, et al (2019) Features of photothermal transformation in porous silicon based multilayered structures. *Appl Phys Lett* 115:021902. <https://doi.org/10.1063/1.5099010>
4. Gesele G, Linsmeier J, Drach V, et al (1997) Temperature-dependent thermal conductivity of porous silicon. *J Phys D Appl Phys* 30:2911–2916. <https://doi.org/10.1088/0022-3727/30/21/001>
5. Chepela L, Lishchuk P, Nkenfack IM, et al (2025) Peculiarities in thermal transport of nanostructured silicon arrays with different morphology. *Sci Rep* 15:31482. <https://doi.org/10.1038/s41598-025-13379-4>
6. Yang L, Huh D, Ning R, et al (2021) High thermoelectric figure of merit of porous Si nanowires from 300 to 700 K. *Nat Commun* 12:3926. <https://doi.org/10.1038/s41467-021-24208-3>
7. Lishchuk P, Vashchuk A, Rogalsky S, et al (2023) Thermal transport properties of porous silicon filled by ionic liquid nanocomposite system. *Sci Rep* 13:5889. <https://doi.org/10.1038/s41598-023-32834-8>
8. Gautier G, Leduc P (2014) Porous silicon for electrical isolation in radio frequency devices: A review. *Appl Phys Rev* 1:011101. <https://doi.org/10.1063/1.4833575>
9. Thakur M, Sinsabaugh SL, Isaacson MJ, et al (2012) Inexpensive method for producing macroporous silicon particulates (MPSPs) with pyrolyzed polyacrylonitrile for lithium ion batteries. *Sci Rep* 2:795. <https://doi.org/10.1038/srep00795>
10. Pacholski C (2013) Photonic crystal sensors based on porous silicon. *Sensors (Switzerland)* 13:4694–4713. <https://doi.org/10.3390/s130404694>
11. Lehmann V (2002) Electrochemistry of Silicon. Wiley

12. Isaiev M, Mankovska Y, Kuryliuk V, Lacroix D (2023) Thermal transport properties of nanoporous silicon with significant specific surface area. *Appl Phys Lett* 122:. <https://doi.org/10.1063/5.0148434>
13. Volz SG, Chen G (1999) Molecular dynamics simulation of thermal conductivity of silicon nanowires. *Appl Phys Lett* 75:2056–2058. <https://doi.org/10.1063/1.124914>
14. Kuryliuk V V., Olikh OY (2026) Thermal conductivity of nanoporous silicon: Molecular dynamics simulations and machine learning prediction. *Low Temp Phys* 52:50–59. <https://doi.org/10.1063/10.0042162>
15. Chepela L, Lishchuk P, Shevchenko V, et al (2022) Fabrication and Photoacoustic Characterization of Multilayered Structures Based on Porous Silicon. In: 2022 IEEE 41st International Conference on Electronics and Nanotechnology (ELNANO). IEEE, pp 178–181 <https://doi.org/10.1109/ELNANO54667.2022.9927023>
16. Rosencwaig A, Gersho A (1976) Theory of the photoacoustic effect with solids. *J Appl Phys* 47:64–69. <https://doi.org/10.1063/1.322296>
17. Lishchuk P, Isaiev M, Osminkina L, et al (2019) Photoacoustic characterization of nanowire arrays formed by metal-assisted chemical etching of crystalline silicon substrates with different doping level. *Phys E Low-dimensional Syst Nanostructures* 107:131–136. <https://doi.org/10.1016/j.physe.2018.11.016>
18. Thompson AP, Aktulga HM, Berger R, et al (2022) LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Comput Phys Commun* 271:108171. <https://doi.org/10.1016/j.cpc.2021.108171>
19. Zi Jian, Zhang Kaiming, Xie Xide (1990) Modification of Stillinger-Weber potentials for Si and Ge. *Phys Rev B* 41:12915–12918. <https://doi.org/10.1103/PhysRevB.41.12915>
20. Isaiev M, Kyrychenko N, Kuryliuk V, Lacroix D (2024) Features of phonon scattering by a spherical pore: Molecular dynamics insight. *Appl Phys Lett* 124:. <https://doi.org/10.1063/5.0200817>
21. Xu J, Wei H, Bao H (2023) Physics-informed neural networks for studying heat transfer in porous media. *Int J Heat Mass Transf* 217:124671. <https://doi.org/10.1016/j.ijheatmasstransfer.2023.124671>
22. Zhu Y, Zabaras N, Koutsourelakis P-S, Perdikaris P (2019) Physics-constrained deep learning for high-dimensional surrogate modeling and uncertainty quantification without labeled data. *J Comput Phys* 394:56–81. <https://doi.org/10.1016/j.jcp.2019.05.024>
23. Ho CY, Powell RW, Liley PE (1972) Thermal Conductivity of the Elements. *J Phys Chem Ref Data* 1:279–421. <https://doi.org/10.1063/1.3253100>
24. Air Properties - Thermal Conductivity vs. Temperature and Pressure Charts and Calculator. <https://www.engineeringtoolbox.com/air-properties-viscosity->

25. Wang M, Pan N, Wang J, Chen S (2007) Mesoscopic simulations of phase distribution effects on the effective thermal conductivity of microgranular porous media. *J Colloid Interface Sci* 311:562–570. <https://doi.org/10.1016/j.jcis.2007.03.038>
26. Wang M, Wang J, Pan N, Chen S (2007) Mesoscopic predictions of the effective thermal conductivity for microscale random porous media. *Phys Rev E* 75:036702. <https://doi.org/10.1103/PhysRevE.75.036702>
27. Melhem A, De Sousa Meneses D, Andreazza-Vignolles C, et al (2015) Structural, Optical, and Thermal Analysis of n-Type Mesoporous Silicon Prepared by Electrochemical Etching. *J Phys Chem C* 119:21443–21451. <https://doi.org/10.1021/acs.jpcc.5b04984>
28. Lettieri S, Bernini U, Massera E, Maddalena P (2005) Optical investigations on thermal conductivity in n- and p-type porous silicon. *Phys status solidi* 2:3414–3418. <https://doi.org/10.1002/pssc.200461194>
29. Boarino L, Monticone E, Amato G, et al (1999) Design and fabrication of metal bolometers on high porosity silicon layers. *Microelectronics J* 30:1149–1154. [https://doi.org/10.1016/S0026-2692\(99\)00078-6](https://doi.org/10.1016/S0026-2692(99)00078-6)
30. Srinivasan R, Jayachandran M, Ramachandran K (2007) Photoacoustic studies on optical and thermal properties of p-type and n-type nanostructured porous silicon for (100) and (111) orientations. *Cryst Res Technol* 42:266–274. <https://doi.org/10.1002/crat.200610811>
31. Shinoda H, Nakajima T, Ueno K, Koshida N (1999) Thermally induced ultrasonic emission from porous silicon. *Nature* 400:853–855. <https://doi.org/10.1038/23664>
32. Obraztsov AN, Okushi H, Watanabe H, Timoshenko VY (1997) Optical Absorption in Porous Silicon Studied by Photoacoustic Spectroscopy. *Phys status solidi* 203:565–569. [https://doi.org/10.1002/1521-3951\(199710\)203:2<565::AID-PSSB565>3.0.CO;2-G](https://doi.org/10.1002/1521-3951(199710)203:2<565::AID-PSSB565>3.0.CO;2-G)
33. Lysenko V, Perichon S, Remaki B, et al (1999) Thermal conductivity of thick meso-porous silicon layers by micro-Raman scattering. *J Appl Phys* 86:6841. <https://doi.org/10.1063/1.371760>
34. Fang Z, Hu M, Zhang W, et al (2008) Thermal conductivity and nanoindentation hardness of as-prepared and oxidized porous silicon layers. *J Mater Sci Mater Electron* 19:1128–1134. <https://doi.org/10.1007/s10854-007-9485-0>
35. Benedetto G, Boarino L, Spagnolo R (1997) Evaluation of thermal conductivity of porous silicon layers by a photoacoustic method. *Appl Phys A Mater Sci Process* 64:155–159. <https://doi.org/10.1007/s003390050457>
36. Gomès S, David L, Lysenko V, et al (2007) Application of scanning thermal microscopy for thermal conductivity measurements on meso-porous silicon thin films. *J Phys D Appl Phys* 40:6677–6683. <https://doi.org/10.1088/0022->

37. Newby PJ, Canut B, Bluet J-M, et al (2013) Amorphization and reduction of thermal conductivity in porous silicon by irradiation with swift heavy ions. *J Appl Phys* 114:014903. <https://doi.org/10.1063/1.4812280>
38. Lucklum F, Schwaiger A, Jakoby B (2014) Highly insulating, fully porous silicon substrates for high temperature micro-hotplates. *Sensors Actuators, A Phys* 213:35–42. <https://doi.org/10.1016/j.sna.2014.04.004>
39. Ould-Abbas A, Bouchaour M, Sari N-EC (2012) Study of Thermal Conductivity of Porous Silicon Using the Micro-Raman Method. *Open J Phys Chem* 02:1–6. <https://doi.org/10.4236/ojpc.2012.21001>
40. Andrusenko D, Isaiev M, Tytarenko A, et al (2014) Size evaluation of the fine morphological features of porous nanostructures from the perturbation of heat transfer by a pore filling agent. *Microporous Mesoporous Mater* 194:79–82. <https://doi.org/10.1016/j.micromeso.2014.03.045>
41. Piera Maccagnani, Renato Angelucci, Paolo Pozzi, et al (1999) Thick Porous Silicon Thermo-Insulating Membranes. *Sensors Mater* 11:131–147
42. Kojda D, Hofmann T, Gostkowska-Lekner N, Habicht K (2022) Characterization and modeling of the temperature-dependent thermal conductivity in sintered porous silicon-aluminum nanomaterials. *Nano Res* 15:5663–5670. <https://doi.org/10.1007/s12274-022-4123-y>
43. Dubyk K, Nychyporuk T, Lysenko V, et al (2020) Thermal properties study of silicon nanostructures by photoacoustic techniques. *J Appl Phys* 127:. <https://doi.org/10.1063/5.0007559>
44. Amato G, Angelucci R, Benedetto G, et al (2000) Thermal Characterisation of Porous Silicon Membranes. *J Porous Mater* 7:183–186. <https://doi.org/10.1023/A:1009630619528>
45. Wolf A, Brendel R (2006) Thermal conductivity of sintered porous silicon films. *Thin Solid Films* 513:385–390. <https://doi.org/10.1016/j.tsf.2006.01.073>
46. Lishchuk P, Andrusenko D, Isaiev M, et al (2015) Investigation of Thermal Transport Properties of Porous Silicon by Photoacoustic Technique. *Int J Thermophys* 36:2428–2433. <https://doi.org/10.1007/s10765-015-1849-8>
47. Nar S, Kusiak A, Mareus R, et al (2024) Investigation of mesoporous silicon thermal conductivity: Effect of nanographene insertion. *Microporous Mesoporous Mater* 366:112943. <https://doi.org/10.1016/j.micromeso.2023.112943>
48. Bernini U, Maddalena P, Massera E, Ramaglia A (1999) Thermal characterization of porous silicon via thermal wave interferometry
49. Bernini U, Lettieri S, Massera E, Rucco PA (2003) Investigation of thermal transport in n-type porous silicon by photo-acoustic technique. *Opt Lasers Eng* 39:127–140. [https://doi.org/10.1016/S0143-8166\(01\)00135-X](https://doi.org/10.1016/S0143-8166(01)00135-X)

50. Lang W, Drost A, Steiner P, Sandmaier H (1994) The Thermal Conductivity of Porous Silicon. *MRS Proc* 358:561. <https://doi.org/10.1557/PROC-358-561>
51. Lee Y, Hwang GS (2012) Mechanism of thermal conductivity suppression in doped silicon studied with nonequilibrium molecular dynamics. *Phys Rev B* 86:075202. <https://doi.org/10.1103/PhysRevB.86.075202>
52. Asheghi M, Kurabayashi K, Kasnavi R, Goodson KE (2002) Thermal conduction in doped single-crystal silicon films. *J Appl Phys* 91:5079–5088. <https://doi.org/10.1063/1.1458057>
53. Erfantalab S, Parish G, Keating A (2022) Determination of thermal conductivity, thermal diffusivity and specific heat capacity of porous silicon thin films using the 3ω method. *Int J Heat Mass Transf* 184:122346. <https://doi.org/10.1016/j.ijheatmasstransfer.2021.122346>
54. Valalaki K, Nassiopoulou AG (2014) Thermal conductivity of highly porous Si in the temperature range 4.2 to 20 K. *Nanoscale Res Lett* 9:318. <https://doi.org/10.1186/1556-276X-9-318>
55. Song D, Chen G (2004) Thermal conductivity of periodic microporous silicon films. *Appl Phys Lett* 84:687–689. <https://doi.org/10.1063/1.1642753>
56. Valalaki K, Nassiopoulou AG (2014) Porous silicon as an efficient local thermal isolation platform on the Si wafer in the temperature range 5–350k. In: 2014 11th International Workshop on Low Temperature Electronics (WOLTE). IEEE, pp 61–64
57. Valalaki K, Nassiopoulou AG (2013) Low thermal conductivity porous Si at cryogenic temperatures for cooling applications. *J Phys D Appl Phys* 46:295101. <https://doi.org/10.1088/0022-3727/46/29/295101>
58. Tonda A (2025) Review of PySR: high-performance symbolic regression in Python and Julia. *Genet Program Evolvable Mach* 26:7. <https://doi.org/10.1007/s10710-024-09503-4>
59. Angelis D, Sofos F, Karakasidis TE (2023) Artificial Intelligence in Physical Sciences: Symbolic Regression Trends and Perspectives. *Arch Comput Methods Eng* 30:3845–3865. <https://doi.org/10.1007/s11831-023-09922-z>
60. Cranmer M (2023) Interpretable Machine Learning for Science with PySR and SymbolicRegression.jl. 1–24. <https://doi.org/https://doi.org/10.48550/arXiv.2305.01582>