

Thermal Conductivity of Nanoporous Silicon: Molecular Dynamics Simulations and Machine Learning Prediction

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Abstract

The thermal conductivity of nanoporous silicon (p-Si) was investigated using equilibrium molecular dynamics simulations and machine learning techniques. Several interatomic potentials were evaluated, with the Tersoff potential selected for its stability and accuracy. Thermal conductivity values were computed over a wide range of temperatures and porosities. A algorithm was used to derive an analytical expression describing its dependence on temperature and porosity. Additionally, Random Forest and Gradient Boosting models were trained to reconstruct heat current autocorrelation functions and predict thermal conductivity, outperforming Support Vector Regression. The combined approach enables accurate, data-efficient prediction of thermal transport in porous nanostructures, supporting the design of materials for thermal management and energy conversion applications.

Keywords: *nanoporous silicon, thermal conductivity, molecular dynamics, symbolic regression, machine learning*

Introduction

In recent years, nanostructured materials have attracted significant interest for their potential in thermal insulation and heat dissipation applications [1, 2]. For instance, as 3D integration advances in micro- and nanoelectronics, there is a growing need for low thermal conductivity materials that remain compatible with CMOS processes. Furthermore, for energetically autonomous systems, the development of effective nanomaterials exhibiting high thermoelectric conversion efficiency is also crucial [3]. The thermal behavior of nanomaterials is significantly influenced by their structural dimensions and the manner in which phonons propagate through their frameworks [4]. In such materials, thermal phonons are frequently scattered at surfaces and interfaces, thereby significantly lowering overall thermal conductivity [5]. It is noteworthy that nanoporous structures have attracted significant interest due to their large specific surface area and shortened phonon mean free path, which further suppresses heat transport [6, 7].

Nanoporous silicon (p-Si), produced by electrochemical anodization of crystalline silicon, has attracted significant attention because its optical, electrical, and thermal properties can be readily tuned by adjusting the porosity. This controllability enables a wide range of potential applications

for *p*-Si in areas such as highly sensitive sensors [8], lithium-ion batteries [9], optoelectronics, micro- and nanoelectronics [10], as well as MEMS technologies [11]. It has been demonstrated that nanostructured silicon with tailored porosity exhibits thermal conductivity that is two to three orders of magnitude lower than that of bulk crystalline silicon ($\sim 140 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$) [12]. This renders it an appealing candidate for utilization in thermal sensors [13], thermal insulation and thermoelectric generators in silicon-based microsystems [14]. In order to gain deeper insight into the mechanisms of phonon transport in *p*-Si, it is crucial to undertake comprehensive thermal characterization. Furthermore, it is imperative to possess precise knowledge of the thermal behavior of this material to ensure its effective integration into practical devices.

Molecular dynamics (MD) simulations have become an indispensable tool for investigating thermal transport phenomena in nanostructured materials, providing valuable atomistic insights that are often inaccessible through experiments alone. In particular, MD methods have been extensively utilized to predict the thermal conductivity of porous silicon and analogous systems, elucidating the profound impact of nanoscale characteristics, such as pore size, shape, and distribution, on phonon scattering and heat conduction [15-18]. The integration of machine learning (ML) approaches with atomistic modelling has emerged as a promising strategy to efficiently predict and optimize the properties of complex materials by uncovering hidden structure-property relationships. Two primary approaches integrate ML with MD. The first one employs machine learning interatomic potentials in simulations, enabling the study of large-scale emergent phenomena in specific materials with accuracy close to that of *ab initio* MD [19, 20]. The second approach uses MD simulation results from a limited number of cases as input data to build and train ML models; these models are then applied to a much wider range of predictions [21, 22]. Both methods have been successfully used to assess the thermal properties of various materials [23-27], including porous structures [28]. As previous studies have shown that such integrated frameworks can significantly accelerate the design of advanced nanostructured materials for thermal management and energy conversion applications. Unfortunately, to the best of our knowledge, no similar studies have been conducted on porous silicon.

In this study, molecular dynamics and machine learning methods were employed to calculate the thermal conductivity of nanoporous silicon. A series of interatomic interaction potentials were tested to predict heat transport in silicon. The equilibrium molecular dynamics approach was used to determine the dependence of the thermal conductivity on temperature and porosity. The resulting dataset was then processed and generalized using machine learning models, allowing the thermal conductivity of *p*-Si to be estimated over a wide range of temperatures and porosities.

Methods

The thermal conductivity of the *p*-Si was calculated via equilibrium molecular dynamics (EMD). All MD simulations were performed using the LAMMPS package [29]. The EMD simulation setup considered in this paper is schematically illustrated in Fig. 1. The simulation box is a cube consisting of $L^3=10a \times 10a \times 10a$ unit cells, where a is the unit-cell lattice vector in the Si. The porosity of the structure was varied by changing the pore radius R and was calculated as $\eta = \frac{4\pi R^3}{3L^3}$.

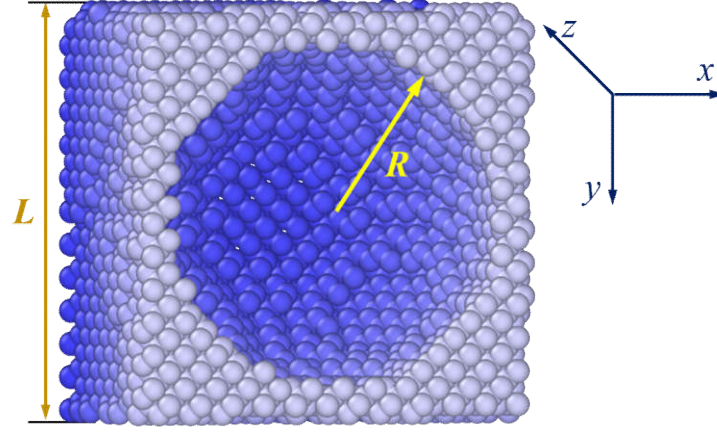


Figure 1. Schematic illustration of the EMD simulation setup: L – size of the Si supercell (cube),
 R – pore radius.

The pore was introduced as a spherical cavity by removing atoms from the silicon lattice and was placed at the center of the simulation box to ensure symmetry and minimize boundary effects. While real materials often exhibit randomly distributed pores of irregular shape, modern fabrication techniques also enable periodic porous structures [30, 31]. Furthermore, recent studies have demonstrated that the effective thermal conductivity of porous silicon is not only determined by the overall porosity but also strongly depends on the pore morphology and their spatial correlations. For a given porosity, different pore shapes (e.g., cylindrical, slit-like, or irregular) can lead to markedly different phonon scattering rates and thus to distinct thermal conductivities, often accompanied by anisotropy in heat transport [32, 33]. Moreover, interactions between neighboring pores, such as pore–pore coupling and percolation effects, have been shown to further reduce the thermal conductivity compared to isolated pores [34; 35]. In the present work, we restrict our attention to the case of spherical pores created by atom removal in molecular dynamics simulations, which provides a simplified but instructive model system. This allows us to isolate the effect of porosity itself, while future studies may extend to more complex pore geometries and correlated pore networks.

For each temperature and porosity, an initial simulation was performed in the isobaric–isothermal (NPT) ensemble to generate thermally equilibrated configurations. The system was then further equilibrated in an isochoric–isothermal (NVT) ensemble. In both the NPT and NVT simulations, the temperature was controlled using a Nosé–Hoover thermostat. The simulation time for each ensemble was 0.5 ns, and the integration of Newton’s equations of motion was carried out

using the Verlet algorithm with a time step of 1 fs. After reaching equilibrium, the system was switched to a constant-volume and constant-energy (NVE) ensemble to determine the thermal conductivity k using the Green–Kubo method. In this method k was estimated by integrating the heat current autocorrelation function (HCACF) as follows:

$$k = \frac{1}{3Vk_B T^2} \int_0^{t_c} \langle \mathbf{J}(t) \mathbf{J}(0) \rangle dt, \quad (1)$$

where V is the volume of the system, t is the time, the brackets $\langle \rangle$ is the ensemble-averaged HCACF and \mathbf{J} is the heat current vector that is defined as

$$\mathbf{J}(t) = \frac{1}{V} \left[\sum_{j=1}^N \mathbf{v}_j E_j - \sum_{\alpha=1}^2 h_{\alpha} \sum_{j=1}^{N_{\alpha}} \mathbf{v}_{\alpha j} \right] + \frac{1}{V} \left[\frac{1}{2} \sum_{j=1}^N \sum_{\substack{j=1, \\ j \neq i}}^N \mathbf{r}_{ij} (\mathbf{v}_{ij} \cdot \mathbf{F}_{ij}) \right], \quad (2)$$

Here, \mathbf{v}_j and E_j are the velocity and energy of the j -th particle; \mathbf{r}_{ij} and \mathbf{F}_{ij} denote the distance and the interaction force between the i -th and j -th particles; N is the total number of particles in the system; and h_{α} is the average partial enthalpy of component α . Obviously, that t_c value (the upper limit of the integral or the MD simulation time) must be sufficiently large for the system to reach equilibrium. In essence, the thermal conductivity k was determined as the saturation value of the $k(t_c)$ curve. To reduce statistical errors, our MD simulations were run for more than 10 ns on average, and five independent simulations were performed for each specific condition. For a structure with a given porosity, calculating the thermal conductivity on a cluster of 128 AMD EPYC cores at the same temperature typically took 10–12 hours.

The primary goal of applying Machine Learning (ML) methods was to enable the rapid estimation of the thermal conductivity of porous silicon across arbitrary values of porosity p ($0 \leq p < 1$) and temperature T . A key consideration when selecting ML approaches is the limited availability of thermal conductivity data – only a few dozen values can realistically be obtained from MD simulations within a feasible timeframe for model development. As a result, conventional ML methods that require training dataset containing tens or hundreds of thousands of samples are not suitable in this context.

As a result, two distinct approaches were used. The first approach employed Symbolic Regression (SR), an algorithm that derives a mathematical expression to describe a given dataset. Unlike conventional regression methods, which require predefined input variables and adjust numerical coefficients to achieve the best fit, SR simultaneously identifies both the structure of the equation and its parameters [36]. It uses evolutionary algorithms to uncover functional relationships and numerical coefficients between input and output variables. A key advantage of SR is its ability to produce interpretable results in the form of analytical expressions. Moreover, this method does not require large amounts of training data to achieve high predictive accuracy [36, 37].

SR was implemented in Python using the open-source PySR package [38]. Data preprocessing was limited to normalizing temperature values to 300 K. During training, the loss function was defined as the mean weighted squared error (MWSE) and was minimized:

$$\text{MWSE} = \frac{1}{N} \sum_{i=1}^N \omega_i (\hat{y}_i - y_i)^2. \quad (3)$$

Here, N represents the number of values in the training set, y_i denotes the true thermal conductivity (result of MD simulation), while \hat{y}_i indicates the predicted value; ω_i is the weighting coefficient, in this study, statistical (reciprocal) weighting was applied, meaning $\omega_i = 1 / y_i$. The use of weighting coefficients is motivated by the fact that the range of target values for thermal conductivity (TC) spans two orders of magnitude (from 1 to 226 W/mK). At the same time, the absolute errors of the values calculated using MD increase with thermal conductivity (see Fig. 3). The weighting was introduced to prevent the model from adapting primarily to large TC values (corresponding to low porosity and temperature).

In the second approach, classical algorithms – specifically Random Forest (RF), Gradient Boosting (GB), and Support Vector Regression (SVR) – were used to build models predicting the $k(t_c)$ curve. This strategy significantly increased the size of the training dataset. The input descriptor set included porosity, temperature, and simulation time. To standardize the features and target values, they were normalized to have zero mean and unit standard deviation. The models were implemented using Python's Scikit-learn toolkit. Model parameters were optimized using the Optuna framework, which employed the TPE sampler and Hyperband pruner for efficient hyperparameter selection. A 5-fold cross-validation scheme was applied during model tuning. To determine thermal conductivity, the predicted $k(t_c)$ curves were processed in the same way as those obtained from MD simulations.

The evaluation metrics used to assess forecast quality were the mean squared error (MSE), mean absolute percentage error (MAPE), and coefficient of determination (R^2), as defined in Eqs. (4)-(6).

$$\text{MSE} = \frac{1}{N} \sum_{i=1}^N (\hat{y}_i - y_i)^2, \quad (4)$$

$$\text{MAPE} = \frac{1}{N} \sum_{i=1}^N \frac{|\hat{y}_i - y_i|}{y_i} \times 100\%, \quad (5)$$

$$R^2 = 1 - \frac{\sum_{i=1}^N (\hat{y}_i - y_i)^2}{(\hat{y}_i - \bar{y})^2}, \quad (6)$$

where \bar{y} is the mean of the true values. MSE was used for model tuning, while all three metrics were applied to evaluate the prediction quality of the trained models.

Results and discussion

1. Evaluation and Selection of Interatomic Potentials. The accuracy of MD simulations strongly depends on the choice of interatomic potential. Therefore, the initial stage of this study focused on evaluating several well-known potentials based on three key criteria: (i) computational performance, which is particularly relevant for high-throughput simulations and machine learning dataset generation; (ii) agreement between simulated and experimental temperature-dependent thermal conductivity of singlecrystalline silicon; and (iii) potential stability for highly porous structures over a wide temperature range. Clearly, the latter criterion plays the most significant role in selecting an interatomic potential for calculating the thermal properties of a porous material. The tested potentials included MEAM [39], Tersoff [40], EDIP [41], Stillinger-Weber (SW) [42], modified Stillinger-Weber (SW-mod) [43], and a machine learning-based potential SNAP [44]. The results are summarized in Figures 2 and 3.

As shown in Figure 2, the EDIP potential demonstrated the highest computational performance, reaching nearly 5000 MD steps per second on a 128-core node. Tersoff, SW, and SW-mod potentials achieved approximately 3000 steps per second, while MEAM exhibited ten times lower performance than EDIP. The SNAP potential was the slowest, with only ~30 steps per second under identical simulation and hardware conditions.

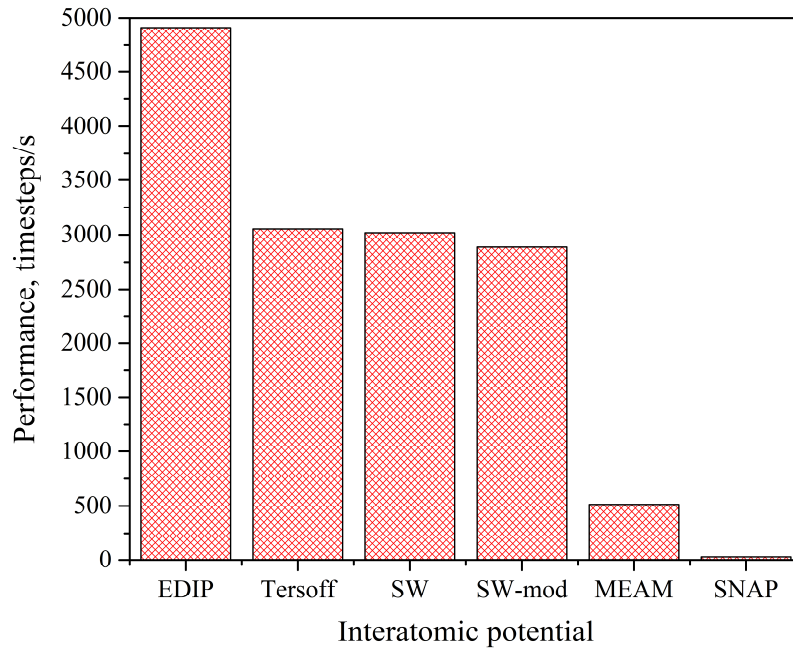


Figure 2. Comparison of the computational performance of various interatomic potentials for calculating the thermal conductivity of singlecrystalline silicon. Structure size: $10a \times 10a \times 10a$; number of cores per node: 128.

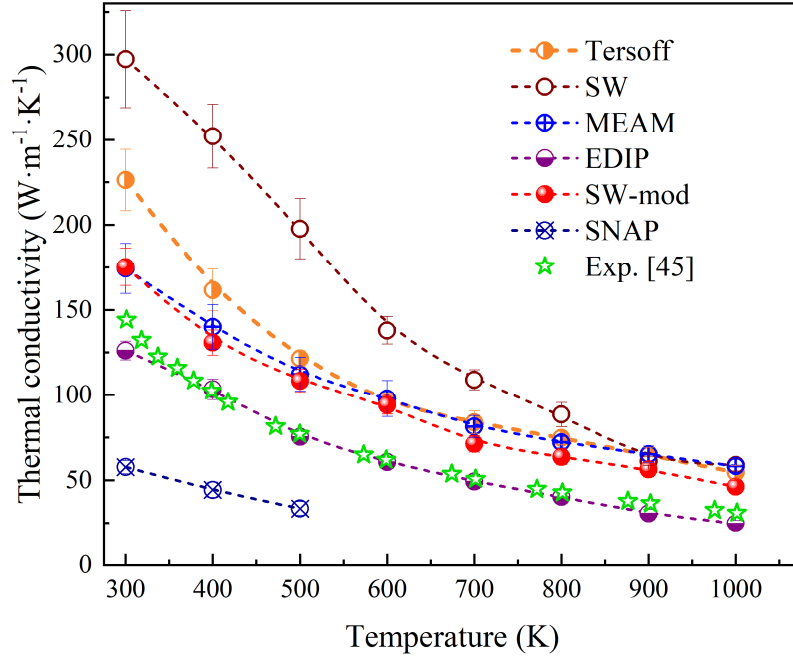


Figure 3. Calculated temperature dependence of thermal conductivity of singlecrystalline silicon using different interatomic potentials, compared with experimental data adapted from [45].

Thermal conductivity values calculated using MEAM, Tersoff, SW, and SW-mod consistently exceeded the experimental results reported in Ref. [45] across the entire temperature range, with deviations ranging from 48% to 106%. In contrast, the SNAP potential significantly underestimated the thermal conductivity, indicating inadequate parameterization for heat transport simulations. The smallest deviation between the calculated and experimental $k(T)$ dependencies was obtained using the EDIP potential. However, this should not be regarded as an inherent advantage of EDIP, since thermal conductivity calculated via MD simulations is typically higher than experimental values due to the use of idealized model structures – defect-free and mono-isotopic.

Moreover, further testing of the potentials revealed that, for highly porous structures at elevated temperatures, the porous architecture became unstable with certain potentials, leading to pore collapse and the formation of nearly amorphous configurations – see Figure 4. As shown in Table 1, similar instabilities were observed for the SW, SW-mod and EDIP potentials.

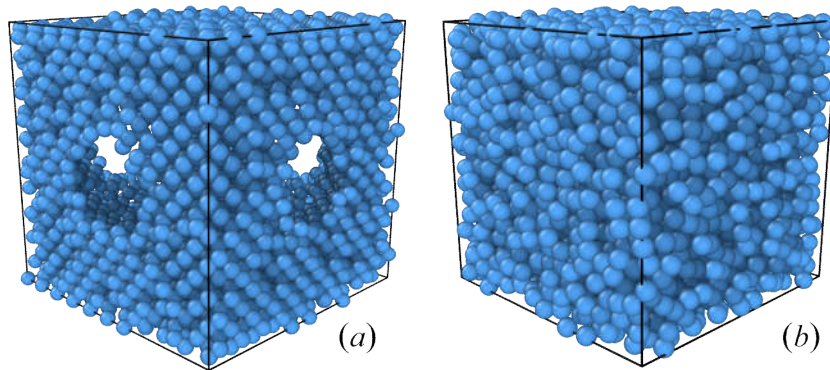


Figure 4. Atomic configurations of porous silicon with 50% porosity, obtained after structure equilibration at 800 K using Tersoff potentials (a) and EDIP (b).

Table 1. Stability of interatomic potentials in MD simulations of thermal conductivity for *p*-Si

Potential	Stability
MEAM	+
Tersoff	+
EDIP	-
Stillinger-Weber	-
modified Stillinger-Weber	-
SNAP	+

As a result, the Tersoff potential was chosen for the remainder of the study. An additional argument in favor of the Tersoff potential is the calculated temperature dependence of k , which is often approximated as follows [46]:

$$k \propto T^{-b}. \quad (7)$$

Fitting the calculated $k(T)$ for singlecrystalline Si using Eq. (7) yielded $b=1.15\pm0.03$, which is close to both the theoretical expectation ($b=1.0$ for semiconductors and dielectrics) and the experimental value (1.25 ± 0.01) [45]. For comparison, the values for other potentials are EDIP 1.36 ± 0.09 , SW 1.5 ± 0.1 , SW-mod 1.08 ± 0.05 , and MEAM 0.92 ± 0.02 .

2. Generation of Molecular Dynamics Data for Machine Learning. The next stage of the study involved generating a dataset of MD simulation results for training machine learning models aimed at predicting the thermal properties of porous silicon structures. Two competing requirements had to be balanced. On the one hand, the simulated data needed to span a wide range of porosity and temperature values and capture all key dependencies of thermal conductivity on these parameters. On the other hand, limitations in computational resources had to be considered. Therefore, MD simulations were performed to obtain temperature-dependent thermal conductivity values at several porosity levels using 100 K intervals, as well as the dependence of thermal conductivity on pore volume fraction at room temperature. Fig. 5a present selected results for the temperature and porosity dependence of thermal conductivity, calculated using the Tersoff potential.

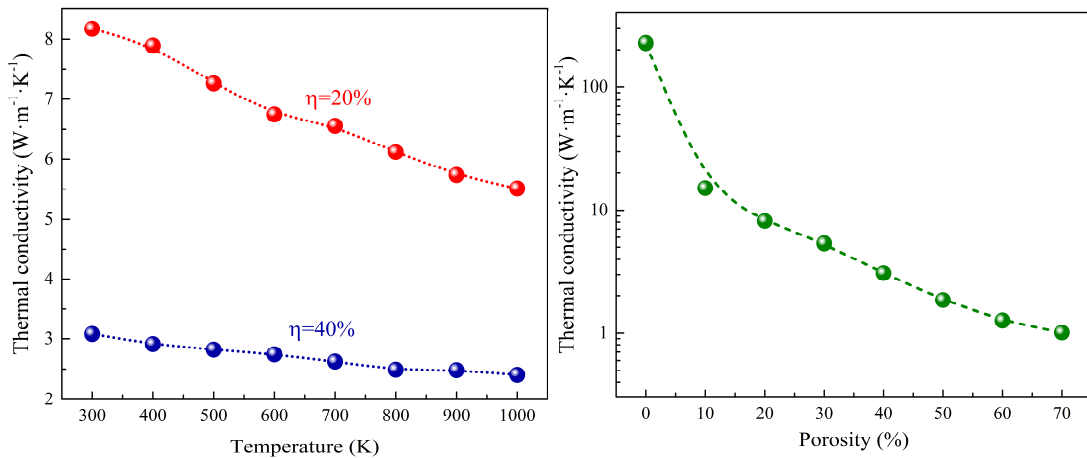


Figure 5. Dependence of thermal conductivity on temperature for *p*-Si with 20% and 40% porosity (a) and on porosity for *p*-Si at $T=300$ K porosity (b). Calculations were performed using the Tersoff interatomic potential.

It should be noted that the observed trends are consistent with literature data: thermal conductivity decreases with increasing temperature, and the form of the $k(T)$ dependence evolves as the system becomes increasingly disordered. A monotonic decrease in thermal conductivity with increasing porosity is also observed (Fig. 5b), attributed to increased phonon-boundary scattering at pore surfaces. Thus, this dependency aligns with general expectations, further supporting the validity of the performed calculations.

The presented data served as a foundation for the development and training of ML models for predicting the heat transport behavior of porous silicon. In addition, a set of p -Si thermal conductivity values was calculated to test the ML models at specific temperatures and porosities within the ranges of 300–1000 K and 0–80%, respectively. In summary, 29 thermal conductivity values (or $k(t_c)$ dependencies for classical ML algorithms) obtained from MD were used for training, and 9 for testing, corresponding to a 76:24 split.

3. Machine Learning-Based Prediction of Thermal Transport Properties in Porous Silicon.

Using the results of MD simulations with the Tersoff potential (Figs. 3, 5) and the Symbolic Regression algorithm, we derived an analytical expression describing the dependence of porous silicon's thermal conductivity on temperature and porosity. By adjusting parameters such as the population size, the maximum expression complexity, and the multiplicative coefficient penalizing complexity, we obtained a formula with a MAPE of no more than 2.89% and a median APE of 1.96% on the training set (see Fig. 6a). The resulting analytical expression is:

$$k = \left(-7.024 + \frac{7.481}{p^{0.55} + (T_n - 0.105) / (\sin[T_n / (4.486 \cdot p - 0.251)] + 27.09)} \right) \exp(-p), \quad (8)$$

where $T_n = T / 300$. For the test set, the average error is approximately 10%. Figure 6b presents the obtained $k(T, p)$ dependence within the temperature range of 300-1000 K and the porosity range of 0–80%. The corresponding MD simulation results are also shown in the figure.

As shown in Fig. 6b, the MD calculations do not fully cover the parameter space. However, in symbolic regression (SR), the key objective is to identify an analytical expression that captures the underlying patterns in the data rather than merely approximating them numerically [36, 37]. Thus, SR does not require exact reproduction of all training values; its primary goal is to recover the correct functional form. Consequently, SR can potentially reconstruct the true equation even from incomplete data, which sets it apart from the “black-box” nature of standard ML models that generalize poorly without additional input. At the same time, validation of the derived expression against known physical laws or asymptotic behavior remains crucial, since the ability to reproduce trends beyond the training domain provides strong evidence of its correctness.

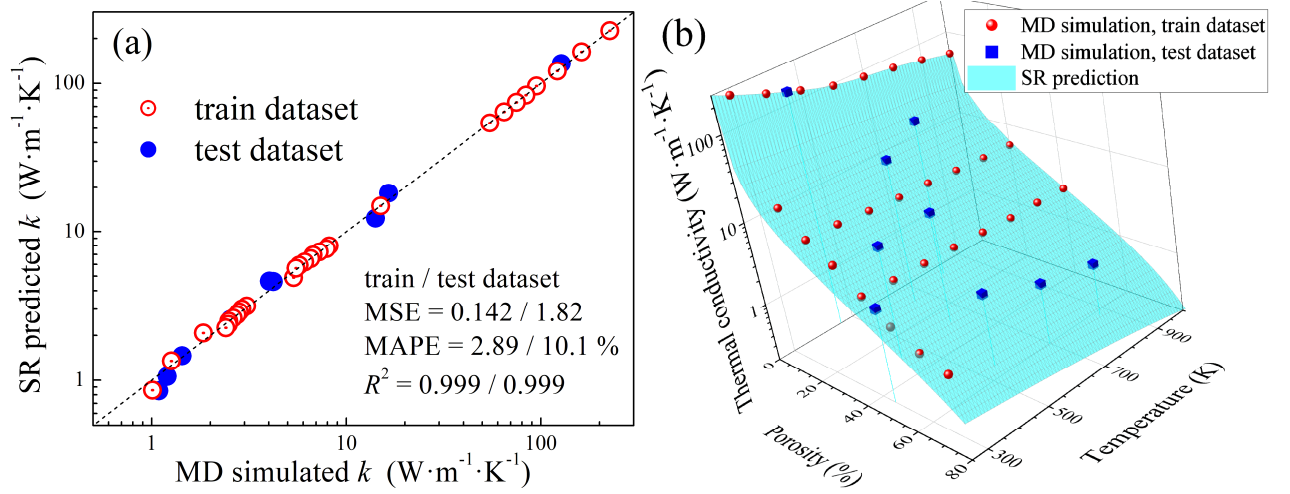


Figure 6. (a) Comparison of SR predicted k and MD calculated k (true value) for p -Si. Open and closed markers indicate training and test datasets, respectively. The black lines are the identified lines serving as the references. (b) Dependence of the thermal conductivity of porous silicon on temperature and porosity. The points represent the results of MD simulations, while the surface corresponds to Eq. (8).

Due to the limited experimental data on porous silicon, the analysis is focused on the predicted $k(T)$ and $k(p)$ dependencies. At the same time, it is more appropriate to focus on the character of these dependencies rather than on the absolute thermal conductivity values, since passivation of the pore surface by air molecules can significantly alter k , and this factor is rarely controlled in experiments.

As noted above, an increase in temperature should correspond to a decrease in thermal conductivity (see Eq. (7)), and partial amorphization should modify the $k(T)$ dependence with increasing disorder. In particular, experiments [46,47] have shown that the exponent b decreases with increasing porosity. Figure 7a summarizes the values of b obtained from various sources. Overall, the results from both MD calculations and SR predictions generally agree with physical expectations and experimental data. A slight increase in b at high porosity may indicate limitations in applying Eq. (8) for $p > 0.5$. However, the non-monotonic behavior of $b(p)$ is also observed experimentally.

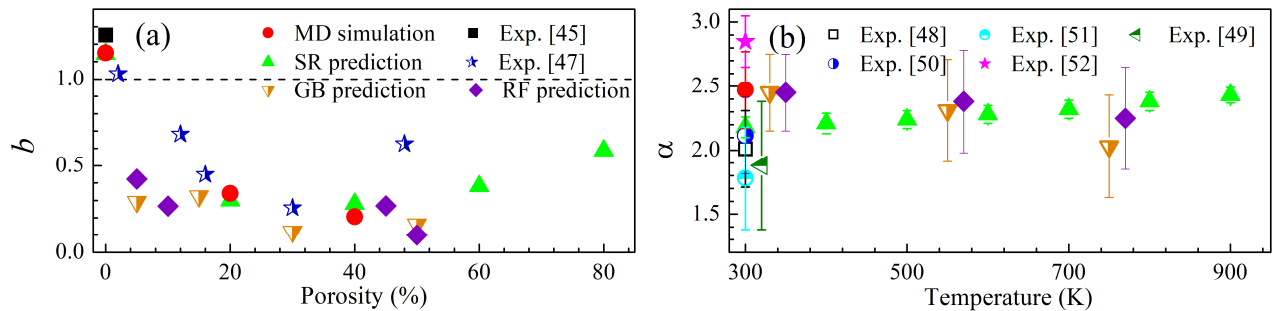


Figure 7. Degree indicators from Eqs. (7) (a) and (9) (b), obtained from MD calculations, SR prediction, and experimental data. The dotted horizontal line in panel (a) represents the theoretical expectation for semiconductors and dielectrics.

The Looyenga effective medium model is most often used [48,49] to describe the dependence of thermal conductivity on porosity. This model accounts for percolation strength and assumes the following power dependence:

$$k \propto (1-p)^\alpha. \quad (7)$$

Moreover, the value of α may depend on the type of conductivity of the semiconductor matrix [49] and is practically independent of temperature. Figure 7b presents the values of α obtained by approximating $k(p)$ dependencies from both our calculations and various experimental studies of p -type silicon. To the best of our knowledge, data for non-room temperatures are not available unfortunately. Nevertheless, the figure shows that the dependencies derived from Eq. (8) yield α values with only weak temperature dependence, and their values near room temperature agree well with experimental data, consistent with physical expectations.

The initial data for each point in Figs. 3 and 5 consisted of MD simulation results for k at 10,000 values of t_c . This dataset was used for training classical the ML models. The training results are shown in Fig. 8. It is evident that the performance metrics of SVR are lower than those of RF and GB, which demonstrate similar levels of accuracy.

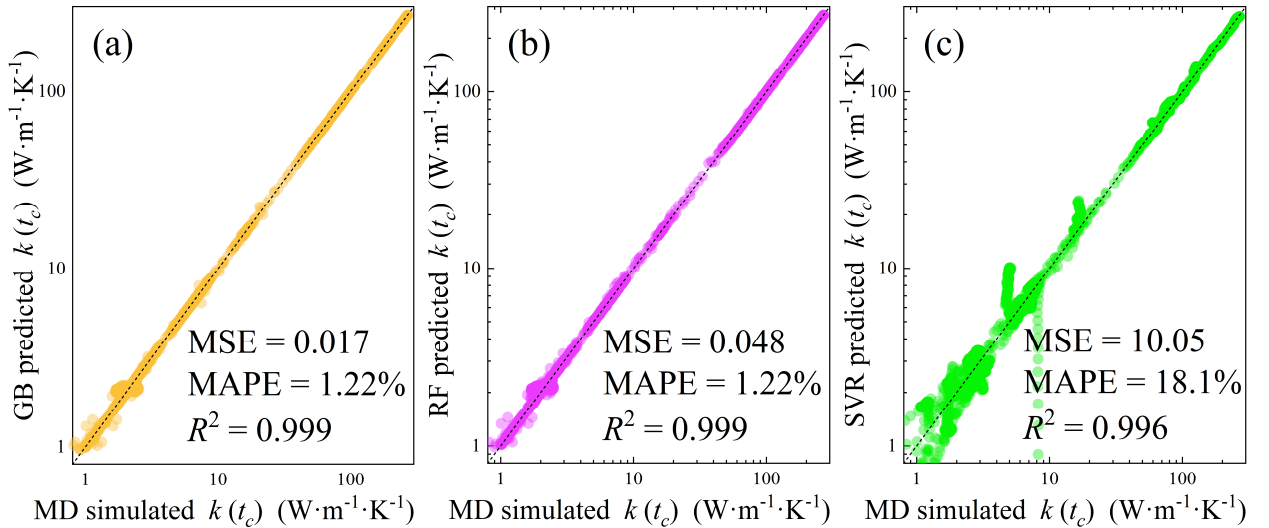


Figure 8. Comparison of k values at different t_c , calculated by MD simulations and predicted by Gradient Boosting (a), Random Forest (b), and Support Vector Regression (c) for the training dataset. The black lines indicate reference lines.

Figure 9 shows the typical $k(t_c)$ dependencies obtained from MD simulations and ML model predictions for the training (a) and test (b) datasets. It should be noted that RF and GB reproduce the training curves $k(t_c)$ with high accuracy; the deviations seen in Figures 8a and b are confined to the initial parts of the curves and do not affect the thermal conductivity values, which are determined in the saturation region. For the test set, however, both RF and GB tend to overestimate the thermal conductivity (Fig. 9b). In contrast, SVR performs considerably worse, with large discrepancies from the reference values already visible for the training set and becoming even more pronounced for the test set.

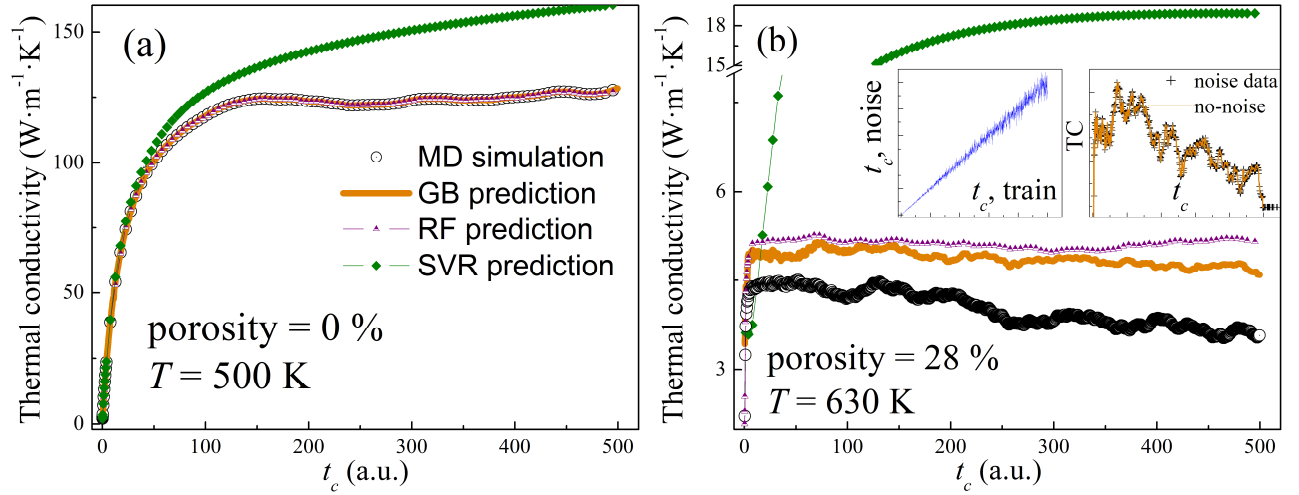


Figure 9. Dependencies of k on t_c from MD (black circles) and ML predictions for different porosity and temperature values in the training (a) and test (b) sets. The inset shows the dependence of noisy on noise-free t_c values (left) and GB predictions with noisy inputs (symbols) versus noise-free inputs (solid line) (right).

In all cases, MD calculations were performed for the same t_c values, so the training set contained only these points. To test the robustness of the models, predictions of $k(t_c)$ were also generated for perturbed data, where t_c values were multiplied by $(1 + \varepsilon)$, where ε is drawn from a normal distribution with mean 0 and standard deviation 0.05. The inset in Fig. 9a illustrates that adding noise does not alter the shape of the predicted curves. Although only GB results are shown, the same behavior was observed for the other algorithms.

Fig. 10 summarizes the thermal conductivity values extracted from the $k(t_c)$ curves for the training and test sets. Gradient Boosting provides the best accuracy on the test set (MAPE = 20.8%, median APE = 16.1%), although the errors are notably higher than for training data. Random Forest yields slightly larger deviations (MAPE = 28.3%, median APE = 23.6%), with the error increasing as k decreases (i.e., with rising temperature and/or porosity). In contrast, the poor performance of SVR, evident even on the training set, makes it unsuitable for the tasks addressed in this study.

RF and GB were also employed to predict $k(T)$ and $k(p)$ dependencies at T and p values beyond the MD simulation range (since, given the accuracy of the training curves, there was no reason to consider regions with MD results). The exponents of the power laws extracted from these predictions are summarized in Fig. 7. Similar to SR, both the trends and absolute values agree with general physical expectations, further confirming the feasibility of the proposed ML oriented approach for estimating the thermal conductivity of porous silicon.

Conclusion

This study evaluated the suitability of several interatomic potentials for calculating the thermal conductivity of porous silicon via molecular dynamics (MD) simulations and confirmed the adequacy of the Tersoff potential. Thermal conductivity was then computed over a broad range of

temperatures and porosity values. Based on these data, a Symbolic Regression algorithm was employed to derive an analytical expression describing the dependence of thermal conductivity on temperature (300-1000 K) and porosity (0–80%). Furthermore, it was demonstrated that Random Forest and Gradient Boosting algorithms can reliably estimate thermal conductivity by reconstructing the time dependence of the heat current autocorrelation function. **The realism of the ML model predictions is supported by the agreement between the predicted dependencies of thermal conductivity on temperature and porosity and the trends expected from physical models and experimental data.** In contrast, Support Vector Regression yielded significantly less accurate results and was deemed unsuitable for this task.

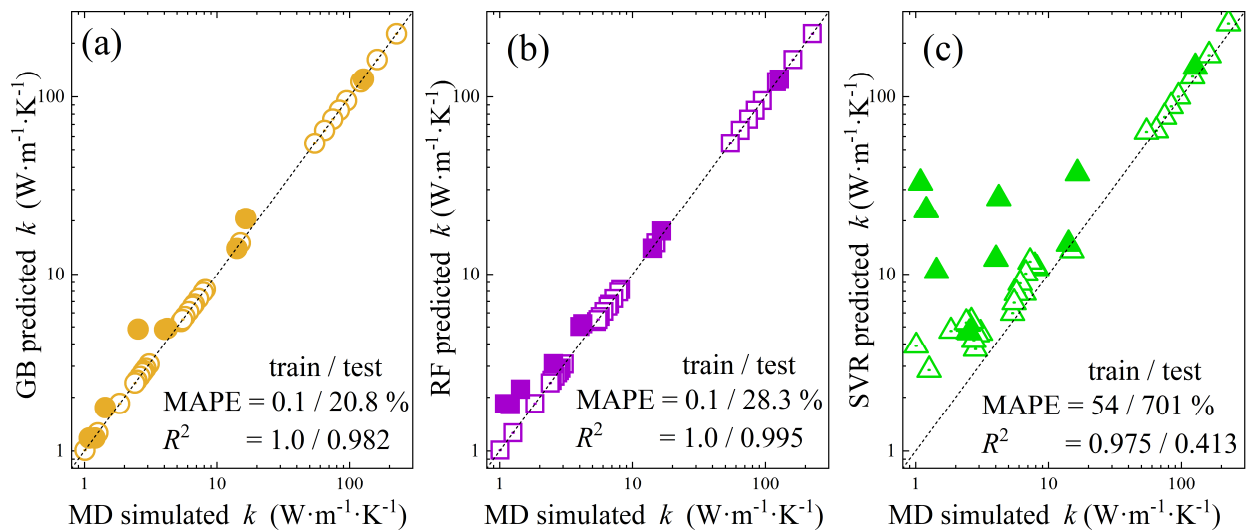


Figure 10. **Comparison between MD-calculated thermal conductivity and predictions obtained from Gradient Boosting (a), Random Forest (b), and Support Vector Regression (c) for porous silicon. Open and closed markers indicate training and test datasets, respectively. Solid black lines represent reference trends.**

Acknowledgments

The work was supported by National Research Foundation of Ukraine (project No. 2023.05/0024).

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