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

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**Abstract**

*Text*

**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 (~140 W⋅m−1⋅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 thermal properties of complex materials by uncovering hidden structure-property relationships [19, 20]. The utilization of such integrated frameworks has the potential to markedly expedite the design process for advanced nanostructured materials intended for thermal management and energy conversion applications.

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 [21]. The EMD simulation setup considered in this paper is schematically illustrated in Fig. 1. The simulation box is a cube consisting of *L*3=10*a*×10*a*×10*a* 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 .

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

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:

, (1)

where *V* is the volume of the system, *t* is the time, the brackets  is the ensemble-averaged HCACF and **J** is the heat current vector that is defined as

, (2)

Here, **υ***j* and *Ej* are the velocity and energy of the *j*-th particle; **r***ij* and **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. 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.

ML method

**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 two key criteria: (i) computational performance, which is particularly relevant for high-throughput simulations and machine learning dataset generation; and (ii) agreement between simulated and experimental temperature-dependent thermal conductivity of singlecrystalline silicon. The tested potentials included MEAM [22], Tersoff [23], EDIP [24], Stillinger-Weber (SW) [25], modified Stillinger-Weber (SW-mod) [26], and a machine learning-based potential SNAP [27]. 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.

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

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| Figure 3. Calculated temperature dependence of thermal conductivity of singlecrystalline silicon using different interatomic potentials, compared with experimental data adapted from [28]. |

Thermal conductivity values calculated using MEAM, Tersoff, SW, and SW-mod consistently exceeded the experimental results reported in Ref. [28] across the entire temperature range, with deviations ranging from 48% to 106%. These discrepancies are largely attributed to the idealized nature of the simulated structures, which lack defects and isotopic disorder present in real crystals. In contrast, the SNAP potential significantly underestimated the thermal conductivity, indicating inadequate parameterization for heat transport simulations.

Among all tested potentials, EDIP showed the best agreement with the experimental temperature dependence *k*(*T*), and given its superior computational efficiency, it was initially selected for further studies of porous silicon. However, subsequent simulations revealed that for highly porous structures and elevated temperatures, the porous architecture (Fig. 1) became unstable, leading to pore collapse and near-amorphous configurations. Similar instabilities were observed with the SW and SW-mod potentials. As a result, the Tersoff potential was chosen for the remainder of the study. An additional argument in favor of Tersoff is that fitting the calculated *k*(*T*) dependence for monocrystalline Si with the function *k*=*AT*−*b* yielded a value of *b*=1.1, which is close to the theoretical expectation *b*=1.0 for semiconductors and dielectrics.

**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. Figures 4 and 5 present selected results for the temperature and porosity dependence of thermal conductivity, calculated using the Tersoff potential.

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| Figure 4. Temperature dependence of thermal conductivity of *p*-Si with 20% and 40% porosity calculated using the Tersoff potential. |

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. Specifically, the exponent *b* in the empirical relation *k*=*AT*−*b* decreases with porosity, indicating enhanced phonon scattering due to partial amorphization. A monotonic decrease in thermal conductivity with increasing porosity is also observed (Fig. 5), attributed to increased phonon-boundary scattering at pore surfaces.

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| Figure 5. Dependence of thermal conductivity on porosity for *p*-Si at *T*=300 K, calculated using the Tersoff potential. |

These simulations were performed across a wide range of temperatures and porosities, and the resulting data served as a foundation for the development and training of ML models for predicting the heat transport behavior of porous silicon.

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

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