Modeling of electronic and phonon thermal conductivity of silicon in a wide temperature range

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Abstract. In the present article, using the methods of mathematical modeling, the thermal conductivity of silicon was obtained in a wide temperature range \(0.3 \leq T \leq 3\,\text{kK}\), including the region of semiconductor–metal phase transformations. As it is known, there are two mechanisms of heat transfer in a solid: elastic lattice vibrations and free electrons, therefore, in the study of the thermal conductivity of silicon, the lattice and electronic components were taken into account. The lattice (phonon) thermal conductivity in this work was determined within the framework of the atomistic approach. The Stillinger–Weber and Kumagai–Izumi–Hara–Sakai interaction potentials were used for modeling. The results of the comparison of the phonon thermal conductivity obtained from the simulation results with the used interaction potentials are presented. The modeling of the thermal conductivity of the electronic subsystem of silicon with intrinsic conductivity in this work is based on the use of the quantum statistics of the electron gas using the Fermi–Dirac integrals. The total thermal conductivity of silicon, obtained as the sum of the electronic and phonon components, is compared with the experimental data.

1. Introduction
Due to its unique properties, silicon is one of the most demanded materials in many application areas [1–13], such as micromachining [1], pulse laser deposition (PLD) [3, 4], laser-induced breakdown spectroscopy (LIBS) [5], which have become traditional and new, rapidly developing areas such as surface nanostructuring [6, 7], chemical and physical synthesis [7–9], the production of nanomaterials [10–13] and their application in the problems of biomedicine [9, 10].

In recent decades, processing of silicon by short and ultrashort pulses of laser radiation has been developing rapidly and opens up additional opportunities for obtaining new materials. Fundamental mechanisms, such as ultrafast melting, separation, and material removal, which underlie the interaction of laser radiation with a silicon target, are priority research objects. The studies of the mechanisms underlying the phase transformations in semiconductors caused by melting and evaporation also remain the subject of discussion. In recent years, to study these interaction mechanisms, both experimental [1–6,14,15] and theoretical [16–20] studies have been carried out, mainly for metal targets. The tool for the theoretical study of processes, including nonequilibrium ones, is mathematical modeling. The adequacy of the results of modeling of the processes occurring in materials under the influence of various external conditions is determined by the reliability and completeness of the thermophysical, thermodynamic, optical mechanical, electrical and kinetic properties of the material under study in a wide range of parameters.

In this regard, much attention is paid to the problem of determining the properties of silicon
and its plasma in a wide range of parameters: temperature, pressure, intensity, duration and wavelength of laser radiation.

The most important characteristic of heat transfer of silicon is thermal conductivity, the determination of which is a difficult task, the complexity of which is associated with the variety of processes that take place in silicon when the parameters change.

Extensive experimental and theoretical material has made it possible to establish [21–24] that silicon belongs to semiconductors, in which, during melting, the destruction of covalent bonds occurs, with a change in short-range order, and a sharp increase in the concentration of conduction electrons, leading to the transition of silicon into a metallic state. In the vicinity of the solid–liquid phase transition point, all properties of crystalline silicon undergo qualitative changes and differ significantly from the analogous characteristics of metals.

The thermal conductivity of solid-state silicon is mainly determined by the phonon (lattice) conductivity, the contribution of the electronic subsystem is insignificant. With increasing temperature, the contribution of the conductivity of free carriers—electrons and holes—increases. Therefore, the thermal conductivity, which varies in a wide temperature range, must be determined for each of the subsystems [23–25].

Mathematical modeling is a universal tool for the theoretical study of material properties. The modern description of properties in a wide temperature range, including the solid-liquid phase transition in semiconductors, as well as in metals, is carried out within the framework of two classes of models: continual [23, 26, 27] and atomistic [25, 28, 29].

In this work, the properties of the electronic subsystem of silicon are modeled using quantum statistics. The characteristics of the phonon subsystem of silicon in the solid-liquid system are investigated within the framework of the atomistic approach.

The aim of this work is to determine the phonon, electronic and total thermal conductivity of silicon in a wide temperature range ($0.3 \leq T \leq 3 \, \text{kK}$), including the semiconductor–metal phase transition region. The obtained dependences are planned to be used in continuous modeling of laser melting and evaporation of a silicon target. The magnitude of the near-surface temperature gradient arising during fast laser heating directly depends on the thermal conductivity of the target. The paper may also be of interest for the analysis of the laser experiments with silicon, for example, such as [30, 31].

2. Methods and approaches

2.1. Modeling of thermal conductivity of the phonon subsystem

In the present work, the lattice (phonon) thermal conductivity of silicon was determined within the framework of the atomistic approach. Atomistic modeling of the properties of the phonon subsystem is based on the molecular dynamics (MD) approach based on solving the system of Newtonian equations of motion for each particle in three-dimensional space, which allows one to consider directly the behavior of each particle and obtain detailed information on the kinetics and mechanisms of laser melting and evaporation of a silicon target [28]. When using MD models to study various properties of matter, the choice of interaction potentials between particles plays an important role, since the reliability of the results obtained directly depends on it [32]. The interatomic potential, on which the accuracy of the results depends, is crucial for molecular dynamics modeling.

The problem of constructing the interatomic interaction potential is especially acute in the materials with covalent bonds, which include silicon. The development of the potential for silicon has a number of features and is more complex than for metals. Under normal conditions, silicon has a diamond structure characterized by low compactness with a coordinate number equal to 4, which is much less than that of metals (8–12). With an increase in pressure in silicon, new structures are formed—a simple cubic one and face-centered cubic one with an increasing coordination number, but little different in energy [33, 34]. After melting, liquid silicon first
acquires the properties of a semi-metal, and then of a metal [23, 24, 35–37]. The coordination number increases to 6, and the density exceeds the density of the solid phase. The presence of these features significantly complicates the task of constructing the interatomic interaction potential for silicon. The choice of interaction potentials for MD simulation was carried out on the basis of test calculations carried out in [32]. By comparing the interaction potentials for modeling silicon in [32], it was found that the semiempirical Stillinger–Weber (SW) and Kumagai–Izumi–Hara– Sakai (KIHS) potentials [38–40] are the most acceptable. Based on the conclusions of [32], in this work, the SW and KIHS potentials were used for MD simulation.

The SW potential was one of the first to be used for simulation of semiconductors [38]. This potential represents the sum of two-particle and three-particle terms. The three-particle term includes the angles formed by bonds between three particles. Therefore, for a given potential, the most favorable configuration is when these angles are as close as possible to the corners of the diamond-like tetrahedral structure. The SW potential gives a fairly realistic description of crystalline silicon. However, its inherent features create a number of problems when simulating the liquid phase of a semiconductor, in particular, it cannot correctly predict the energies of non-tetragonal structures found under pressure; the coordination number of the liquid is very small; the surface structures are incorrect. Thus, it becomes difficult to use the potential in conditions other than those for which it was designed.

The KIHS potential [40] is a modification of the Tersoff many-particle potential [41, 42]. The KIHS potential, like the Tersoff potential, is based on the concept of bond order, which states that the bond strength between two atoms is not constant, but depends on the local environment. The KIHS modification makes it possible to simulate a wider range of situations, since it removes a number of problems inherent in the Tersoff potential in modeling the elastic constants and the melting point.

Within the framework of the MD approach, two kinds of the lattice thermal conductivity $\kappa_{\text{lat SW}}(T)$ and $\kappa_{\text{lat KIHS}}(T)$ were determined using the direct method (DM) [43]. DM is non-equilibrium molecular dynamics (NEMD) technique, where heat source and sink regions are created in a simulation cell to establish a constant heat flow along the direction of interest. Thermal conductivity $\kappa_{\text{lat}}$ was determined from the known heat flow $W$ using the Fourier law

$$W = -\kappa_{\text{lat}} \frac{\partial T}{\partial x},$$

where $W$ is the heat flow, and $x$ is the coordinate in along the direction of the flow. A series of calculations was carried out to determine the lattice thermal conductivity. The modeling area was considered in the form of a parallelepiped with dimensions of $10 \times 10 \times 20$ unit cells (lattice constant 0.543 nm) with periodic boundary conditions along three axes. The time step was chosen depending on the temperature: from 3 fs at 0.3 kK to 1 fs at 4 kK and higher. For the crystal, the calculations were performed for 5 different sizes of the region from 20 to 320 unit cells with a constant cross section of $10 \times 10$ cells. The maximum number of atoms was 256 000. For the liquid state, only one calculation was performed for a size of 40 cells, for large sizes the results were approximately the same.

The heat flow $W$ was calculate as

$$W = \frac{dQ}{2SNvdx},$$

where $dQ = Ndt\delta Q_N$ is the total deposited energy; $\delta Q_N$ is the energy deposited during 1 time step; $N$ is the number of time steps; $dt$ is the size of the time step; $S$ is the cross-section of the region. The division by 2 is due to periodic boundary conditions.

A scaling procedure was used to determine the thermal conductivity coefficient: the thermal conductivity was determined for several lengths of the modeling region along $x$. Then the inverse thermal conductivity $1/\kappa_{\text{lat}}$ was plotted versus the inverse length $1/L$. The resulting thermal conductivity was determined from the extrapolation of the data at $1/L \rightarrow 0$ [43].
A detailed presentation of the problem statement, as well as an analysis of the obtained temperature dependences of such characteristics of silicon as density, change of the sample linear size, and the coefficient of linear expansion, are presented in [44] and are not presented in this article.

MD modeling of the thermal conductivity of silicon was carried out using the well-known applied package LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [45]. It supports many pairs and many-particle short-range potentials, has the ability to write atomic configurations to a text file, and also has built-in thermostats and barostats. The computational algorithm is based on the Verlet finite-difference scheme [46]. The velocity and pressure for the ensemble of particles were corrected using the Berendsen’s thermostat and barostat [47].

2.2. Modeling of thermal conductivity of the electron subsystem

Modeling the thermal conductivity of the electron subsystem of silicon with intrinsic conductivity in this work is based on the use of the quantum statistics of the electron gas. With this approach, the basis is the knowledge of the law of distribution of carriers over the energy states. The electrons in the conduction band and holes in the valence band of silicon can be regarded as an ideal Fermi gas, for which the distribution of carriers over energy states obeys the Fermi–Dirac (FD) law [23, 24, 48]. Based on these suppositions, the properties of the electronic subsystem of silicon are determined. The most important of these is the concentration of electrons \(N_e\) in the conduction band or the concentration of holes \(N_h\) in the valence band. In semiconductors, unlike metals, the concentration of charge carriers depends on temperature. At low temperatures in semiconductors, the valence band is completely occupied and, according to the Pauli principle, the movement inside the valence band is impossible, and therefore the electron gas is non-degenerate, and the concentration of conduction electrons is low. The allowed bands in semiconductors (conductivity and valence) are separated by a forbidden band, which is an obstacle to the interband movement of electrons. The band gap \(E_g(T, N_e)\) is a fundamental characteristic of silicon, which depends in a complex way on temperature and the concentration of carriers in the conduction band [23, 37]. With increasing temperature, the band gap decreases, and hot electrons transfer energy to the lattice. In this case, the concentration of free charge carriers in the conduction band increases, determined by the processes of generation and recombination of electrons from the conduction band and holes from the valence band, which occur continuously and in parallel. In such a situation, the electron gas degenerates. In the molten state, semiconductors acquire metallic properties.

According to the quantum-statistical approach, the thermal conductivity of the electronic subsystem of silicon, taking into account the degree of carrier degeneracy, is determined as [36]

\[
\kappa_e(T) = N_e(T)\mu_e(T) \frac{k_B^2 T}{e} \left[ \frac{F_2(\eta_e)}{F_0(\eta_e)} - 4 \left( \frac{F_1(\eta_e)}{F_0(\eta_e)} \right)^2 \right],
\]

where \(e\) is the electron charge, \(F_0(\eta_e), F_1(\eta_e), F_2(\eta_e)\), are the Fermi–Dirac integrals of the orders \(j = 0, 1, 2\) for the electrons; \(N_e(T)\) is the intrinsic concentration of charge carriers is determined using the integral Fermi–Dirac of the order \(j = 1/2, F_{1/2}(\eta_e)\) [47], \(\mu_e(T) = \mu^0_e(T)/F_0(\eta_e)\) is the mobility of the charge carriers; \(\eta_e = (E_C - E_F)/(k_B T)\) is the reduced Fermi energy for electrons, here \(k_B\) is the Boltzmann constant, \(E_C\) is the energy of the bottom of the conduction band, \(E_F\) is the Fermi energy, determined from the electroneutrality condition [49]; \(\mu^0_e(T)\) is the mobility of the carriers for a non-degenerate semiconductor. In papers [50, 51], a method for calculating the mobility of nondegenerate charge carriers \(\mu^0_e(T)\) taking into account electron–hole scattering, which was used for the calculation, is presented. In this approach, it is assumed that, in the general case, the electron or hole mobility is a function of the following three components: lattice mobility, impurity scattering mobility, and electron–hole scattering mobility.
To calculate the Fermi–Dirac integrals of integer and half-integer orders in this work, we used the approximations proposed in the paper [52].

3. Modeling results

3.1. Thermal conductivity of the phonon subsystem

The results of the modeling of the thermal conductivity of the silicon lattice $\kappa_{\text{lat}}(T)$ with KIHS and SW potentials in the range $0.3 < T < 3$ kK after statistical processing are shown in figure 1. In our MD calculations of lattice thermal conductivity by the direct method, we aimed to maintain a single-phase state in the computational domain. Results that lead to a biphasic state have been discarded. To the point of equilibrium melting, the values of thermal conductivity were extrapolated from both the solid and liquid phases. In figure 1, these values near the line of separation of the solid and liquid phases are shown by filled markers.

Regardless of the interaction potential used, as the results show, in the temperature range under study, the behavior of the lattice thermal conductivity is decreasing with temperature. As you can see, the variants of the dependence of thermal conductivity obtained with different potentials do not coincide. The values of thermal conductivity in the solid phase, $0.3 < T < 1.685$ kK, obtained with the SW potential exceed the values obtained with the KIHS potential by $\approx 2–3$ times. The same ratio is maintained in the liquid phase.

At the equilibrium melting temperature $T_m = 1.685$ kK, in the solid phase the values of the thermal conductivity are as follows: for the KIHS potential, $\kappa_{\text{lat KIHS}} = 8.62$ W/(m K); for the SW potential, $\kappa_{\text{lat SW}} = 17$ W/(m K). In the liquid phase at the same temperature, $\kappa_{\text{lat KIHS}} = 0.986$ W/(m K), $\kappa_{\text{lat SW}} = 3.6$ W/(m K). Thus, for both potentials the calculations show a jump of the lattice thermal conductivity by 88.6% for KIHS potential, and by 78.6% for SW one (see figure 1). The magnitude of the jump for SW potential is by 10% less than for KIHS one.

Figure 1. Temperature dependence of the lattice thermal conductivity according to calculations (1) with the KIHS potential; (2) with SW potential; (3) the results of calculations with the SW potential in [29].
The calculations were carried out up to $T = 3$ kK. At $T = 3$ kK, $\kappa_{\text{lat KIHS}} = 0.74$ W/mK and $\kappa_{\text{lat SW}} = 1.96$ W/(m K), and the relation between them is $\kappa_{\text{lat SW}} / \kappa_{\text{lat KIHS}} = 2.66$.

The markers in figure 1 show the results of calculation with SW potential from [29]. The comparison of the MD results obtained in this work with the SW potential and the alternative results shows good agreement. In the solid phase, the agreement is almost complete. In the liquid phase, the difference is $\approx 45\%$.

3.2. The ratio of the electronic and lattice thermal conductivity of silicon

The thermal conductivity of the silicon electron gas was determined in the temperature range $0.3 \leq T \leq 3$ kK. The calculation results are shown in figure 2 (red line with markers). To compare the electronic and phonon thermal conductivity, figure 2 shows the variants of the thermal conductivity of the silicon lattice, calculated in this work with the SW and KIHS potentials. With increasing temperature in the entire investigated range, the thermal conductivity of electrons increases, in contrast to the constantly decreasing thermal conductivity of the lattice. The simulation results show that the thermal conductivity of the electron gas in the range $0.3 \text{kK} \leq T \leq T_m$ is significantly lower than the thermal conductivity of the lattice. At low temperature $0.3 \leq T < 1$ kK, thermal conductivity of the electrons takes the value from $1.22 \times 10^{-7}$ to $9.48 \times 10^{-2}$ W/(m K). At $T = 0.35$ kK, $\kappa_e(T)$ is only $8.07 \times 10^{-5}\%$ of $\kappa_{\text{lat SW}}(T)$ and $1.83 \times 10^{-7}\%$ of $\kappa_{\text{lat KIHS}}(T)$, while at $T = 0.95$ kK $\kappa_e(T)$ is $0.13\%$ of $\kappa_{\text{lat SW}}(T)$ and $0.4\%$ of $\kappa_{\text{lat KIHS}}(T)$. The values of the electronic thermal conductivity in this temperature range are so small because of the large width of the band gap, which prevents an increase in the carrier concentration in the conduction band.

As the temperature rises, the band gap decreases, the concentration of the carriers increases, which results in the increase of the electronic thermal conductivity. In the range $1 \text{kK} \leq T < T_m$ the electronic thermal conductivity increases by 2 orders, still being lower than the phonon one: $\kappa_{\text{lat SW}}(T) > \kappa_{\text{lat KIHS}}(T) > \kappa_e(T) = 4.123$ W/(m K). At the equilibrium melting temperature
\( T = T_m \) the band gap vanishes according to the theoretic [21, 23, 25] and experimental [22, 29] data. Because of that the concentration of the carriers and thermal conductivity increase sharply \((\kappa_e(T) = 39.9\ \text{W}/(\text{mK}), \text{see figure 2})\). The thermal conductivity of the phonons at \( T = T_m \) decreases abruptly taking the value of \( \kappa_{\text{lat SW}}(T) = 3.6\ \text{W}/(\text{mK}) \) and \( \kappa_{\text{lat KIHS}}(T) = 0.986\ \text{W}/(\text{mK}) \) (see figure 2), which is by one order less than the electron component for SW and by two orders for KIHS.

For \( T > T_m \), the increase in the thermal conductivity of electrons slows down, since molten silicon acquires metallic properties and the carrier concentration becomes almost constant. In this temperature range, the thermal conductivity of electrons significantly exceeds the phonon thermal conductivity. At \( T = 2\ \text{kK} \) the electronic thermal conductivity \( \kappa_e(T) = 40.627\ \text{W}/(\text{mK}) \) is many times higher than the phonon one: for SW by 13 times, \( \kappa_{\text{lat SW}}(T) = 2.95\ \text{W}/(\text{mK}) \); and for KIHS by 45 times, \( \kappa_{\text{lat KIHS}}(T) = 0.896\ \text{W}/(\text{mK}) \). At the temperature \( T \approx 3\ \text{kK} \), the electronic thermal conductivity is \( \kappa_e(T) \approx 44\ \text{W}/(\text{mK}) \), and exceeds the thermal conductivity of phonons: \( \kappa_{\text{lat SW}}(T) = 1.96\ \text{W}/(\text{mK}) \), by \( \approx 22\ \text{times} \), and \( \kappa_{\text{lat KIHS}}(T) = 0.738\ \text{W}/(\text{mK}) \), by \( \approx 60\ \text{times} \).

In work [53], at a temperature of 1.7 kK, from molecular dynamics modeling, using 3 hybrid functionals with different sizes of computational cells, 5 values of electronic thermal conductivity were obtained, differing by \( \approx 1.5–2\ \text{times} \). In this work, the value of the electronic thermal conductivity, at the same temperature, is \( \kappa_e(T) = 39.926\ \text{W}/(\text{mK}) \), which is 3–5% different from the closest values obtained in [53]. Due to the lack of experimental data on electronic thermal conductivity, a comparison was made between the calculated data obtained in this work with the experimental data on total thermal conductivity [54] and experimental and calculated work [55] at \( T = 1.7\ \text{kK} \) from the side of the liquid phase; the difference is 22.5% and 31.9%, respectively.

### 3.3. Full thermal conductivity

Since the transfer of thermal energy is carried out by free charge carriers and phonons, the total thermal conductivity \( \kappa \) is determined by the lattice thermal conductivity \( \kappa_{\text{lat}}(T) \) and the thermal conductivity of free carriers \( \kappa_e(T) \):

\[
\kappa(T) = \kappa_{\text{lat}}(T) + \kappa_e(T).
\]

The results of MD simulation of the lattice thermal conductivity of silicon with the SW and KIHS potentials make it possible to obtain two versions of the total thermal conductivity, including as a phonon component either \( \kappa_{\text{lat SW}}(T) \) or \( \kappa_{\text{lat KIHS}}(T) \):

\[
\kappa_{\text{SW}}(T) = \kappa_{\text{lat SW}}(T) + \kappa_e(T),
\]

\[
\kappa_{\text{KIHS}}(T) = \kappa_{\text{lat KIHS}}(T) + \kappa_e(T).
\]

Both versions of the total thermal conductivity of silicon in the range \( 0.3 < T < 3\ \text{kK} \) are shown in figure 3. The markers in the figure show the experimental data [54].

The behavior of the total thermal conductivity as a function of temperature is completely determined by the behavior of its components. The above comparison of the components of thermal conductivity obtained from the simulation results shows that, in contrast to metals, in the solid phase the thermal conductivity of silicon is completely determined by the lattice conductivity, which at a low temperature exceeds the electronic one by more than 1000 times (see figure 2). The consequence of calculating the phonon thermal conductivity with two potentials is a noticeable difference between the branches of the total thermal conductivity of solid-state silicon (see figure 3). Both variants of total thermal conductivity differ from the experimental data. In the range \( 0.3 < T < 1.5\ \text{kK} \), the thermal conductivity \( \kappa_{\text{SW}}(T) \) obtained with the SW potential exceeds the experimental values by \( \approx 25\% \). In a small range of \( 1.5 < T < 1.58\ \text{kK} \), the values of calculations and experiments practically coincide (the difference is \( \approx 2\% \), and
Figure 3. Temperature dependences of the thermal conductivity of silicon: 1—equation (6), the thermal conductivity of the lattice is calculated with the KIHS potential; 2—equation (5), the lattice thermal conductivity is calculated with the SW potential. The markers are experimental data [54].

At a higher temperature \( T \leq 1.68 \text{ kK} \) the differences are \( \approx 18\% \). The comparison of the experimental values of thermal conductivity and those obtained using the KIHS potential shows that the difference in the range \( 0.3 < T < 1.68 \text{ kK} \) is about 90%.

At the semiconductor–metal phase transition for the thermal conductivities calculated with both potentials, an abrupt increase in values is obtained, despite the fact that both variants of the lattice thermal conductivity decrease abruptly in this range (see figures 1 and 2). The compensation of the values of the lattice component in the total thermal conductivity occurs due to a significant increase in the thermal conductivity of electrons in this temperature range. In the experimental values of thermal conductivity, an abrupt increase in values at the semiconductor–metal transition is also observed. The abrupt increase in the calculated thermal conductivities at the phase transition is 51.5% for \( \kappa_{SW}(T) \), 68.85% for \( \kappa_{KIHS}(T) \). For the experimental data, the abrupt increase is 51.26%.

At \( T > T_m \), the difference between the \( \kappa_{KIHS}(T) \) and \( \kappa_{SW}(T) \) values from each other and from the experimental values is not as large as in the solid phase. This is due to the fact that the total thermal conductivity in the liquid phase is determined by the thermal conductivity of electrons. The difference from the experimental values is \( \approx 16\% \) for \( \kappa_{SW}(T) \), and \( \approx 21\% \) for \( \kappa_{KIHS}(T) \).

4. Conclusions
The thermal conductivity of silicon in a wide range of temperature (0.3 \( \leq T \leq 3 \text{ kK} \)), including the area of semiconductor–metal phase transformations, has been obtained by mathematical modeling. The total thermal conductivity is obtained as the sum of the electronic and phonon thermal conductivities. The modeling of the thermal conductivity of the electronic subsystem of silicon with intrinsic conductivity in this work is based on the use of the quantum statistics of the
electron gas using the Fermi–Dirac integrals. The phonon thermal conductivity was obtained by a direct method within the framework of MD simulation. For MD calculations, the SW potentials and the modification of the Tersoff potential—KIHS—were used. The results of MD simulation of the lattice thermal conductivity of silicon with these potentials made it possible to obtain two versions of the total thermal conductivity, including the phonon thermal conductivity obtained with the SW potential or with the KIHS potential.

The comparison of the modeling results with experimental data [54] shows good agreement. The analysis of the modeling results and their comparison with the experimental data show that the values of the total thermal conductivity of solid-state silicon obtained from the MD simulation with the SW potential are in better agreement with the experimental results. The same conclusion is obtained by comparing the thermal conductivity calculated with the SW potential and the experimental values in the region of the semiconductor–metal phase transition. In the liquid phase, both variants of silicon thermal conductivity have slight differences between themselves and with the experimental data. In this case, preference is also given to the SW potential for MD calculations of the lattice thermal conductivity of silicon, since comparison with the experimental values of the total thermal conductivity $\kappa_{SW}(T)$ shows greater agreement than the result obtained with the KIHS potential.

Thus, in MD modeling of silicon for processes occurring in temperature range $0.3 \leq T \leq 3$ kK, including the phase transition region, the classical Stillinger–Weber potential has an advantage.

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