

Estimation of phonon relaxation time for silicon by means of using the velocity autocorrelation function of atoms in molecular dynamics

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Abstract. Results of the *ab initio* molecular dynamics calculations of silicon crystals are presented by means of analysis of the velocity autocorrelation function and determination of mean phonon relaxation time. The mean phonon relaxation time is crucial for prediction of the phonon-associated coefficient of thermal conductivity of materials. A clear correlation between the velocity autocorrelation function relaxation time and the coefficient of thermal diffusivity has been found. The analysis of the results obtained has indicated a decrease of the velocity autocorrelation function relaxation time t with increase of temperature. The method proposed may be used to estimate the coefficient of thermal diffusivity and thermal conductivity of the materials based on silicon and of other wide-bandgap semiconductors. The correlation between kinetic energy fluctuations and relaxation time of the velocity autocorrelation function has been calculated with the relatively high coefficient of determination $R^2 = 0.9396$. The correlation obtained and the corresponding approach substantiate the use of kinetic energy fluctuations for the calculation of values related to heat conductivity in silicon-based semiconductors (coefficients of thermal conductivity and diffusivity).

Key words: silicon, molecular dynamics, relaxation time of the velocity autocorrelation function, coefficient of thermal diffusivity.

1. Introduction

The demand for high voltage and high current electronic devices poses technical challenges for power conversion beyond those normally associated with electrical and electronic systems. There are many ways to remove heat from a power electronic device. However, nearly all of them are based on the same common principle: to move heat away from the device to the ambient medium by means of convection, conduction or radiation [1]. Thus research on the thermal conductivity properties of semiconductors used in the electronic devices and their proper modification constitutes a massive undertaking [2–4].

The coefficient of thermal conductivity is one of the fundamental characteristics of many materials. Because of the large variety of materials used in modern electronics, the problem of determining their heat characteristics is extremely important [5]. The value of the coefficient of thermal conductivity and its dependence on external factors (temperature, pressure, etc.) is indispensable for the proper design of corresponding devices in electronics [6, 7].

The interest in thermal conductivity studies of materials has grown in the last years also due to the development of effective thermoelectric devices. Thermoelectric materials can convert waste heat directly into electrical energy, which is increasingly

important under the challenges of growing energy demand [8–13]. The performance of thermoelectric materials can be estimated by the dimensionless figure of merit $ZT = S^2\sigma T/\kappa$, where S , σ , T are the Seebeck coefficient, electrical conductivity and absolute temperature, respectively. κ is the coefficient of thermal conductivity, which is composed of electronic contribution κ_e and phonon contribution κ_p . A high value of ZT means a high $S^2\sigma$ and a low κ . To achieve high ZT by the decrease of κ_p , one should use the proper nanostructure of material [14].

Though neglecting electrons removes the ability to model the associated electrical and thermal transport, one can still consider many of the relevant thermal issues in devices. These include the transport of phonons in superlattices and across material interfaces and grain boundaries, the dissipation of heat in integrated circuits (the dimensions of field effect transistors are approaching tens of nanometers), and low-dimensional effects in structures such as quantum dots and nanotubes [15]. Analysis of thermal transport in dielectrics is typically done in the phonon space, which provides a wave-based description of lattice dynamics. For a harmonic solid, the phonon system corresponds to a set of independent harmonic oscillators, yet harmonic theory is only exact at zero temperature. As temperature increases, anharmonic (higher-order) effects, which are difficult to model theoretically, become more evident.

Among several theoretical techniques used for determination of thermal conductivity of semiconductors, the method of molecular dynamics (MD) is often applied to resolve the problem [16–18]. MD simulations come as a suitable tool for the analysis of dielectrics at finite temperature and for the bridging

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of real and phonon space analysis techniques [15]. Most importantly, MD simulations allow for natural inclusion of anharmonic effects and for atomic-level observations.

The Green-Kubo method is one of the two main MD approaches used for calculation of thermal conductivity of materials. According to this approach, the net flow of heat in a solid, described by the heat current vector J , fluctuates at about zero at equilibrium. In the Green-Kubo method, the coefficient of thermal conductivity κ is related to how long it takes these fluctuations to dissipate, and for an isotropic material it is given by [19]:

$$\kappa = \frac{1}{k_B VT^2} \int_0^\infty \frac{\langle J(t) \cdot J(0) \rangle}{3} dt, \quad (1)$$

where $\langle J(t) \cdot J(0) \rangle$ is the heat current autocorrelation function (HCACF). The Green-Kubo approach is valid in the case of small deviations from equilibrium and for long times (i.e. the hydrodynamic limit) and should be applied to simulations in the microcanonical ensemble [15]. Thus the coefficient of thermal conductivity κ is proportional to the amplitude of fluctuation of heat current J . In turn, the later value of J should also be proportional to the value of standard deviation for energy during MD at certain temperature T .

One of the alternative ways to calculate lattice thermal conductivity is to use the Debye-Callaway model [20] within the relaxation time approach [21]. In the model, the relaxation time due to the phonon-phonon scattering can be written as a function of Debye temperature (Θ), phonon velocity (v) and the Grüneisen parameter (γ). The simple Debye-Callaway model is the computationally feasible methodology used in the experimental community to estimate lattice thermal conductivity based on experimentally measured parameters (Θ , v , and γ) [21].

In our previous theoretical studies of silicon using the molecular dynamics (MD) method [22–24], the temperature dependences of the values responsible for the corresponding dependences of the coefficient of thermal conductivity κ and thermal diffusivity D were analyzed on the basis of known relations [25],

$$\kappa = \frac{1}{3} \rho C_V v^2 \tau_{ph}, \quad (2)$$

$$D = \frac{1}{3} v^2 \tau_{ph}, \quad (3)$$

where ρ is the density of material, C_V is the specific heat at constant volume V , v is the mean acoustic phonon velocity and τ_{ph} is the mean phonon relaxation time. According to the results obtained in [23], the expected relative temperature change of product $\rho C_V v$ from relation (2) in the wide temperature range of 200–1000 K is placed within the value of 10%. This conclusion was formulated on the basis of the temperature dependences of specific heat at constant volume $C_V(T)$ and the elastic constant $C(T)$ obtained from MD studies [23]. According to the known reference information, the relative change of silicon density $\Delta\rho/\rho$ does not exceed 1% in the temperature range of 200–1000 K. On the other hand, the coefficient of

thermal conductivity of silicon κ decreases nearly five times in this temperature range [26]. These results indicate that the temperature dependence of the mean phonon relaxation time $\tau_{ph}(T)$ is mainly responsible for the temperature dependence of the coefficient of thermal conductivity $\kappa(T)$. This conclusion substantiates the necessity of studying the dependences of the mean phonon relaxation time τ_{ph} on external factors: temperature, pressure, etc.

In one of the recent molecular dynamics studies of silicon thermal conductivity, the phonon mean free path L_{ph} ($L_{ph} = v\tau_{ph}$) has been proposed to be equal to the interferometric coherence length L_{coher} [27]. This coherence length L_{coher} , in turn, was determined from the condition of the interferometric minimum, $\Delta = \Lambda/2$, for two phonons of wavelength Λ and path difference Δ [27]. This coherence-based approach indicates that the maintenance of a certain correlation between atomic vibrations is one of the main conditions for keeping the corresponding level of thermal conductivity of materials. This conclusion inclines us to use the time-dependent velocity autocorrelation function (VACF) to obtain the mean phonon relaxation time τ_{ph} .

In the present research, the correlation between relative fluctuations of kinetic energy $\Delta E_k / \langle E_k \rangle$ and relaxation time t of the velocity autocorrelation function and phonon relaxation time τ_{ph} at MD simulations of silicon crystal shall be studied for the first time. If the degree of such correlation is high, then the $\Delta E_k / \langle E_k \rangle$ value may be used for estimation of phonon relaxation time τ_{ph} and the coefficient of phonon-related thermal conductivity.

2. Method of calculation

The equilibrium-type *ab initio* MD calculations of the crystal have been performed within the framework of density functional theory (DFT) using the VASP package [28]. The projector augmented wave (PAW) method with cutoff energy of 400 eV for the plane waves was employed [29] together with the corresponding pseudopotentials. For the exchange and correlation terms, the gradient-corrected Perdew-Burke-Ernzerhof (PBE) functional was used. MD calculations of silicon-related crystals were performed at the macro-canonical NVT ensemble for different temperatures at the optimized crystal structure of the super cell of $3 \times 3 \times 3$. Most results of MD calculations have been obtained for the simulation time of up to 15 ps with the time steps of 1.5 fs. The nMoldyn 3.0 program was used for post-MD analysis [30]. According to [30], the velocity autocorrelation functions (VACF) $C_{vv}(t)$ may be calculated using the MD data by the following relation:

$$C_{vv}(t) = \frac{1}{3N} \sum_{\alpha=1}^N w_{\alpha} \langle v_{\alpha}(0) \cdot v_{\alpha}(t) \rangle, \quad (4)$$

where, $\langle v_{\alpha}(0) \cdot v_{\alpha}(t) \rangle$ denotes the averaged value of the scalar products $v_{\alpha}(0) \cdot v_{\alpha}(t)$ for atom velocities for ion of the α -type, w_{α} is the weight coefficient, t is the time and N is the number of atoms in a supercell.

Table 1

Effective relaxation time τ for different MD temperatures T of silicon obtained using relation (3). Mean acoustic velocity v has been calculated using relation (3) and the reference data for thermal diffusivity D [32]

| T/K | 200 | 300 | 400 | 500 |
|-----------------------------------|--------|------|------|------|
| $D/\text{cm}^2\text{s}^{-1}$ [32] | 2.23 | 0.86 | 0.52 | 0.37 |
| τ_1/ps | 8.0 | 6.4 | 5.3 | 4.6 |
| v_1/ms^{-1} | 9145 | 6349 | 5425 | 4912 |
| τ_2/ps | 4.4 | 3.7 | 3.0 | 2.7 |
| v_2/ms^{-1} | 12 330 | 8350 | 7211 | 6411 |

| T/K | 600 | 700 | 800 | 1000 |
|-----------------------------------|------|------|------|------|
| $D/\text{cm}^2\text{s}^{-1}$ [19] | 0.29 | 0.24 | 0.19 | 0.14 |
| τ_1/ps | 4.2 | 3.7 | 3.9 | 3.0 |
| v_1/ms^{-1} | 4551 | 4411 | 3823 | 3742 |
| τ_2/ps | 2.5 | 2.3 | 2.4 | 1.5 |
| v_2/ms^{-1} | 5899 | 5595 | 4873 | 5291 |

Due to the relatively strong bonding between atoms in solids, the corresponding relatively strong correlation of atomic velocities takes place. But, on the other hand, due to the finite acoustic velocity in solids and the statistical character of atomic parameters, the velocity correlation is a decreasing function of time and distance to other atoms. So, the mean phonon relaxation time τ_{ph} , mentioned above in the introduction, may be associated with the velocity autocorrelation function relaxation time τ .

3. Results and discussion

To estimate the effective relaxation time τ of VACF, the absolute value of VACF has been fitted initially by the following exponential function:

$$|C_{vv}(t)| = a \exp\left(-\frac{t}{\tau}\right). \quad (5)$$

The relaxation time τ obtained (5) has been taken as an approximation of the mean phonon relaxation time τ_{ph} used for

presentation of thermal diffusivity D in kinetic theory of heat transfer (see Eq. (3)).

The absolute values of VACFs for silicon at different MD temperatures and the corresponding exponential fits are presented in Fig. 1 for the case of the approximation procedure in the simulation time range from 0 ps to 7.5 ps. The corresponding values for the fit parameter τ_1 and the calculated mean acoustic velocity v_1 are presented in Table 1. The latter value obtained may be compared with the reference longitudinal velocity of about 8500 ms^{-1} at the temperature of 300 K [31]. However, we have found that the approximated value of relaxation time τ depends on the simulation time range used. For the smaller simulation time range of 0–5.0 ps, the value of relaxation time τ_2 is smaller and the mean acoustic velocity v_2 is larger (Table 1). It is known that the relative temperature decrease of the mean phonon relaxation time is several times larger than the relative temperature decrease of the elastic stiffness coefficient and, subsequently, the corresponding acoustic velocity [23].

The form of the temperature dependence $\tau_2(T)$ obtained (Fig. 2) is similar to the form of the experimental temperature dependence of thermal diffusivity $D(T)$ [32, 33].

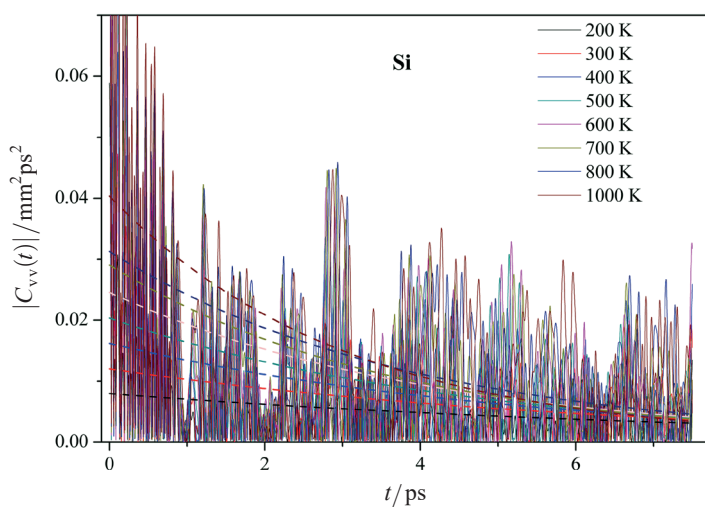


Fig. 1. Time dependences of absolute value of velocity autocorrelation function $|C_{vv}(t)|$ for $3 \times 3 \times 3$ supercell of silicon (solid lines) for different temperatures of MD in the range of 200–1000 K and corresponding exponential approximations (dashed lines)

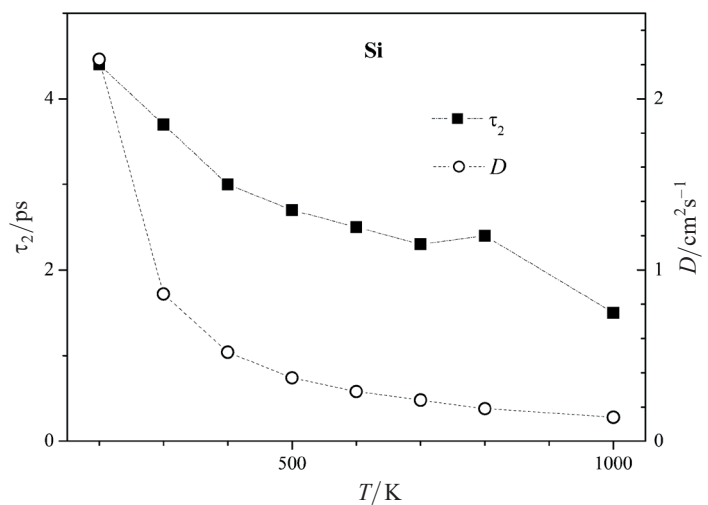


Fig. 2. Temperature dependences of the experimental coefficient of thermal diffusivity $D(T)$ [32] (circles) and the fitting parameter $\tau_2(T)$ (5) (squares), corresponding to the set of VACFs $|C_{vv}(t)|$ presented in Fig. 1 for silicon

The temperature decrease of effective velocity $v(T)$ observed in the temperature range of 200–1000 K (Table 1) is however larger than the expected decrease of about 3%. The latter magnitude is based on the corresponding temperature decreases of the largest elastic constants c_{11} ($\Delta c_{11}/c_{11} = -0.06$) [34–36], the density ρ ($\Delta\rho/\rho = -0.01$) of silicon and the known relation for velocity v of acoustic (phonon) waves:

$$v = \sqrt{\frac{c}{\rho}}. \quad (6)$$

The reference longitudinal v_L and transversal v_T velocities of acoustic waves for the direction [100] of silicon at the temperature of about 300 K, obtained from the experimental data of elastic constants [34–36], are equal to: $v_L = 8430 \text{ ms}^{-1}$ and $v_T = 5840 \text{ ms}^{-1}$. The expected effective velocity v_2 at the temperature near $T = 300 \text{ K}$ (Table 1) is close to the reference longitudinal one, i.e. $v_L = 8430 \text{ ms}^{-1}$. This comparison may confirm the validity of our supposition related to the equality of the VACF effective relaxation time τ and the mean phonon relaxation time τ_{ph} . However, one should remember that velocity v_2 corresponds to the simulation time range of 0–5.0 ps, the upper limit of which corresponds approximately to double the effective relaxation time τ_2 (Table 1).

Taking into account that all types of phonon polarizations (acoustical, optical, longitudinal and transversal one) may take part in the process of heat conductivity [37], effective velocity v at the temperature $T = 300 \text{ K}$ may differ from the reference value for longitudinal acoustic waves, i.e. $v_L = 8430 \text{ ms}^{-1}$ [34–36]. The latter value is probably one of the largest among other phonon velocities taking part in the process of thermal conductivity. This is caused by the known fact, i.e. that the value of phonon thermal conductivity of silicon originates mainly from the acoustic phonons [37].

The relatively large temperature decrease of effective velocity $v_2(T)$ in the range of 300–1000 K ($\Delta v_2/v_2 \sim 0.4$, see Table 1) may be substantiated by the temperature-stimulated increase of participation of higher frequency vibrations, forming the optical branches of phonons. Because the group velocity of optical phonons is much smaller than that for the acoustic ones, the effective velocity v of phonons at higher temperatures may be smaller than that predicted by the simplified relation (6). Besides, the higher the frequency of acoustic phonons (Ω), the smaller the corresponding group velocity $v = d\Omega/dK$, which is associated with the process of thermal conductivity (see Equations (2) and (3)).

What is obtained from molecular dynamics simulation is the configuration or microstate of the system (the positions and momenta of every single atom) at any given time included in the simulation – a quantity that cannot be measured experimentally. And how to relate the microscopic configuration to macroscopic quantities that can be measured experimentally (observables), such as temperature (1), is the subject of statistical mechanics [38].

$$\langle E_k \rangle = \frac{1}{2} f k_B T, \quad (7)$$

where E_k is the kinetic energy and $f = 3N - 3$ are the degrees of freedoms for the system (crystal) with N atoms.

Statistical mechanics are concerned with statistical *ensembles*, an ensemble being a theoretical construct holding a large number of copies (sometimes infinitely many) of essentially the same system, i.e. a collection of systems described by the same set of microscopic interactions, and sharing a common set of macroscopic control variables such as internal energy E , volume V and number of atoms (or moles) N [39].

From the known Maxwell-Boltzmann distribution for kinetic energies, one can obtain the relations for relative variance in single-particle kinetic energy $\varepsilon_k = 1/2 m_k v^2$,

$$\frac{\Delta \varepsilon_k^2}{\langle \varepsilon_k \rangle^2} = \frac{\langle \varepsilon_k^2 \rangle - \langle \varepsilon_k \rangle^2}{\langle \varepsilon_k \rangle^2} = \frac{\langle v_k^4 \rangle - \langle v_k^2 \rangle^2}{\langle v_k^2 \rangle^2} = \frac{2}{3}, \quad (8)$$

and the relative variance in instantaneous temperature T or N -particle kinetic energy E_k [40],

$$\frac{\Delta T^2}{\langle T \rangle^2} = \frac{\Delta E_k^2}{\langle E_k \rangle^2} = \frac{2}{f} = \frac{2}{3N - 3}. \quad (9)$$

Here the values ΔT and ΔE_k are correspondingly standard deviations of T and E_k .

For the case of absence of limitation on the degrees of freedom, the value f should be equal to $3N - 3$ [40]. However, interactions between atoms in solids may lead to the change of the value of f and, consequently, the value of $\langle E_k \rangle / \Delta E_k$ (9). Such an interaction may change the correlation of the positions and velocities of neighboring atoms, which in turn may be temperature-dependent. In the latter case, one may expect to observe, for example, temperature-dependent phonon relaxation time, phonon mean free path and, as a result, the coefficient of thermal conductivity.

Another example of probable change in the above – mentioned value of f could be the temperature-stimulated structural phase transition in solids. In this case, one may expect more or less distinct change of the f value with temperature as it nears the temperature of phase transition of a crystal.

To verify the validity of our supposition, that due to interatomic correlations the temperature dependence of VACF relaxation time $\tau(T)$ and the relative temperature changes of kinetic energy $\Delta E_k / \langle E_k \rangle (T)$ are dependent on one another, we have performed MD calculations for the silicon crystal at different temperatures within the range of 200–1000 K. The MD calculations within the NVE ensemble were performed for the silicon supercell $3 \times 3 \times 3$ containing 216 atoms. The fitted linear dependence of the coefficient of determination (COD) $R^2 \approx 0.94$ between the values τ and $\Delta E_k / \langle E_k \rangle$ indicates the relatively high degree of correlation between these values (Fig. 3).

The linear fit, $y = a + b \cdot x$, of the dependence between the values of $\Delta E_k / \langle E_k \rangle$ and τ is characterized by the relatively high coefficient of determination $R^2 = 0.9296$ (Fig. 3), which stands as clear proof of the validity of this relation. Here ΔE_k is the standard deviation of kinetic energy E_k , and $\langle E_k \rangle$ is the

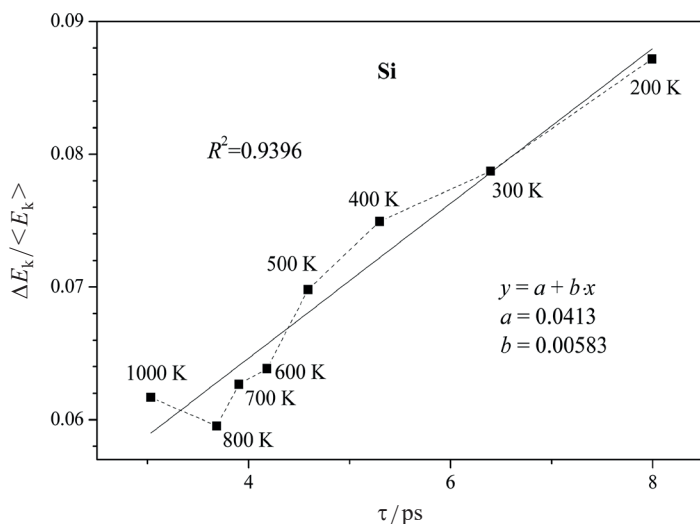


Fig. 3. Correspondence between VACF relaxation time t and relative change of kinetic energy $\Delta E_k / \langle E_k \rangle$ of silicon obtained on the basis of MD calculations at different temperatures within the range of 200–1000 K

averaged value of kinetic energy. This relation could be useful for estimation of temperature-dependent mean phonon relaxation time τ_{ph} and the coefficient of phonon thermal diffusivity D of silicon by means of calculating the value of $\Delta E_k / \langle E_k \rangle$. Evidently, the fitting parameters a and b found (Fig. 3) are characteristic for silicon. Due to the straightforward calculation of the value of $\Delta E_k / \langle E_k \rangle$ on the basis of the molecular dynamics run, the proposed approach may be applied also for study of the coefficient of phonon thermal diffusivity D and thermal conductivity κ_{ph} as functions of different factors: chemical composition, temperature, pressure, etc.

4. Conclusions

In view of the thermal conductivity problem in semiconductors, a new approach to estimate the mean phonon relaxation time τ_{ph} has been proposed using the DFT-based MD and the corresponding analysis of VACF. The mean phonon relaxation time τ_{ph} can be estimated with sufficiently good accuracy as the effective relaxation time τ of the VACF calculated within the range of MD simulation time $\Delta t \approx 2\tau$. The proposed approach has been checked successfully using MD calculation of silicon crystals within the temperature range of 200–1000 K.

The relative fluctuations of the silicon crystal kinetic energy $\Delta E_k / \langle E_k \rangle$ have been found to be in inverse dependence with temperature. Clear correlation with the relatively high coefficient of determination $R^2 = 0.9296$ has been revealed between the fluctuations of the silicon crystal kinetic energy $\Delta E_k / \langle E_k \rangle$ and the corresponding relaxation time τ of the velocity autocorrelation function and the phonon relaxation time. This substantiates the use of the proposed approach for the calculation of values related to heat conductivity in silicon-based semiconductors.

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