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Monte Carlo simulation of thermoelectric properties in silicon nanofilms: diffusive seebeck coefficient analysis[☆]

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ABSTRACT

A silicon based nanofilm is examined by using self-consistent electron-phonon transport model. An ensemble Monte Carlo solver for electrons is coupled with a phonon bath that can have a non-uniform temperature. In this simulator, the electron-phonon scattering rates depend on the local temperature and the boundary conditions are also temperature dependent. Using this simulation tool, the thermoelectric properties can be studied, at the microscopic level, in doped semiconductor nanostructures of different sizes and with different types of interfaces. In the present work, the only electronic so-called diffusive Seebeck coefficient of silicon-based nanofilms is investigated as the phonon drag effect is not considered. The influence of the average temperature, temperature gradient, device size, and carrier concentration are investigated.

1. Introduction

Thermoelectric (TE) conversion has emerged as a promising phenomenon for energy harvesting, particularly for low voltage devices [1]. The efficiency of these TE devices is assessed using the figure of merit $ZT = S^2\sigma T/k$, where S , σ , T , and k represent the Seebeck coefficient, electrical conductivity, temperature, and thermal conductivity of the device, respectively. While bulk silicon has long been studied as a TE material, its ZT value of 0.01 [2] falls short for practical applications. Numerous factors can influence this efficiency, such as the device's size, doping level, and temperature gradient.

Enhancing the ZT can be achieved either by reducing the thermal conductivity or/and by improving and enhancing the electrical properties. Previous experimental [3,4] and theoretical [5] results proved that reducing the thermal conductivity can be done by nanostructuring primarily attributed to scattering at rough boundaries. Another work [6] which was focused on the electronic part of the picture indicates that confinement due to nanostructuring helps in increasing the power factor ($PF=S^2\sigma$). Thus, nanostructuring has acquired in the last years a prominent role in several cutting-edge researches in thermoelectricity due to their unique electronic and thermal properties. Among appealing nanostructures, polytype nanowires as in [7] and dual doped nanowires could be interesting to investigate their thermoelectric performance in

the future. In the present work, an ensemble Monte Carlo (MC) Code for electrons presented in [8] has been modified to study the I-V characteristics in the presence of temperature gradient. This enables the estimation of the Seebeck coefficient (S) of a silicon based nanofilm under the influence of size, temperature, temperature gradient and doping. In our model, the electron-phonon scattering rates vary locally according to the local temperature. Besides, the boundary conditions at terminal contacts are also temperature dependent. The model excludes the phonon drag effect, focusing solely on extracting the diffusion part of the Seebeck coefficient. This MC approach of solving the Boltzmann transport equation is well suited for such investigation since it naturally includes all stochastic features of carrier transport, and it can provide a deep insight into the TE transport at the microscopic level.

2. Model and simulated device

In Fig. 1, a silicon nanofilm with an N-doping of 10^{17} cm^{-3} and a length (thickness) of $1 \mu\text{m}$ in the cross-plane configuration is schematized. This nanofilm is sandwiched between 2 Ohmic contacts regions at both ends with an N-doping of 10^{19} cm^{-3} and a length of 10 nm. These ohmic contacts acts as reference material for the extraction of the Seebeck coefficient for the device in the middle. Thermal gradient (here 280 K-320 K) and voltage differences are applied between contacts. The

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particle Monte Carlo code [8] used here is self-consistently coupled to the Poisson's equation. It is based on an analytical conduction band structure of bulk silicon which consists of six ellipsoidal non parabolic Δ valleys along [100] directions. Their effective masses and non-parabolicity coefficient are $m_l = 0.916 \cdot m_0$, $m_t = 0.19 \cdot m_0$, and $\alpha = 0.5$, respectively. This conduction band description is sufficient since the studies are only conducted close to equilibrium and in low energy scales. The parameters used for intravalley and intervalley electron-phonon scatterings mechanisms are given in [9], and the dependence of the scattering rates on temperature is detailed in [10]. The surface roughness scattering is considered specular to allow comparison with the bulk case.

3. Results

In Fig. 2 (a), non-uniform ($T_{\text{phonon}} = [280 \text{ K}-320 \text{ K}]$) and uniform ($T_{\text{phonon}} = [300 \text{ K}-300 \text{ K}]$) temperature profiles applied along the device are shown in addition to the temperature of electrons (T_{electron}) after moving and scattering inside the device without any voltage bias applied ($V_{\text{applied}} = 0 \text{ V}$). When a non-uniform phonon temperature is applied to the device, the electron temperature is not constant and very close to the phonon one. This occurs because the temperature difference between electrons and phonons tends to be limited by the inelastic electron-phonon scattering. In Fig. 2 (b), the obtained I-V curve for the device is presented in the case of the non-uniform temperature (black dots) and in the case of a uniform temperature of 300 K (red dots). A linear regression (depicted by the red and black solid lines) was applied to the simulated current data points. The total device's Seebeck coefficient, under non-uniform temperature profile, was obtained by dividing the open voltage (extracted as the voltage corresponding to zero current from the linear fit) V_{oc} , by the temperature difference ΔT . The mobility of the total device was obtained from the slope of the linear fit. The obtained total Seebeck coefficient (S) was determined to be $451 \pm 12 \mu\text{V}/\text{K}$. The mobility of the device was determined to be $612 \pm 8 \frac{\text{cm}^2}{\text{V}\cdot\text{s}}$. The difference in S between 10^{17} cm^{-3} and 10^{19} cm^{-3} N-doped bulk silicon without the phonon-drag effect, i.e. only diffusion part, was calculated by [11] to be $378 \mu\text{V}/\text{K}$ at 300 K (where in their work the phonon drag part was shown to take a strong and crucial role).

In Fig. 3, at a bias voltage of 0 V, 0.05 V, and 0.1 V the kinetic energy of electrons, the electrostatic potential, and the electric field profiles along the length of the simulated device are plotted. As previously mentioned, the increase in electron energy along the device (Fig. 3 (a)) primarily stems from the initial imbalance between electron and phonon energies. The effect of the applied voltage on the kinetic energy is barely noticeable due to the small applied voltages.

Fig. 3 (b) shows the electrostatic potential difference between the contacts and the device's middle due to doping variation. The non-uniform electron temperature drives electrons from hot to cool regions, altering their distribution. This causes a linearly decreasing electrostatic potential even when no voltage bias is applied. As V_{app} increases, the potential flattens at $V_{\text{app}} = V_{\text{oc}}$ where the applied field counteracts this movement and forces uniform distribution. For $V_{\text{app}} > V_{\text{oc}}$, the field dominates, reversing the imbalance and creating a linear increase in the potential. The electric field which is the negative derivative of the potential along the device, is presented in the inset of Fig. 3 (b). Understanding the impact of non-uniform temperature profiles and applied voltage on electron kinetics not only enriches our understanding of thermoelectric transport mechanisms but also offers valuable insights for the designing better thermoelectric devices.

In Fig. 4, the total diffusive Seebeck coefficient (which is the difference between the one of the low doping material - 10^{17} cm^{-3} - and the reference material, i.e. contacts at 10^{19} cm^{-3}) was calculated for different average temperatures and for different temperature gradients at 300 K. The Seebeck coefficient decreases as the temperature increases, primarily due to higher scattering rates, which hinder electron movement toward the colder side. On the other hand, the Seebeck coefficient seems to be constant and barely changes for various temperature differences in Fig. 4(b). The slight variation can be attributed to simulation uncertainty. This was also observed in [12], where in their TE device the Open Circuit Voltage V_{oc} seems to increase linearly with the increase of temperature gradient which ensures that the obtained results are consistent, and the Seebeck coefficient is not affected.

This difference in the diffusive thermopower was also investigated with respect to different device's length and doping at 300 K and plotted in Fig. 5. The Seebeck coefficient slightly increases with device length because longer devices experience more scattering, enhancing energy distribution asymmetry. In shorter, ballistic devices, the energy distribution remains more uniform, resulting in a lower Seebeck coefficient. In contrast, Fig. 5(b) shows that the diffusive Seebeck coefficient for bulk silicon decreases with increasing carrier concentration. This decline is attributed to the reduced energy difference between carriers and the Fermi level. Our results, when compared to those in [11], are found to be close, where the coupled Boltzmann transport equations are solved.

4. Conclusion

The device's Seebeck coefficient and thermoelectric transport properties were investigated for a silicon-based nanofilm by using an ensemble Monte Carlo solver for electrons considering a phonon bath

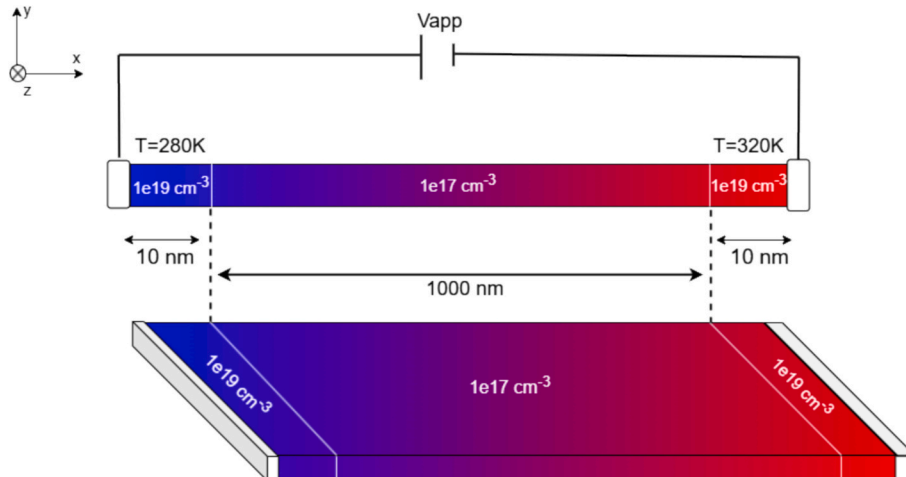


Fig. 1. Schematic view of the TE device studied.

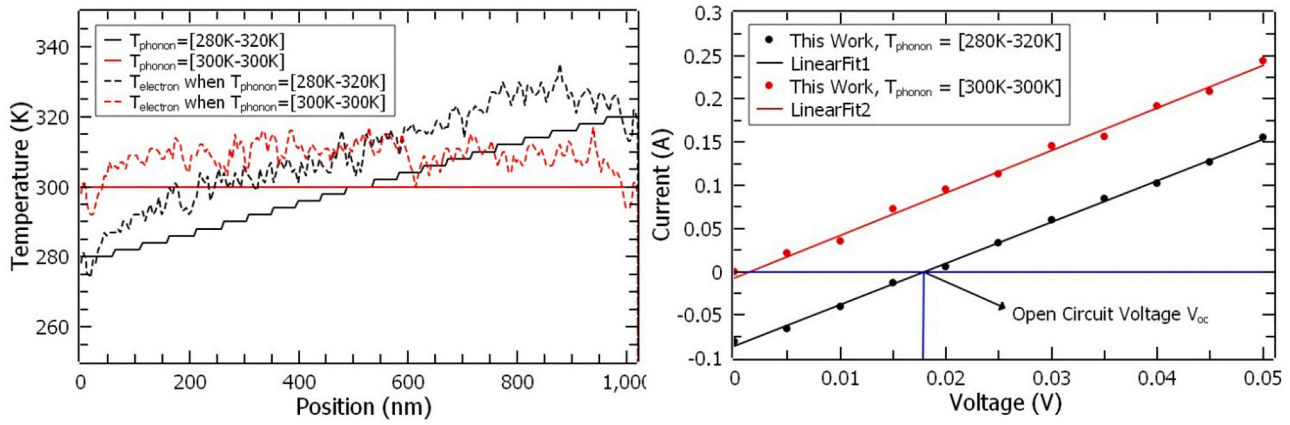


Fig. 2. (a) Non-uniform (black solid line) and uniform (red solid line) applied temperatures in addition to the calculated temperature of electrons (dashed lines) along the device length. (b) Simulated I-V curves (dots) and their linear regression (solid lines). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

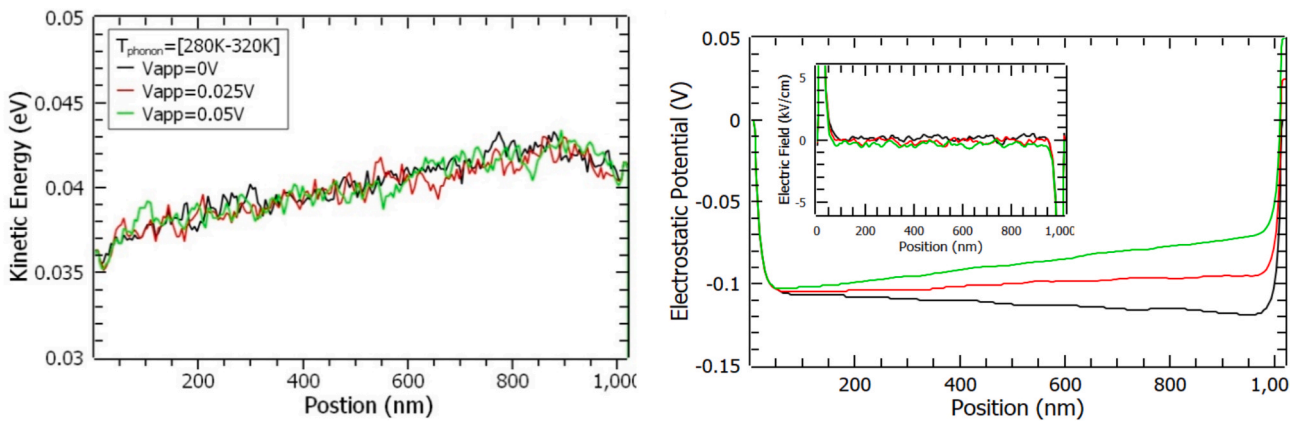


Fig. 3. Electrons kinetic energy (a) and electrostatic potential created (b) as a function of the position. Inset: corresponding electric field.

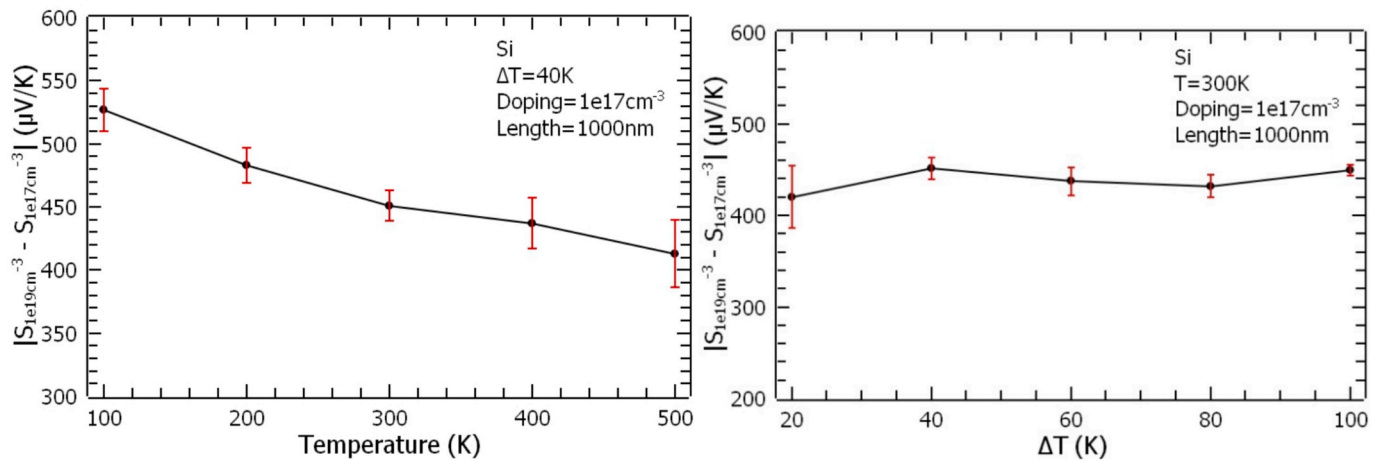


Fig. 4. Seebeck coefficient of the simulated nanofilm with respect to different (a) temperatures and (b) temperature gradients at 300 K.

with a non-uniform temperature. The obtained Seebeck coefficient in this work seems to be comparable and consistent with previous experimental and simulation works, and the computed microscopic thermoelectric transport results are expected to help designing better thermoelectric devices. In future work, different polytype and dual doping nanowires will be investigated, and phonon drag effects will also be implemented in our simulator, which will provide a more accurate

tool to optimize and test the TE device performance in these kinds of nanostructures.

CRedit authorship contribution statement

Mohammad Ghanem: Writing – original draft. **Philippe Dollfus:** Supervision. **Jerome Saint-Martin:** Supervision.

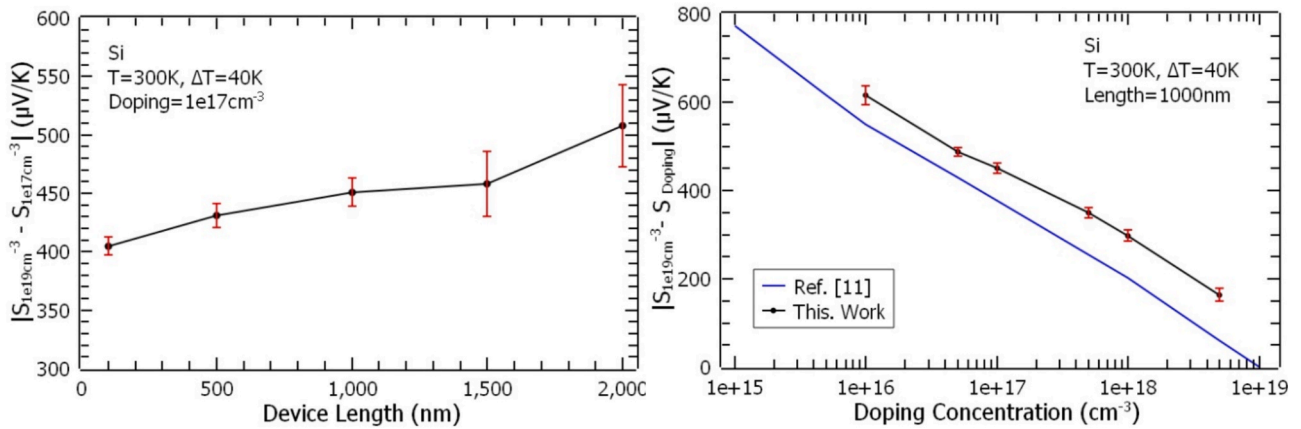


Fig. 5. Seebeck coefficient of the simulated nanofilm with respect to different (a) device length and (b) carrier concentration at 300 K.

Declaration of competing interest

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Data availability

Data will be made available on request.

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