

Monte Carlo Modeling of Phonon Drag Effects on Thermoelectric Transport in Silicon Nanostructures with doping modulation

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Abstract—Silicon nanofilms, with and without doping modulation, are investigated using an original ensemble Monte Carlo solver that explicitly couples electron transport to a phonon bath with a spatially non-uniform temperature. This advanced approach enables a fully self-consistent microscopic description of thermoelectric transport, including phonon drag effects, which are usually neglected or treated phenomenologically. The developed framework provides real-space resolution of electrothermal transport and enables a detailed analysis of thermoelectric properties in silicon nanostructures with varying dimensions and interface characteristics. It captures size-dependent effects, in particular, the space-charge layer resulting from the modulation of the potential barrier, as well as nonlocal transport phenomena that strongly influence the thermoelectric behavior of short doping-modulated nanostructures.

Keywords— Thermoelectrics, Monte Carlo, Simulation, Phonon drag, Doping modulation-, Seebeck coefficient.

I. INTRODUCTION

Thermoelectric (TE) conversion is a promising technology for solid-state cooling and low-power energy harvesting because it directly converts heat into electricity without moving parts [1]. Its performance is commonly characterized by the dimensionless figure of merit, $ZT = S^2 \sigma T / \kappa_{th}$, where S is the Seebeck coefficient, σ the electrical conductivity, T the absolute temperature, and κ_{th} the thermal conductivity. Since the electrical conductivity and the Seebeck coefficient are generally antagonistic with respect to the carrier concentration, improving the thermoelectric power factor $S^2 \sigma$ remains one of the major challenges in thermoelectric material design.

Nanostructuring [2],[3] has emerged as an effective strategy for enhancing thermoelectric performance by independently tailoring electron and phonon transport. In particular, doping-modulated nanostructures [4], [5] have attracted considerable attention because they can exploit energy-filtering mechanisms and built-in electric fields to increase the Seebeck coefficient while maintaining a relatively high electrical conductivity. However, the transport in such

structures is inherently non-local and governed by strong electrostatic fields and non-equilibrium carrier dynamics, limiting the applicability of conventional analytical models based on bulk transport coefficients.

At room temperature, another important contribution to thermoelectric transport is the phonon-drag effect, which results from momentum exchange between charge carriers and nonequilibrium phonons [6]. Although this effect has been extensively investigated in bulk materials, its incorporation into real-space transport simulations of nanostructures remains challenging, particularly when electrostatic effects and spatially varying doping profiles must be considered simultaneously.

In this work, an original electro-thermal ensemble Monte Carlo approach [7], incorporating phonon drag effect [8], is employed to investigate the thermoelectric properties of silicon nanofilms with and without doping modulation.

II. MODEL

A. Electrothermal Ensemble Monte Carlo Simulator

To solve the Boltzmann transport equation for electrons, we used an in-house particle-based ensemble Monte Carlo solver self-consistently coupled with Poisson's equation. The model uses an analytical conduction-band model consisting of six non-parabolic ellipsoidal Δ valleys. Both inter- and intravalley electron-phonon scattering, as well as electron-charged-impurity scattering, are taken into account. All the effective masses and scattering parameters used in the model were reported in [9].

This electron transport model is coupled to a phonon bath with a spatially non-uniform temperature. Accordingly, the electron-phonon scattering rates are evaluated using the local phonon temperature, while the boundary conditions are treated in a temperature-dependent manner. Full details of the electrothermal model and its numerical implementation are provided in [10].

B. Phonon drag implementation

More recently, we proposed an extension of our electrothermal model presented previously, originally developed to evaluate self-heating effects in electronic devices, in order to capture thermoelectric phenomena. To achieve this, the implementation of the phonon-drag effect is essential.

In our approach, presented in details in [8], the phonon-drag effect is incorporated at the particle level through an additional term in the treatment of electron-phonon scattering. Then, after each electron-acoustic-phonon scattering event (assumed as elastic without considering the phonon drag effect), the final electron wave vector, denoted $\vec{k}_f$, is given by:

$$\vec{k}_f = \vec{k}_0 + \vec{q}_0 \quad (1)$$

where $\vec{k}_0$ is the electron wave vector selected isotopically on the iso-energy surface without considering any momentum exchange (valid when the phonon bath is at equilibrium), and $\vec{q}_0$ represents the exchange wave vector (i.e. phonon wave vector) associated with the phonon-drag effect, due to the out of equilibrium distribution of phonon population. Then, the final electron energy is updated accordingly.

In the present implementation, only the momentum exchange along the transport direction is considered and a constant momentum transfer $\vec{q}_0 = q_x \hat{x}$ is used. The value of $q_x \hat{x}$ is obtained from the average momentum exchanged between the electrons and a nonequilibrium phonon bath characterized by the distribution $N_{0,\lambda} + \delta N_\lambda$ where $N_{0,\lambda}$ is the equilibrium Bose-Einstein distribution $N_{0,\lambda}$ and δN_λ stands for its deviation from equilibrium. The average momentum is therefore given by:

$$\langle q_x \rangle = \frac{\int \int \int (N_{0,\lambda} + \delta N_\lambda) \cdot q_x \cdot dq_x dq_y dq_z}{\int \int \int (N_{0,\lambda} + \delta N_\lambda) \cdot dq_x dq_y dq_z} \quad (2)$$

One important issue of this approach is the evaluation of the nonequilibrium phonon population δN_λ . In the present work, we assume that the phonon population remains close to equilibrium. Under this assumption, δN_λ is obtained from the analytical solution of the linearized phonon Boltzmann transport equation.

III. MODULATED DOPING STRUCTURES

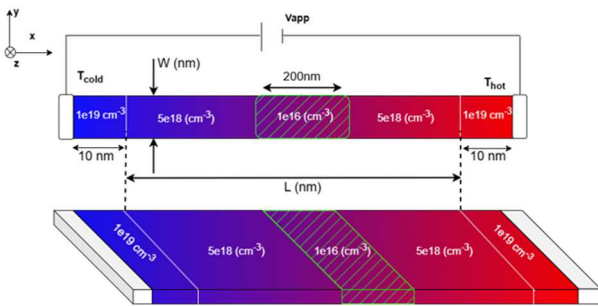


Fig. 1. Schema of studied thermoelectric devices.

A key advantage of the present approach is its ability to resolve real-space profiles beyond the bulk configuration. This capability is particularly important for doping-modulated structures, which combine lightly and heavily doped regions. Such devices are expected to exploit the high Seebeck

coefficient of the lightly doped region while benefiting from the high electrical conductivity of the heavily doped region.

In this work, we have simulated devices schematized in Fig. 1. The central and active part, where we want to optimize the thermoelectric properties, consists of a slab of a lightly doped N-type region of 10^{16} at./cm^3 sandwiched between heavily doped N-type silicon regions of $5 \times 10^{18} \text{ at./cm}^3$. Near the two electrodes a highly N-doped region of 10^{19} at./cm^3 is used as a reference material for the Seebeck coefficient extraction as explained in [8].

In this work, the distance L between the two reference materials, where the voltage and temperature difference are applied, is fixed at $1 \mu\text{m}$, while the slab length is varied. The device is assumed to be infinitely extended in the transverse (y and z) directions, as specular boundary conditions are applied at the external interfaces.

IV. RESULTS

As detailed in [8], the thermoelectric properties of the device schematized in Fig. 1 are extracted from the current-voltage I-V characteristics computed for a given temperature difference, $\Delta T = T_{\text{hot}} - T_{\text{cold}}$. For each value of ΔT , the corresponding open-circuit voltage V_{oc} was determined. The Seebeck coefficient of the material under investigation was then obtained from the ratio $V_{\text{oc}}/\Delta T$ after subtracting the contribution of the reference materials.

A. Seebeck coefficient without doping modulation

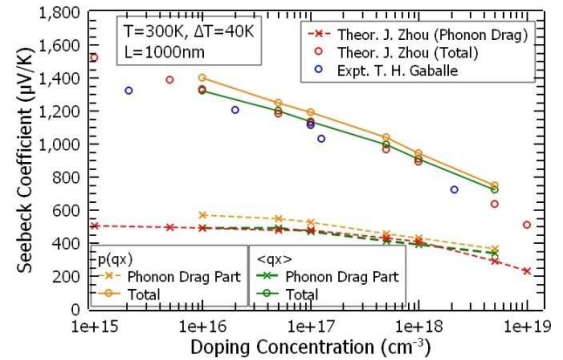


Fig. 2. Bulk Si, total Seebeck coefficient (circles) and phonon drag contribution (crosses) as a function of doping concentration vs. previous theoretical [11] and experimental works [12] at 300K

Fig. 2 compares the calculated Seebeck coefficient of bulk silicon with experimental measurements over a wide range of doping concentrations at room temperature. In this validation case, the device does not contain any doping-modulated slab, allowing a direct comparison with bulk experimental data. The predicted total Seebeck coefficient is in good agreement with the measurements reported in the literature [12]. Moreover, the phonon-drag contribution predicted by our model is consistent with values reported by other theoretical studies [11].

These results validate the implementation of the phonon-drag model and demonstrate that the proposed Monte Carlo framework provides a physically consistent and quantitative description of thermoelectric transport in bulk silicon, forming a reliable basis for the investigation of more complex nanostructures with spatially varying doping profiles.

B. Microscopic results in doping modulated devices

Our Monte Carlo simulator provides a microscopic picture of thermoelectric transport. As an illustration, Fig. 3 presents the spatial profiles of the local carrier kinetic energy of electrons and the electrostatic potential along the transport direction (x direction) for different lengths of the lightly doped slab. The simulations were performed under short-circuit conditions (zero voltage bias), assuming a linear lattice (phonon) temperature profile between the two contacts.

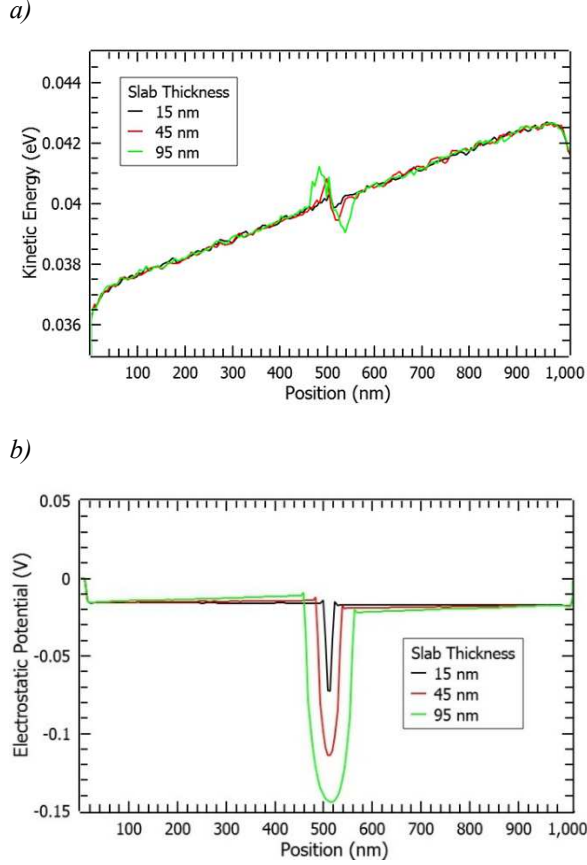


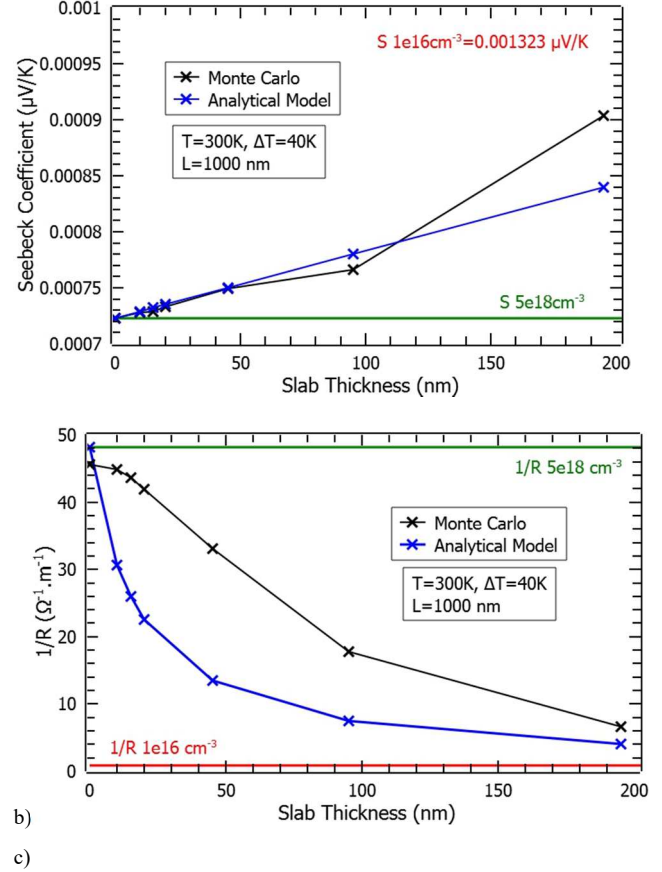
Fig. 3. (a) Electron kinetic energy (proportional to electronic temperature) and (b) electrostatic potential profiles for different slab lengths 15 nm, 45 nm and 95 nm at 300 K for temperature difference of 40 K without any voltage bias.

Since the average electron kinetic energy is equal to $\frac{3}{2}k_B T_e$, where k_B is the Boltzmann's constant and T_e is the local electron temperature, the nearly linear profile shown in Fig. 3(a) indicates that the electron temperature remains close to the local lattice temperature throughout most of the device. Noticeable deviations are only observed in the vicinity of the lightly doped region.

These deviations are explained by the corresponding electrostatic potential profile presented in Fig. 3(b). For all presented slab lengths shorter than 95 nm, the lightly doped region is not fully depleted, resulting in a sharp potential variation and, consequently, the formation of strong electric fields on both sides of the low-doped region. These electric fields significantly modify the carrier transport, causing it to deviate from the conventional low-field mobility regime.

As electrons enter the depletion region near the low doped slab, they are initially cooled by the decelerating electric field, leading to a reduction in their kinetic energy. They are subsequently heated as they traverse the opposite side of the potential barrier. These local cooling and heating phenomena are characteristic of local thermoelectric effects that can only be captured using a spatially resolved transport model.

a)



b)

c)

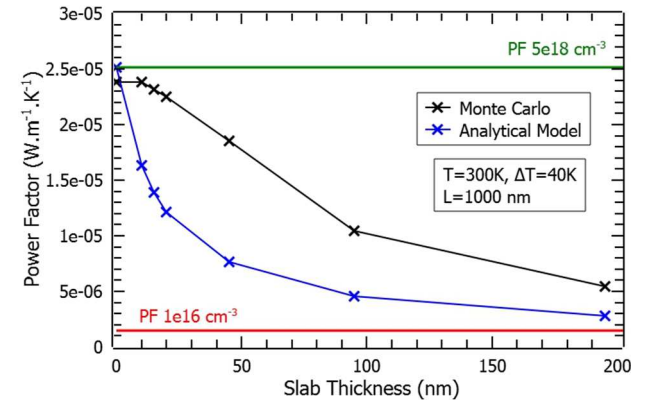


Fig. 4. a) Total Seebeck coefficient S (with phonon drag) and b) total conductance $1/R$ as a function of the slab length (with a modulated doping of 10^{16} cm^{-3}) in c) Power factor S/R a $1 \mu\text{m}$ long device (with a doping level of $5 \cdot 10^{18} \text{ cm}^{-3}$ in the background). Monte Carlo results (black) vs. series resistance model (blue).

C. Seebeck parameter in doping modulated devices

Fig. 4(a) shows that the Seebeck coefficient increases nearly linearly with the length of the lightly doped region for slab lengths below approximately 100 nm. For larger slab

lengths, however, the Monte Carlo (MC) predictions deviate significantly from this linear trend, yielding substantially higher Seebeck coefficients. For comparison, a simple analytical model based on a length-weighted average of the bulk Seebeck coefficients of the lightly (10^{16} at./cm^3) and heavily ($5 \times 10^{18} \text{ at./cm}^3$) doped regions predicts a linear increase of the Seebeck coefficient over the entire range of slab lengths.

D. Electrical conductance in doping modulated devices

Electrical conductance is even less accurately described by a simple series-resistance model, in which the resistance of each region is assumed to scale linearly with its length while neglecting carrier redistribution and nonequilibrium transport at the interfaces. Such a model predicts that the total resistance is dominated by the highly resistive lightly doped slab, resulting in an linear increase in resistance with slab length L_{slab} , or equivalently a conductance decreasing as $\frac{1}{L_{\text{slab}}}$.

The Monte Carlo simulations show a different behavior, as shown in Fig. 4(b). For short slab lengths, the conductance remains significantly higher than predicted by the analytical model. This discrepancy originates from the strong built-in electric fields generated by the doping modulation, which extend across a large fraction of the lightly doped region. These fields accelerate the carriers and produce a highly nonequilibrium transport regime that cannot be described by local transport coefficients. As the slab length increases, the influence of the depletion regions becomes progressively confined to the slab edges, and the transport gradually approaches the diffusive limit.

E. Power factor in doping modulated devices

The combined inaccuracies in the analytical predictions of both the Seebeck coefficient S and the electrical conductance G naturally lead to large errors in the estimation of the thermoelectric power factor, ($PF = S^2 \cdot G$). Figure 4(c) shows that the Monte Carlo simulations consistently predict significantly larger power-factor values than the analytical model over the entire range of slab lengths.

Overall, these results demonstrate that doping-modulated structures cannot be accurately described using conventional effective-medium or series-resistance approaches. A spatially resolved microscopic transport model is required to correctly predict their thermoelectric performance and to identify device geometries that maximize the power factor.

It should be noted that the doping concentration of the heavily doped regions remains below the value that maximizes the thermoelectric power factor, which is typically achieved for concentrations around $5.10^{19} \text{ at./cm}^3$. The doping-modulated structures investigated in this work were primarily intended to validate the proposed methodology rather than to optimize the device performance.

V. CONCLUSION

In this work, we have developed a real-space electron Monte Carlo framework incorporating the phonon-drag effect through a microscopic treatment of electron-phonon momentum exchange. The model accurately reproduces the Seebeck coefficient of bulk silicon over a wide range of doping concentrations, providing a solid validation of the proposed approach.

The simulations indicate that doping modulation can significantly enhance the Seebeck coefficient while only moderately reducing the electrical conductance. More important, the transport properties are shown to be governed by the interplay between built-in electric fields, space-charge regions, nonequilibrium carrier dynamics, and finite-size effects. As a consequence, conventional analytical models based on bulk transport coefficients fail to accurately predict the thermoelectric performance of these nanostructures.

The proposed framework therefore provides a physically consistent and predictive tool for the investigation and optimization of doping-engineered thermoelectric devices. Furthermore, it can be readily coupled to advanced phonon transport solvers, such as phonon Monte Carlo methods [13], to achieve a fully self-consistent description of electron-phonon transport under nonequilibrium conditions.

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