2012

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Kim, Raseong and Lundstrom, Mark S., "Computational study of energy filtering effects in one-dimensional composite nano-structures" (2012). *Department of Electrical and Computer Engineering Faculty Publications*. Paper 141.
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Computational study of energy filtering effects in one-dimensional composite nano-structures

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(Received 21 August 2011; accepted 16 December 2011; published online 25 January 2012)

Possibilities to improve the Seebeck coefficient S versus electrical conductance G trade-off of diffusive composite nano-structures are explored using an electro-thermal simulation framework based on the non-equilibrium Green's function method for quantum electron transport and the lattice heat diffusion equation. We examine the role of the grain size d , potential barrier height Φ_B , grain doping, and the lattice thermal conductivity κ_L using a one-dimensional model structure. For a uniform κ_L , simulation results show that the power factor of a composite structure may be improved over bulk with the optimum Φ_B being about $k_B T$, where k_B and T are the Boltzmann constant and the temperature, respectively. An optimum Φ_B occurs because the current flow near the Fermi level is not obstructed too much while S still improves due to barriers. The optimum grain size d_{opt} is significantly longer than the momentum relaxation length λ_p so that G is not seriously degraded due to the barriers, and d_{opt} is comparable to or somewhat larger than the energy relaxation length λ_E so that the carrier energy is not fully relaxed within the grain and $|S|$ remains high. Simulation results also show that if κ_L in the barrier region is smaller than in the grain, S and power factor are further improved. In such cases, the optimum Φ_B and d_{opt} increase, and the power factor may improve even for Φ_B (d) significantly higher (longer) than $k_B T$ (λ_E). We find that the results from this quantum mechanical approach are readily understood using a simple, semi-classical model. © 2012 American Institute of Physics. [doi:10.1063/1.3678001]

I. INTRODUCTION

For a high efficiency of thermoelectric (TE) energy conversion, the figure of merit $ZT = S^2 G T / K$ should be maximized.¹ The figure of merit is the product of the Seebeck coefficient S , the electrical conductance G , and the temperature T , divided by the thermal conductance K , which is the sum of the electronic contribution K_e and the lattice contribution K_L . It has been difficult to increase ZT because its components are interdependent.² Recently, the application of nanotechnology has achieved significant breakthroughs in TE devices - mostly due to the reduced K_L .³⁻⁸ Another possibility to improve ZT is by improving the power factor, $S^2 G$. Some success has been reported,⁹ but it is not easy to obtain a dramatic improvement in $S^2 G$ unlike the case of K_L , where orders of magnitude of suppression can be achieved by material and surface engineering.^{5,6} Possibilities being explored include reduced dimensionality,^{10,11} thermionic emission devices with non-conserved lateral momentum,¹²⁻¹⁴ and composite band structures.⁹

Recently, nano-composite materials are attracting attention as a way to improve ZT . Nano-composite materials are fabricated by thermal processing and powder metallurgy,^{15,16} and they are composed of grains and grain boundaries, where the grain is a doped crystalline region, and the grain boundaries are potential barriers introduced by point defects, etc.¹⁷ Although much of the experimental improvement still comes

from the reduced K_L ,^{4,7,8} there are reports that the power factor may also be improved.^{18,19}

Currently, the design of nano-composite TE materials is largely empirical. Theoretical and simulation studies can help understand the physics of nano-composite materials and the optimization of the material design. Previous studies¹⁹⁻²² adopt semi-classical approaches using the Boltzmann transport equation (BTE) treating the effect of grain boundaries as a scattering mechanism with some relaxation time. As the grain size shrinks and approaches the electron wave length,²³ however, it becomes essential to treat quantum effects. In a recent paper, Minnich *et al.*²⁴ pointed out that several of the characteristic lengths in nano-composites are shorter than the electron wave length, which is expected to invalidate the BTE.

Our goal in this paper is to computationally explore the possibilities to improve the S versus G trade-off and the power factor of diffusive composite nano-structures using a fully quantum mechanical approach. We use an electro-thermal simulation framework similar to that developed in our previous work²⁵ to explore the TE properties of one-dimensional (1D) composite nano-structures. We address following questions: (1) "Can the power factor of composite nano-structures, in principle, exceed that of a uniform material? If so, what are the conditions for which an enhanced power factor can be expected?;" (2) "Can we interpret the fully quantum mechanical results in semi-classical terms?" Surprisingly, we find that the results from our quantum mechanical model can be readily understood in terms of the existing semi-classical understanding. We also find that significant increase in the power factor can result from engineering the lattice heat flow across the grain boundary.

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This paper is organized as follows. In Sec. II, we explain our model device and simulation methods to compare TE performance across composite and bulk structures. In Sec. III, simulation results for S versus G and power factor are presented for composite structures with uniform and non-uniform lattice thermal conductivities and compared with those for bulk. In that section, we also clarify the condition under which the power factor of a composite structure can be improved over bulk. In Sec. IV, we identify special features of 1D composite structures and discuss the expected features of three-dimensional (3D) composite nano-structures. The limitations of our model are also discussed in that section. Conclusions follow in Sec. V.

II. APPROACH

A. Model device

Figure 1 shows the schematic of our model device to treat 1D composite nano-structures with x being the transport direction. A 1D channel of length L is connected to two ideal reservoirs²⁶ contact 1 and contact 2, which are maintained under equilibrium with Fermi levels E_{F1} and E_{F2} . For a fixed $L = 300$ nm, we vary the number of barriers within the channel to change the grain size d . If there are five barriers in the channel, for example, $d = 60$ nm. Note that when we define d , we do not consider the finite thickness of the barrier l_b , which is 5 nm in our model device. To describe the potential barrier and grain doping, we define two quantities, i.e., the barrier height Φ_B and the conduction band edge in the grain $E_{C,g}$. We assume rectangular potential barriers. Note that $E_{F1} \equiv E_F$ always lies at 0 eV, and the values of Φ_B and $E_{C,g}$ are defined from this reference. We assume 1D model structures that allow us treat dissipative quantum transport rigorously with a modest computational burden.²⁶ The model device is simple, but note that we follow a common process in scientific research—first reduce a problem to its simplest possible form, then understand the essential physics, and finally add the problem-specific details. Our paper focuses on understanding the essential physics of the problem.

B. Simulation methods

In this work, we use an electro-thermal simulation framework similar to that developed in our previous work.²⁵ We assume that the potential profiles depicted in Fig. 1 are fixed and do not solve the Poisson scheme self-consistently. Fixing the potential profile helps us clearly understand the effect of varying d and carrier scattering on the TE performance of a composite structure. Electron transport is described by the non-equilibrium Green's function method with hopping parameters from the effective mass m^* .^{26,27} For our model device, we assume $m^* = 0.25m_0$, where m_0 is the free electron mass. It should be noted that the lattice heat diffusion equation is still solved self-consistently with electron transport because it is essential to treat both to calculate the TE properties of a diffusive composite structure.²⁵ For carrier scattering, we assume an optical phonon process with a deformation potential D_0 ,²⁶ which can be related to the conventional optical phonon deformation potential D_{op} ²⁸ as

FIG. 1. (Color online) Schematic of the model device to treat 1D composite nano-structures where x is the transport direction, L is the channel length, d is the grain size, l_b is the barrier thickness, Φ_B is the barrier height, and $E_{C,g}$ is the conduction band edge in the grain. In this work, $L = 300$ nm and $l_b = 5$ nm. The channel is connected to ideal reservoirs contact 1 and contact 2 with Fermi levels E_{F1} and E_{F2} , respectively.

$D_0 = \hbar D_{op}^2 F / (2\rho\omega_o a^3)$,²⁹ where $\hbar$ is the reduced Planck constant, F is the wave function overlap,³⁰ ρ is the mass density, ω_o is the optical phonon frequency, and a is the grid size. We consider optical phonon scattering because it is the simplest way to capture the essential physics of diffusive transport, where both momentum and energy are relaxed. In all following simulations, we use $\hbar\omega_o = 20$ meV with $D_0 = 0.005$ eV² for $a = 0.5$ nm. For these model parameters, we obtain momentum relaxation lengths $\lambda_p = 14 \sim 4.3$ nm (or mobility $\mu = 125 \sim 88$ cm² V⁻¹ s⁻¹) for bulk wires (i.e., 1D channel with no potential barrier) with the conduction band edge E_C lying at $-0.15 \sim 0.1$ eV, which correspond to 3D carrier densities of $7.3 \times 10^{19} \sim 9.6 \times 10^9$ cm⁻³. For the lattice heat conduction, we assume that the lattice thermal conductivity κ_L is uniform (Sec. III A) or it varies along the x -direction (Sec. III B). The wire diameter is assumed to be 3 nm to solve the 1D heat diffusion equation.²⁵

As discussed in our previous work,²⁵ there are two ways to numerically “measure” S , i.e. open-circuit voltage measurement for a temperature difference ΔT or current measurements for finite ΔT and ΔV , where ΔV is the voltage difference between two contacts. The two approaches are equivalent,²⁵ so we calculate S using the current measurement approach, which usually requires fewer simulation runs.

C. Comparing S versus G

Next, we discuss how we generate and compare the S versus G curves for the composite and bulk structures. The S versus G curve of a composite structure for the given Φ_B and $E_{C,g}$ is generated by changing d within a fixed L . For a large d (fewer barriers within the channel), the G is high while $|S|$ is low due to the relaxation of carrier energy in the grain.²⁵ For a smaller d (many barriers within the channel), $|S|$ increases because the carrier energy is less relaxed within the grain while G degrades due to the barriers. In all following simulations, we vary d as 300 (one barrier within the channel), 150, 100, 75, 60, 50, 37.5, 30, 25, 20, 15, 12, 10, and 7.5 nm (40 barriers within the channel), which are basically the divisors of $L = 300$ nm. Then the process is repeated for other composite structures with different Φ_B and $E_{C,g}$ values. For bulk structures, the S versus G curve is generated by changing the doping density, i.e., E_C throughout the device.

III. RESULTS

A. Uniform κ_L

In this section, we present simulation results for a uniform κ_L , which gives a linear lattice temperature T_L profile along the device. We use a κ_L value of 1.5 W/m-K, which is 100 times smaller than that of the bulk silicon to take account that κ_L is dramatically suppressed in wire structures.^{6,31} Figure 2 shows the simulation results for the energy (E) and position (x) resolved current $I(E, x)$ for a composite structure with $\Phi_B = 40$ meV, $E_{C,g} = -0.06$ eV, $\Delta V = 1$ mV and $T_1 = T_2 = 300$ K for $d = 100$ and 30 nm, where T_1 and T_2 are the temperatures of contact 1 and contact 2, respectively. On the barrier, the average energy of the current flow $\langle E \rangle$ is high in both cases due to the filtering of low energy carriers. As d gets larger, the carrier energy is more relaxed within the heavily doped grain region, so $\langle E \rangle$ decays more in Fig. 2(a) than in Fig. 2(b). Therefore, the overall $|S|$ is lower for the device in Fig. 2(a) ($S = -111$ μ V/K) than in Fig. 2(b) ($S = -165$ μ V/K). Note that the decay rate of $\langle E \rangle$ within the grain depends on the relative length of d compared to the energy relaxation length λ_E .^{19,22,25,32} More details of λ_p and λ_E of our model device will be discussed later.

FIG. 2. (Color online) Simulation results for $I(E, x)$ of composite nanostructures with $\Phi_B = 40$ meV, $E_{C,g} = -0.06$ eV, $\Delta V = 1$ mV, $T_1 = T_2 = 300$ K, and a uniform $\kappa_L = 1.5$ W/m-K. The E_{F1} lies at 0 eV, and the brighter color represents the higher intensity of $I(E, x)$. Note that the total current, $I(x) = \int dE I(E, x)$, is constant along x due to charge conservation. In all simulations, an optical phonon process with $\hbar\omega_o = 20$ meV and $D_0 = 0.005$ eV² ($a = 0.5$ nm) is considered. For $d = 100$ nm in (a), $\langle E \rangle$ is more relaxed, and the overall $|S|$ is smaller ($S = -111$ μ V/K) than for $d = 30$ nm in (b) ($S = -165$ μ V/K).

Figure 3 shows the simulation results for $|S|$ versus G and power factor (S^2G) versus G of bulk and composite structures with various Φ_B values (10, 20, 40, 60, 80, and 100 meV) with $E_{C,g} = -0.06$ eV. As explained in Sec. II, the curve for bulk is generated by changing E_C throughout the device. For the results in Fig. 3, $E_C = -0.15 \sim 0.04$ eV. For composite structures, curves are generated by changing d for the given sets of Φ_B and $E_{C,g}$. While the features are less clear in the $|S|$ versus G curve in Fig. 3(a), we see that the maximum S^2G improves for composite structures with Φ_B of 10 ~ 40 meV in Fig. 3(b) with the maximum improvement being about 12% for $\Phi_B = 20$ meV. For $\Phi_B = 60$ meV, the peak value of S^2G is comparable to that of bulk, and as Φ_B gets higher than that, the maximum S^2G of a composite structure becomes smaller than that of bulk as shown in Fig. 3(b). For those high Φ_B values (80 and 100 meV), the degradation of the S versus G trade-off is also clearly seen in Fig. 3(a).

As shown in Fig. 3, for a diffusive composite nanostructure with energy relaxing scattering, there exists an optimum Φ_B that improves the power factor over bulk, and it is around $k_B T \sim 26$ meV where k_B is the Boltzmann constant, and $T = 300$ K. If Φ_B is much higher than that, then S^2G is degraded. These results can be understood in the following

FIG. 3. (Color online) Simulation results for (a) $|S|$ vs G and (b) S^2G vs G for diffusive bulk and composite nano-structures with various Φ_B values (shown in the legend) and $E_{C,g} = -0.06$ eV for a uniform $\kappa_L = 1.5$ W/m-K. As shown in Fig. 3(b), the maximum S^2G improves over bulk for composite structures with $\Phi_B = 10 \sim 40$ meV, and the maximum improvement is about 12% for $\Phi_B = 20$ meV. For $\Phi_B = 60$ meV, the maximum S^2G is comparable to the bulk case, and for the Φ_B higher than that, the maximum power factor becomes inferior to that of bulk.

way. If Φ_B is too low, then the characteristics will approach to those of bulk. If Φ_B is too high, then S improves significantly, but G may be degraded even more. At the optimum $\Phi_B \sim k_B T$, S still improves while G is less degraded because the current flow near E_F is not obstructed too much due to barriers. Note that this interpretation is qualitative, and more quantitative results for the optimum Φ_B may depend on the problem-specific details such as material and scattering parameters as partly discussed in Sec. III B. Figure 4 shows the results for the optimum S and G (S_{opt} and G_{opt}) extracted at the peaks of the S^2G curves of the composite structures for various Φ_B values in Fig. 3(b). The optimum S and G for bulk (values for $E_C \sim 0$ eV in Fig. 3) are also shown as a reference. (Note that S_{opt} for bulk, $-151 \mu\text{V/K}$ in Fig. 4(a), corresponds to the optimum S theoretically reported for 1D conductors with a parabolic band and phonon scattering, $-167 \mu\text{V/K}$ ^{33,34} or equivalently, $-1.94 \times k_B/q$,³⁵ where q is the unit charge. The difference may come from different transport models, i.e., numerical quantum transport simulations (our case) versus analytical semi-classical calculations.^{33,35}) As Φ_B becomes very large, $|S_{\text{opt}}|$ increases significantly in Fig. 4(a), but G_{opt} degrades even more in Fig. 4(b), so the overall power factor in Fig. 4(c) becomes inferior to that of bulk. The peak of $S^2_{\text{opt}}G_{\text{opt}}$ occurs at around $\Phi_B \sim k_B T$. Note that these numerical results are in accordance with the optimum Φ_B values reported in previous studies of heterostructures based on analytical models.^{18,36}

Figure 5 shows simulation results for $|S|$ versus G and S^2G versus G for bulk and composite nano-structures with a fixed $\Phi_B = 40$ meV and various $E_{C,g}$ values of -0.03 , -0.06 , -0.09 , and -0.12 eV, which correspond to 3D doping densities of about $3 \times 10^{19} \sim 6 \times 10^{19} \text{ cm}^{-3}$ for our model device. In Fig. 5(a), it is clearly seen that the S versus G trade-off improves as $|E_{C,g}|$ increases (i.e., grain doping density

FIG. 4. (Color online) (a) $|S_{\text{opt}}|$ and (b) G_{opt} extracted at the peaks of S^2G curves in Fig. 3(b) for composite nano-structures for various Φ_B values. The optimum S and G for bulk are also shown. As Φ_B increases, $|S_{\text{opt}}|$ increases significantly, but G_{opt} degrades accordingly. (c) For a very large Φ_B , the power factor is smaller than that of bulk due to the significantly degraded G . If Φ_B is very low, then the characteristics approach to that of bulk. The optimum Φ_B is $\sim k_B T$.

FIG. 5. (Color online) Simulation results for (a) $|S|$ vs G and (b) S^2G vs G for bulk and composite nano-structures with $\Phi_B = 40$ meV and various $E_{C,g}$ values shown in the legend. The κ_L is uniform. As $|E_{C,g}|$ increases (grain doping increases), the S vs G trade-off improves, and the maximum power factor increases by up to $\sim 33\%$ over bulk for the highest grain doping ($E_{C,g} = -0.12$ eV).

increases). The maximum power factor improvement in Fig. 5(b) is about 33% for $E_{C,g} = -0.12$ eV. There are two reasons for this improvement. First, as $|E_{C,g}|$ increases, the electrical conductivity of the grain increases due to the increased carrier density, so the overall G improves. Secondly, λ_E improves as the $|E_{C,g}|$ increases because the carrier energy increases. Note that the second feature comes from the characteristics of 1D conductors. The carrier mean-free-path λ can be roughly expressed as $\lambda \sim v\tau$, where v is the group velocity, and τ is the relaxation time. For a parabolic band, $v \sim E^{1/2}$, and if the scattering rate ($1/\tau$) is proportional to the density-of-states as in the phonon-type scattering,³⁰ then $\tau \sim E^{1/2}$ for a 1D conductor, and $\lambda \sim E$. As λ_E increases with the increasing $|E_{C,g}|$, the carrier energy is less relaxed within the grain, and the overall $|S|$ increases. Note that in Fig. 5(a), the improvement coming from the second factor, i.e., the improvement of S due to the increased λ_E is dominant as can be seen from the almost vertical movement of the S versus G curve for the increasing $|E_{C,g}|$.

Figure 6 shows the results for the peak values of S^2G ($S^2_{\text{opt}}G_{\text{opt}}$) of the composite nano-structures in Fig. 5 and the S_{opt} and G_{opt} values extracted at those peaks. The optimum values of bulk are also shown as a reference. As summarized in Fig. 6(a), the maximum power factor improves more over

bulk as $|E_{C,g}|$ increases. As shown in Fig. 6(b), G_{opt} somewhat increases as $|E_{C,g}|$ increases while S_{opt} in Fig. 6(c) stays more or less similar. For higher $|E_{C,g}|$ values, due to the significantly improved S for the similar G in Fig. 5, we maintain high $|S_{\text{opt}}|$ with decent G_{opt} values, and $S_{\text{opt}}^2 G_{\text{opt}}$ increases significantly over bulk as shown in Fig. 6(a).

Next, we discuss the effect of grain size d on the TE properties of composite nano-structures. Figure 7 shows the results for the optimum d (d_{opt}) that gives the maximum $S^2 G$ for the cases in Figs. 3 and 5 and the extracted λ_p and λ_E values. Given the simulation results for the transmission (which is between 0 and 1) of bulk wires with $E_C = E_{C,g}$ and different channel lengths L_{ch} , λ_p can be extracted from the slope of the $1/(\text{transmission})$ versus L_{ch} curve.³⁷ The λ_E is extracted using the exponential decay of $\langle E \rangle$ within the grain,¹⁸ and more details are discussed in the Appendix. In Fig. 7(a) (for the results of Fig. 3), λ_E increases as Φ_B increases, and d_{opt} is larger than λ_E and also increases with increasing Φ_B . Note that λ_p is constant in Fig. 7(a) because it is obtained from bulk wires with $E_C = E_{C,g} = -0.06$ eV, and the λ_E increases with Φ_B because roughly $\lambda_E \sim E/(\hbar\omega_0) \times \lambda_p$,³⁰ and the carrier energy E increases with increasing Φ_B . Results in Fig. 7(a) show that d_{opt} is significantly larger than λ_p and comparable to or larger than λ_E , i.e., $d_{\text{opt}} \sim > \lambda_E > \lambda_p$. Note that d should not be much larger than λ_E because if $d \gg \lambda_E$, then the carrier energy is more relaxed within the grain so that the overall $|S|$ approaches to that of heavily doped bulk. The values of d_{opt} for different $|E_{C,g}|$ values for $\Phi_B = 40$ meV in Fig. 7(b) (for the results of Fig. 5) show similar trends. In Fig. 7(b), λ_p increases with increasing $|E_{C,g}|$ because $\lambda \sim E$ for diffusive 1D conductors as discussed previously,³⁰ and λ_E increases accordingly. The extracted d_{opt} is significantly larger than λ_p and somewhat larger than λ_E , i.e., $d_{\text{opt}} \sim > \lambda_E > \lambda_p$. Here we

FIG. 7. (Color online) Simulation results for d_{opt} that maximizes the $S^2 G$ of composite nano-structures for the given Φ_B and $E_{C,g}$ and the extracted values of λ_p and λ_E . (a) For the results in Fig. 3 with a fixed $E_{C,g}$ and various Φ_B values. (b) For the results in Fig. 5 with a fixed Φ_B and various $E_{C,g}$ values. In all cases, $d_{\text{opt}} \sim > \lambda_E > \lambda_p$.

should note that the data points for d_{opt} in Fig. 7 may scatter because they are picked up among discrete values of d , i.e., d_{opt} in Fig. 7 may not be the true optimum but the d values available in our sample and closest to the true optimum. It is virtually impossible to run numerical simulations for all continuous values of d . As described in Sec. II C, the sample d values are the divisors of $L = 300$ nm, and the difference between the two adjacent d values increases as d increases, i.e., the sampling may be poor for large d values. In Fig. 7(a), for example, d_{opt} seems to saturate at 37.5 nm for $\Phi_B = 80$ and 100 meV while λ_p and λ_E are still increasing. We believe, however, that the true optimum d is still increasing but it may be still closer to 37.5 nm than to the next available d sample, 50 nm.

Results in Fig. 7 support the suggestions that composite nano-structures with engineered d may improve the power factor.¹⁸ For $d > \lambda_p$, the overall G is not degraded much due to barriers because the device is already in the highly diffusive limit. For $d < \lambda_E$, carrier energy is not fully relaxed within the grain so that the overall $|S|$ remains high. Usually λ_E is larger than λ_p , so it has been suggested that by engineering d as $\lambda_p < d < \lambda_E$, both conditions can be satisfied. Our results in Fig. 7 suggest that d_{opt} should be significantly larger than λ_p and is comparable to or somewhat larger than λ_E . Note that the detailed conditions for d_{opt} may depend on the specific definitions of λ_p or λ_E . For the λ_E as described in the Appendix, d should be significantly larger than λ_E ($d \sim 10\lambda_E$) to fully relax the carrier energy and see bulk properties (see Fig. 11). For d values comparable to or somewhat larger than λ_E ($d = 1 \sim 2\lambda_E$), we still see significant energy filtering effects as in the cases of Fig. 7. Therefore, the basic idea of using “energy filtering” effects, i.e., engineering d so that low energy carriers are filtered out due to potential barriers while the overall electrical conductivity is not degraded much, still works consistently here.

B. Non-uniform κ_L

Grain boundaries are expected to impede phonon flow as well as electron flow. Accordingly, we should expect κ_L to be lower near the grain boundaries. In this section, we reduce κ_L in the barrier region and explore its effect on the TE performance of the nano-composite materials. Figure 8 shows simulation results for T_L versus x for a composite

FIG. 6. (Color online) Simulation results for the (a) maximum $S^2 G$, (b) G_{opt} , and (c) S_{opt} at the peaks of the $S^2 G$ curves of the composite nano-structures with $\Phi_B = 40$ meV and various $E_{C,g}$ values in Fig. 5. As $|E_{C,g}|$ increases, G_{opt} somewhat increases while $|S_{\text{opt}}|$ remains similarly high, which result in the increasing power factor with increasing $|E_{C,g}|$. This is mainly because λ_E increases with increasing $|E_{C,g}|$ in 1D conductor with phonon-type scattering resulting in the improved S .

FIG. 8. (Color online) Simulation results for T_L vs x for a composite structure with $\Phi_B = 40$ meV, $E_{C,g} = -0.06$ eV, $d = 60$ nm, $\Delta V = 0$, $T_1 = 301$ K, $T_2 = 300$ K, $\kappa_L = 1.5$ W/m-K in the grain, and κ_L in the barrier is smaller than in the grain by the factors shown in the legend (the factor “1” means that κ_L is uniform along the device). To clearly show the x -resolved T_L , only a part of the channel ($80 \text{ nm} < x < 220 \text{ nm}$) is shown, and the barrier regions are marked by dotted lines. As κ_L is suppressed more in the barrier, more temperature gradient is applied across the barrier region.

structure with $\Phi_B = 20$ meV, $E_{C,g} = -0.06$ eV, $d = 60$ nm, $\Delta V = 0$, $T_1 = 301$ K, and $T_2 = 300$ K. The κ_L in the grain remains the same as in Sec. III A (1.5 W/m-K) while κ_L in the barrier is reduced by a factor 1 (i.e., a uniform κ_L), 2, 5, and 10. As shown in Fig. 8, the lattice temperature gradient $dT_L(x)/dx$ applied across the barrier increases as the κ_L in the barrier is reduced more. As discussed in our previous work,²⁵ the overall S of a diffusive composite structure is the weighted average of the x -dependent Seebeck coefficient $S(x)$ with $dT_L(x)/dx$ being the weighting factor as

$$S = \frac{\int_0^L dx S(x) dT_L(x)/dx}{\Delta T}, \quad (1)$$

where $S(x) = -\langle E - E_F \rangle / (qT)$,²⁵ and $\Delta T = \int_0^L dx (dT_L(x)/dx)$. Therefore, the results in Fig. 8 suggest that the overall S is more dominated by the barrier region that has higher $\langle E \rangle$ and $|S(x)|$. Equation (1) implies that for a given ΔT across contacts, what is important is how it is distributed inside the device.²⁵ The overall S is dominated by the region which more of that ΔT is dropped across. When κ_L is smaller in the barrier than in the grain, compared to the case of a uniform κ_L with the same ΔT , a larger portion of ΔT drops across the barrier (i.e., $dT_L(x)/dx$ increases in the barrier) while the portion of ΔT decreases in the grain (i.e., $dT_L(x)/dx$ decreases in the grain) as a result of the continuity of heat flux, $\kappa_L dT_L(x)/dx$. This means a larger (smaller) weighting factor in the barrier (grain) region with a high (low) local $|S(x)|$, which results in the increased overall $|S|$ compared to the case of a uniform κ_L .

Figure 9 shows simulation results for $|S|$ versus G and S^2G versus G for a composite structure with $\Phi_B = 20$ meV, $E_{C,g} = -0.06$ eV, $\kappa_L = 1.5$ W/m-K in the grain, and κ_L in the barrier is reduced by a factor of 1 (i.e., a uniform κ_L), 2, 5, and 10 from that of the grain. As κ_L is reduced more in the barrier, S improves while G stays similar, i.e., the $|S|$ versus G curve in Fig. 9(a) moves in the vertical direction. The G is little affected by the non-uniform κ_L because the self-heating

FIG. 9. (Color online) Simulation results for (a) $|S|$ vs G and (b) S^2G vs G for a diffusive composite nano-structures with $\Phi_B = 20$ meV, $E_{C,g} = -0.06$ eV, $\kappa_L = 1.5$ W/m-K in the grain, and κ_L in the barrier is smaller than that of grain by the factors shown in the legend. As κ_L in the barrier is reduced more, S improves while G stays similar, the maximum S^2G improves significantly ($\sim 28\%$ over bulk for κ_L in the barrier reduced by a factor of 10), and d_{opt} occurs at higher values (S^2G peaks shift to the right).

effects³⁸ are negligible in the linear regime (small ΔV and current). This improved S is directly reflected in the power factor in Fig. 9(b), where the maximum S^2G is improved significantly (maximum $\sim 28\%$ over bulk for κ_L reduced by a factor of 10 in the barrier). We also note that d_{opt} occurs at higher values (e.g., $d_{\text{opt}} \sim 50$ nm for κ_L reduced by a factor of 10 in the barrier) than in the uniform κ_L case ($d_{\text{opt}} \sim 20$ nm in Figs. 3 and 7), and the power factor significantly improves at large d values, where there was little improvement in the uniform κ_L case in Fig. 3. This is because the large temperature gradient in the barrier region selectively picks up the large $|S(x)|$ in the barrier and increases the overall $|S|$. Note that for small values of d (near the left end of the curves), the reduced κ_L in the barrier does not improve S further because $\langle E \rangle$ is not relaxed and $|S(x)|$ is also high in the grain region.

Figure 10 shows simulation results for S^2G versus G for composite structures with $E_{C,g} = -0.06$ eV, various Φ_B values (10, 20, 40, 60, 80, and 100 meV), $\kappa_L = 1.5$ W/m-K in the grain, and κ_L suppressed by a factor of 10 in the barrier. The maximum power factor improvement over bulk is $\sim 36\%$ for $\Phi_B = 40$ meV and $d_{\text{opt}} = 50$ nm. Note that this optimum Φ_B is higher than that of a uniform κ_L (20 meV in Fig. 3(b)), and d_{opt} is also longer than that of the same Φ_B for a uniform κ_L (25 nm in Figs. 3(b) and 7(a)). Recall that in Fig. 3(b)

FIG. 10. (Color online) Simulation results for S^2G vs G for composite structures with $E_{C,g} = -0.06$ eV, $\kappa_L = 1.5$ W/m-K in the grain, and various Φ_B values. The κ_L in the barrier is reduced by a factor 10 from that of the grain. The maximum power factor improvement over bulk is $\sim 36\%$ for $\Phi_B = 40$ meV and $d_{opt} = 50$ nm. As the κ_L is suppressed in the barrier, the optimum Φ_B and d_{opt} increase, and we can achieve power factor improvement even for high Φ_B values (e.g., 80 meV) that showed inferior performance for the uniform κ_L in Fig. 3.

(uniform κ_L), maximum power factors for $\Phi_B = 20$ and 40 meV are similar while $\Phi_B = 20$ meV is slightly better. In Fig. 10(b) (κ_L smaller in the barrier), however, $\Phi_B = 40$ meV gives significantly better performance over $\Phi_B = 20$ meV. We also achieve a power factor improvement even for $\Phi_B = 60$ and 80 meV, which gave no benefit or showed inferior performance in the uniform κ_L case in Fig. 3(b). In summary, a κ_L smaller in the barrier than in the grain enhances the benefit of energy filtering due to potential barriers.

IV. DISCUSSION

So far, we have treated diffusive carrier transport in 1D composite nano-structures and compared the TE properties with those of 1D bulk with the same scattering parameters. Although our simulation results can be reasonably interpreted using some physical models, we should note that realistic nano-composite structures are in 3D.²⁴ Therefore, to project the performance and optimize the design of realistic materials, it will be essential to extend this work to 3D. As a first step, we should clarify 1D characteristic features that affect the TE properties in our simulations but are not expected to occur in the 3D case.

In Sec. III A, we showed that there exists an optimum Φ_B that improves the maximum S^2G of the composite structure over bulk. We believe that this feature will be common to all dimensions because the mechanism that determines the optimum Φ_B , i.e., S improvement with the current flow near E_F not being obstructed much, does not depend on any specific 1D features and should be still valid in 3D. The $E_{C,g}$ -dependence, however, may significantly depend on the dimensionality. As discussed in Sec. III A, $\lambda \sim E^1$ for phonon-type scattering in 1D.³⁰ In 3D, however, a similar type of scattering gives $\lambda \sim E^0$.^{30,39} Therefore, the improvement of S for the increasing $|E_{C,g}|$ is not expected to occur for 3D composite structures if phonon scattering is dominant. One thing to note

is that λ may show different E -dependence if ionized impurity scattering³⁰ is dominant. For unscreened Coulomb scattering, $1/\tau \sim E^{3/2}$, so $\lambda \sim v\tau \sim E^2$ for a 3D parabolic band.³⁰ It should be noted, however, that the scattering rate is proportional to the impurity density,³⁰ so the resulting τ and λ may decrease with increased doping density although their E -dependence suggests an increasing behavior.

In Sec. III B, we explored the κ_L -dependence of power factor. We believe that the further improvement of S and S^2G due to the decreased κ_L in the barrier does not depend on any specific 1D features, and it may be universal in all dimensions. We should note, however, that it is yet uncertain how the percolative transport in 3D composite structures^{40,41} affects the conclusions.

To treat realistic composite nano-structures, there are a few other issues to be resolved. First, a more realistic model is required to treat realistic potential barriers at the grain boundaries. Although we assume fixed potential profiles in this work, treating self-consistent potential profile²⁵ will be important to explore the effects of modulation doping.⁴² In experiments, most of the improvement comes from the reduced κ_L ,^{3,4,7,8} and there are only a few experimental results that actually report improved power factors in composite nano-structures.^{17,19} This may be because in realistic devices, there could be additional degradation of G due to surface roughness scattering at the barrier interface,⁴³ etc. It should be also noted that although we assume a relatively thick potential barrier to avoid direct carrier tunneling and make our analysis simpler, tunneling^{44,45} may be an essential transport mechanism in realistic composite structures. Finally, a more advanced diffusive phonon transport model^{46,47} may be required to treat non-equilibrium phonon transport in nanoscale devices and explore its effect on electron transport.

V. CONCLUSIONS

In this paper, we explored possibilities to improve the S versus G trade-off of diffusive composite nano-structures over bulk by engineering the grain size d , potential barrier, grain doping, and the distribution of κ_L . For a uniform κ_L that gives a uniform lattice temperature gradient along the device, our simulations suggest that the power factor of a composite structure may be improved over bulk with the optimum barrier height Φ_B being about $k_B T$. The optimum Φ_B occurs because the current flow near E_F is not reduced too much while S still improves due to barriers. We believe that this feature will be general in all dimensions. We also clarified the condition of the optimum grain size d_{opt} to maximize the power factor. The d_{opt} is significantly longer than λ_p so that the G is not degraded much due to the barriers, and d_{opt} is comparable to or somewhat larger than λ_E so that the carrier energy is not fully relaxed within the grain and $|S|$ remains high. Our simulations also suggest that if κ_L in the barrier region is smaller than in the grain, S and power factor may be further improved. In such cases, the optimum Φ_B and d_{opt} increase, and the power factor of a composite structure may improve over bulk even for very high Φ_B and large d .

In this paper, we have used a fully quantum mechanical treatment to address the questions raised on the validity of

the BTE.²⁴ Nevertheless, we find that the conclusions are readily understood in simple, semi-classical terms, and our findings are in general agreement with earlier work based on simpler models.¹⁸ Although we have used thick barriers to minimize tunneling, we do not expect this conclusion to change when tunneling is more important.

In conclusion, using a quantum mechanical transport model and a simple 1D model device, we have shown that nano-composite materials should provide useful performance gains in the power factor. The mechanism is an enhancement of Seebeck coefficient with a moderate reduction of electrical conductivity. When non-uniform thermal properties are included, the performance advantages may increase due to the further enhanced Seebeck coefficient.

ACKNOWLEDGMENTS

This work was supported by the Semiconductor Research Corporation under grant number 1871.001 and National Science Foundation under contract number ECS-0609282. Computational support was provided by the Network for Computational Nanotechnology, supported by the National Science Foundation under cooperative agreement EEC-0634750. Authors would like to thank C. Jeong at Purdue University for helpful discussions.

APPENDIX: EXTRACTING λ_E OF NANO-COMPOSITE STRUCTURES

We assume a 1D model structure where a grain with size d is surrounded by two grain boundaries at $x=0$ and $x=d$. In our derivation, we ignore the finite l_b , which is a reasonable approximation to explain our numerical simulation results. Within the grain, $\langle E \rangle$ decays exponentially¹⁸ as

$$d\langle E \rangle_x / dx = -\langle E \rangle_x / \lambda_E, \quad (\text{A1})$$

where the subscript x of $\langle E \rangle$ represents the x -dependence. And then $\langle E \rangle_x$ has an exponential form as $\langle E \rangle_x \sim \exp(-x/\lambda_E)$. The analytical expression for $\langle E \rangle_x$ can be derived using exponential functions and boundary conditions. (Note that the detailed form of the exponential function depends on the definition of the coordinate system.) At the grain boundaries, $\langle E \rangle_x$ has its peak values as

$$\langle E \rangle = \langle E \rangle_{\text{barrier}} \quad x=0, \quad x=d, \quad (\text{A2})$$

where $\langle E \rangle_{\text{barrier}}$ is the $\langle E \rangle$ on the barrier at the grain boundaries. In our model structure, the exponential functions should also satisfy another condition as

$$\langle E \rangle = \langle E \rangle_{\text{grain,bulk}} \quad x=d/2 \quad \text{as} \quad d \rightarrow \infty, \quad (\text{A3})$$

where $\langle E \rangle_{\text{grain,bulk}}$ means $\langle E \rangle$ of a bulk with the grain doping density. Equation (A3) means that as the grain gets large ($d \gg \lambda_E$), the carrier energy is fully relaxed within the grain so that $\langle E \rangle$ should reach the bulk limit. And then we obtain $\langle E \rangle_x$ as

FIG. 11. (Color online) Model calculation results for $\langle E \rangle_x$ using Eq. (A4) with $\langle E \rangle_{\text{barrier}} = 0.1$ eV, $\langle E \rangle_{\text{grain,bulk}} = 30$ meV, $\lambda_E = 20$ nm, and $d = 20, 50, 100$, and 200 nm. As d gets longer, $\langle E \rangle$ is relaxed more within the grain.

$$\begin{aligned} \langle E \rangle_x = & \left(\langle E \rangle_{\text{barrier}} - \langle E \rangle_{\text{grain,bulk}} \right) \\ & \times \left(e^{-x/\lambda_E} + e^{(x-d)/\lambda_E} - e^{-d/\lambda_E} - 1 \right) + \langle E \rangle_{\text{barrier}}. \quad (\text{A4}) \end{aligned}$$

Figure 11 shows the model calculation results for $\langle E \rangle_{\text{barrier}} = 0.1$ eV, $\langle E \rangle_{\text{grain,bulk}} = 30$ meV, $\lambda_E = 20$ nm, and $d = 20, 50, 100$, and 200 nm. As d gets longer, $\langle E \rangle$ relaxes

FIG. 12. (Color online) Simulation (solid) and analytical fitting (symbol) results for a diffusive composite nano-structures with (a) $d = 60$ nm and (b) $d = 30$ nm for $\Phi_B = 20$ meV, $E_{C,g} = -0.06$ eV, $\Delta V = 1$ mV, and $T_1 = T_2 = 300$ K. Using analytical formulas in Eqs. (A4) and (A6) and $\lambda_E = 13.5$ nm, we can reproduce the numerical results well.

more in the grain, and it approaches $\langle E \rangle_{\text{grain,bulk}}$ at $x = d/2$. Results in Fig. 11 show that d should be significantly larger than λ_E ($d \sim 10\lambda_E$) to observe bulk properties within the grain.

For the numerical simulation results in Sec. III, we extract λ_E by fitting the $\langle E \rangle_x$ curves using the formula in Eq. (A4). Figure 12 shows fitting results for the composite nanostructure discussed in Sec. III A, where $\Phi_B = 20$ meV, $E_{C,g} = -0.06$ eV, $\Delta V = 1$ mV, $T_1 = T_2 = 300$ K, and $d = 60$ and 30 nm. The results in Fig. 12 show that the analytical formula with $\lambda_E = 13.5$ nm well describes the simulation results.

One thing to note in Fig. 12 is that the formula in Eq. (A4) does not apply in the grains at the channel ends. To analytically fit $\langle E \rangle_x$ in these regions, we should use different boundary conditions to solve Eq. (A1) as

$$\langle E \rangle = \langle E \rangle_{\text{barrier}} \quad x = 0, \quad (\text{A5a})$$

$$\langle E \rangle = \langle E \rangle_{\text{grain,bulk}} \quad x = d/2 \quad \text{as} \quad d \rightarrow \infty, \quad (\text{A5b})$$

where it is assumed that the last grain boundary at the right end (near contact 2 in Fig. 1) lies at $x = 0$, and the grain is connected to contact 2 at $x = d/2$. And then we obtain

$$\langle E \rangle_x = \left(\langle E \rangle_{\text{barrier}} - \langle E \rangle_{\text{grain,bulk}} \right) e^{-x/\lambda_E} + \langle E \rangle_{\text{grain,bulk}}. \quad (\text{A6})$$

The $\langle E \rangle_x$ at the left end (near contact 1) is simply obtained by flipping the plot from Eq. (A6).

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Computational study of energy filtering effects in one-dimensional composite nano-structures

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Citation: [Journal of Applied Physics](#) **111**, 024508 (2012); doi: 10.1063/1.3678001

View online: <http://dx.doi.org/10.1063/1.3678001>

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