Full Quantum Mechanical Electronic Transport Simulations in Si Quantum Wells and Superlattices for Thermoelectric Applications

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1. Introduction

When a temperature difference is applied across a thermoelectric material, a potential difference which can be used to drive a circuit, results. Thus, thermoelectrics have the potential to turn omnipresent waste heat into a power source. Furthermore, unlike a traditional heat engine, thermoelectric generators have no moving parts, require no or minimal maintenance, are arbitrarily scalable in size, and can also be used for cooling applications when a voltage is applied across them. The main hurdle towards wide-spread application of such technology is the stubbornly low power conversion efficiency of current materials. Recent advances in nanostructured thermoelectrics, however, and especially in Si-based low-dimensional and nanostructured materials, has the potential to uproot this state of affairs [1-4].

The thermoelectric (TE) performance of a material can be quantified by the figure of merit $ZT=\sigma S^2/\kappa$, where σ denotes the electrical conductivity, S the Seebeck coefficient and κ the thermal conductivity. Recent improvements in ZT have been achieved through the use of nano-engineered materials with ultra-low κ, reaching values below the amorphous limit [1-3]. Attempts to improve the numerator, the so-called power factor (σS^2), have proved substantially less successful owing to the often inverse relationship between the conductivity and the Seebeck coefficient. However, the energy filtering of carriers in nanocomposite materials with embedded potential barriers (V_B) (i.e. superlattices) is a promising way to improve σS^2 via improvements in the Seebeck coefficient [4, 5]. Seebeck coefficient enhancement in nanometers-size layer superlattices has been observed in several experimental works. However, improvements over the overall power factor were not due to accompanying losses in σ. In this work, we develop a fully quantum mechanical Non-Equilibrium Green's Function (NEGF) method in 1D to explore the conditions under which σ and S^2 can be simultaneously improved. We show that optimized superlattice structures could provide up to ~30% power factor improvements.

2. Method and Discussion

We use the NEGF method in the effective mass approximation, including both acoustic and optical phonon scattering. Figure 1 illustrates the simulated 1D channel geometry, consisting of a series of potential barriers. The colormap shows the current spectrum and how it fluctuates in energy during emission / absorption of optical phonons. Previous works have indicated that under optimal conditions the transport in the wells needs to be semi-ballistic, where carriers only lose part of their energy before they reach the next barrier [6, 7], and thus, in this work we calibrate the well size Lw, electron-phonon scattering, and barrier height V_B for these optimal conditions. We use Lw=20nm and V_B=0.16eV throughout this work.

Once the model is constructed, we then explore the space of possible superlattice configurations and calculate their corresponding power factors. Two main parameters are examined, the width of the barriers W, and the position of the Fermi level with respect to the barrier height $\eta_F=E_F-E_C$. Figure 2 shows the significance in choosing the right barrier width. Figure 2a shows that if the barriers are too thin, tunneling makes them seem transparent, and their filtering effect is lost (which is detrimental to S). Figure 2b shows that if the barriers are too thick, then carriers relax at the top of them, which increases the channel resistance. The optimal width is somewhere in the middle as shown in Fig. 2c. The influence of the barrier width on the power factor is indicated in Fig. 3. We can observe thin barriers could cause up to ~40% degradation in performance. The optimal value is W~3nm, whereas for larger widths the resistance increases and the power factor drops again.

The behavior of the power factor versus η_F is shown in Fig. 4. As the E_F increases, the power factor increases, with an optimal value around E_F~0.14eV, approximately ~k_BT below V_B. This allows enough hot carriers to overpass the barriers, and blocks the cold carriers, which increases energy filtering and benefits both S and σ. In comparison to the optimized power factor in a uniform material without barriers (magenta line), this is ~15% higher. An additional improvement can be achieved be relaxing the shape of the barriers from perfectly sharp to smooth, which provides power factor values up to ~30% higher compared to the uniform material. The reason behind this is the fact that sharp edges introduce quantum reflections in the transmission, which strongly reduces the conductivity.

The fact that two major performance degrading mechanisms, are of quantum mechanical nature (tunneling and reflections) justifies the choice of our

quantum mechanical model for the optimization of new generation TE materials. We also note that we are currently developing 2D quantum mechanical transport capabilities, which will be used to explore a much richer design space in terms of geometries for even larger improvements in the TE power factor.

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References

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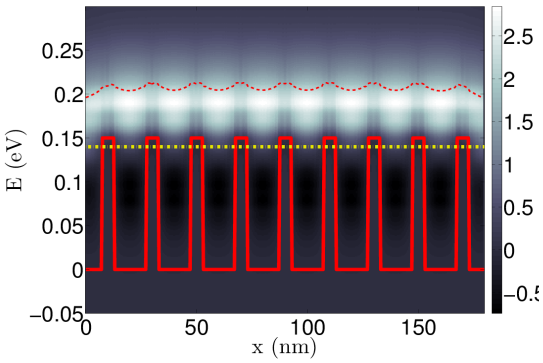

Fig. 1. The potential profile of the barriers in the channel with width of 4nm and height of 0.16 eV. The colormap shows the current density versus position. Superimposed on the image are the potential barriers and the carriers energy expectation value <E>.

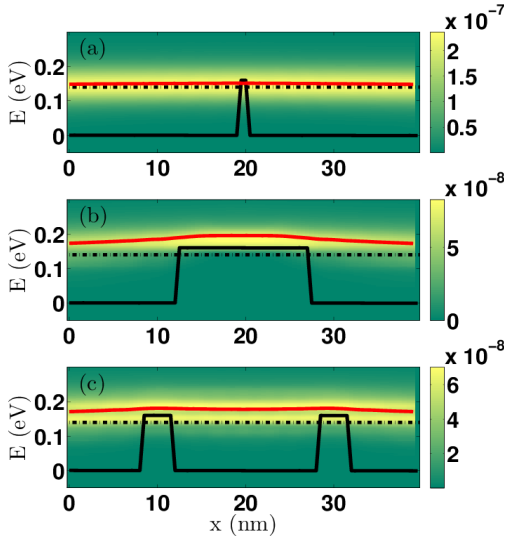

Fig. 2. (a) The case of a thin, transparent barrier, in which most current passes through the barrier. (b) The case of a thick barrier, where most of the current passes over the barrier. (c) The case of an optimal superlattice. Partial energy relaxation is observed in the wells (lowering of the red line in the well regions).

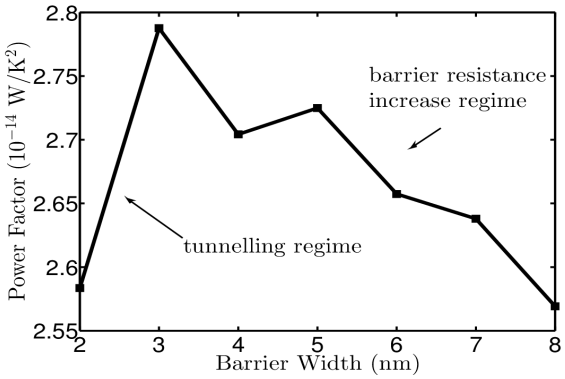

Fig. 3. Power factor versus barrier width. The optimal barrier width is ~3nm, which is thick enough to prevent tunnelling, but thin enough retain the conductance high.

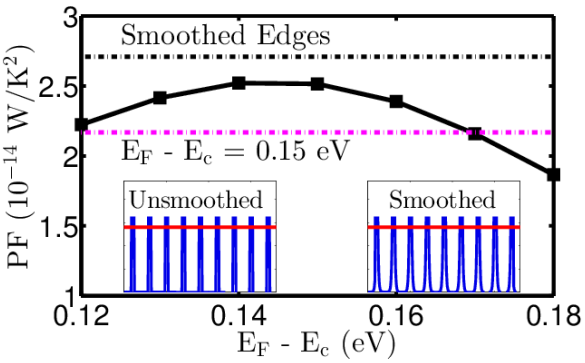

Fig. 4. The thermoelectric power factor of a superlattice material versus the position of the Fermi level E_F with respect to the conduction band edge. The barrier height is V_B=0.16 eV. The optimal power factor of a uniform channel is indicated by the magenta-dashed line, and the optimal power factor of a superlattice with smoothened barriers (as shown in the insets) by the black-dashed line.