# Thermoelectric power factor optimization in nanocomposites by energy filtering using NEGF

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## INTRODUCTION

The thermoelectric (TE) performance of materials is determined by the figure of merit $ZT=\sigma S^2/\kappa$, where $\sigma$ denotes the electrical conductivity, S the Seebeck coefficient and $\kappa$ the thermal conductivity. Large improvements in ZT have recently been reported in nanoscale materials due to drastic reduction in $\kappa$ [1]. On the other hand, much less success has been achieved in improving the power factor ($\sigma S^2$), and ZT still remains low. Energy filtering in nanocomposite materials with embedded potential barriers ($V_B$) is a promising way to improve $\sigma S^2$ via improvements in the Seebeck coefficient [2, 3]. Indeed, the improvement in the Seebeck coefficient of nanometers-size layer superlattices has been demonstrated in several experimental works. Significant benefits to the overall power factor, however, were never observed in these structures due to large reductions in $\sigma$. In this work, we use the Non-Equilibrium Green's Function (NEGF) method to illustrate the design details under which improvements in $\sigma S^2$ can be achieved by energy filtering. We further demonstrate that variation of the design parameters, and most importantly in the barrier heights is a strong detrimental mechanism which can take away most of the energy filtering benefits.

## 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. Figure 1a shows the channel as a series of potential barriers, Fig. 1b shows the extracted local density of states LDOS(E,x) from NEGF, Fig. 1c the charge density in the channel, and Fig. 1d 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 [4, 5]. In addition, it was also indicated that ideally the barrier height needs to extend $\sim k_BT$ above the Fermi level [4, 5]. Thus, in this work we calibrate the geometry, electron-phonon scattering, Fermi level, and barrier height for these optimal conditions.

Once this is done, we proceed by investigating the performance of energy filtering processes under statistical fluctuations in the design parameters. The first parameter we examine is the width of the barrier W. Figure 2 shows the power factor versus W. We can observe that the barriers need to be thick enough to prevent tunneling (which is detrimental to S and could cause up to ~40% degradation in performance), but thin enough for reduced resistivity (so ~2-3nm), since the carrier energy and momentum can relax on top of the barriers and acquire reduced velocities. The next parameter we consider is the actual shape of the barrier. In practice, an ideal rectangular barrier would not be achievable, thus we examine the influence of deviations from the rectangular shape on the performance. Figure 3 shows that the rectangular barriers are ideal (left side), which shows that ~30% improvement can be achieved compared to the bulk TE material case. As we deviate from that shape the power factor drops (approaching the bulk case – right side). Finally, the last parameter we examine, is fluctuations in the height of the potential barriers $V_B$. The results are shown in Fig. 4 (black line). In this case, we vary the barrier heights along the transport path according to a Gaussian distribution. As the variation increases, a large drop is observed in the power factor (black line). We perform the same studies for variations in the barrier position (blue line) and the barrier width (red line), which introduce only small power factor reduction.

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## CONCLUSION

Using the NEGF method we computed the thermoelectric power factor in nanocomposite channels in the presence of energy barriers. We show that ideally, power factor improvements up to 30% can be achieved using energy filtering under optimal conditions. However, we show that this achievement is improvement is sensitive to structure imperfections. Fluctuations in the barrier width and well size do not affect performance significantly, but fluctuations in the barrier shape and most importantly the barrier height (even of the order of 5meV) could take away most of the power factor improvements, and therefore, need to be avoided.

## ACKNOWLEDGEMENT

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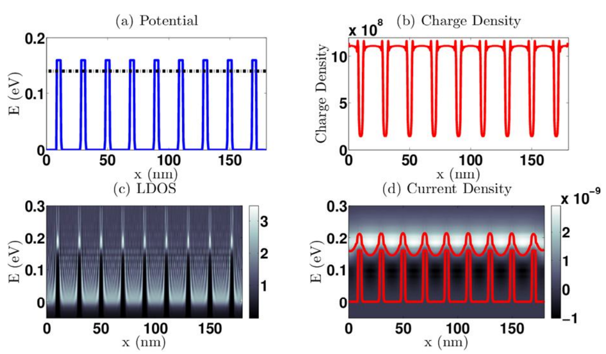


Fig. 1. Sample data for a nanocomposite channel. (a) The potential profile of the barriers in the channel with width of 4nm and height of 0.16 eV. (b) The local density of states in the channel. (c) The charge density. (d) The current density versus position (colormap). Superimposed on the image are the potential barriers and the carriers energy expectation value <*E*>.

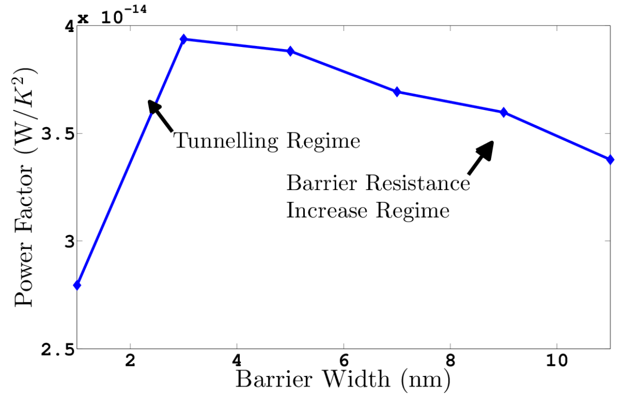


Fig. 2. Power factor versus barrier width. The optimal barrier width is ~3nm, which is thick enough to prevent tunnelling, but thin enough to keep the electrical resistance from barriers low.

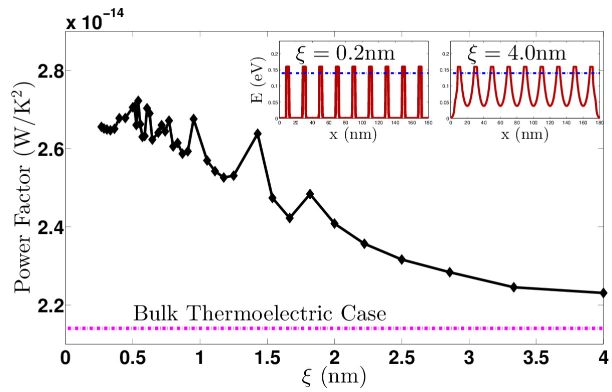


Fig. 3. Power factor versus barrier shape, defined as an exponentially decaying profile, described by a decay length, ξ, from the top of the barrier. The limit ξ=0 corresponds to a square barrier (left side), which is found to be the optimal one.

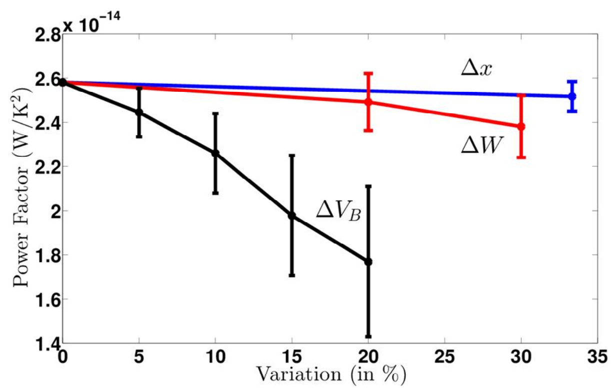


Fig. 4. Power factor ($\sigma S^2$) versus statistical variation of the barrier placement (blue line), width (red line), and height (black line) along the transport path. It is clear that performance is most substantially degraded by barrier height variation.