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Energy filtering optimization for power factor improvements through fully quantum mechanical transport simulations

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Energy filtering is a promising way of achieving large thermoelectric power factors by improving Seebeck coefficients. Materials with embedded potential barriers, such as cross-plane superlattices provide energy filtering in addition to low thermal conductivities, and could potentially achieve high ZTs. The improvement in the Seebeck coefficient of ultra-thin, nanometer-size layer superlattices has been demonstrated in several experimental works. Significant benefits to the power factor, however, were never observed because the electrical conductivity in such materials was drastically reduced. This was intuitively attributed to the presence of the potential barriers and the disorder around the multiple layer interfaces; however, no proper theoretical investigation has yet been conducted.

In this work, using quantum mechanical simulations based on the Non-Equilibrium Green's Function method, we show that power factor improvements can only be observed under very specific conditions. The geometry of the layered material and the shape of the underlying potential profile, need to be properly correlated with the electrons' effective mass, energy, and momentum relaxation times. We show that: i) The barriers need to be thick enough to prevent tunnelling, but thick enough for reduced resistivity; ii) Transport in the potential wells needs to be semi-ballistic; iii) The material needs to be highly degenerate for improved conductivity; and iv) The barrier heights need to be $\sim k_B T$ above the Fermi level. Once these parameters are aligned, power factor improvements up to 50% can be achieved. With regards to structure imperfections, we show that slight variations in the shape and width of the barriers, the well size and its underlying potential, could slightly degrade the power factor. The more detrimental imperfection, however, is the fluctuation in the height of the potential barriers. Fluctuations of the order of 5meV could take away most of the power factor improvements, and therefore, need to be avoided.