A theoretical model for the Seebeck coefficient in superlattices and nanocomposite materials with partial energy relaxation

Vassilios Vargiamidis[1], Mischa Thesberg[2], and Neophytos Neophytou[1]

[1]*School of Engineering, University of Warwick, Coventry, CV4 7AL, U.K.*

[2]*Institute for Microelectronics, Technical University of Vienna, Vienna, A-1040, Austria*

Abstract

Nanostructured materials have shown great potential to achieve improved thermoelectric performance, not only due to lower thermal conductivities, but also due to higher power factors. The power factor improvements come primarily from energy filtering, which results in a higher Seebeck coefficient S. In nanocomposites with feature sizes similar to the electronic mean-free-paths, however, S is not only determined by the bulk Seebeck values of the individual materials but, in addition, by the energy relaxation process of electrons as they propagate over the potential barriers and lose energy to relax into the wells. The intermixture of the properties of the two regions requires involved computational modelling to accurately determine the composite S, usually through 'real-space' Monte Carlo or the quantum mechanical non-equilibrium Green's function (NEGF) method. However, these methods are either complex or time-consuming, or both.

Here we present a simple analytical model for the Seebeck coefficient S of a channel with embedded superlattice (SL) barriers for energy filtering, which explicitly takes into account the details of energy relaxation due to electron-optical phonon scattering. The model mimics either a SL or a nanocomposite, or any material in which carrier transport alternates between potential barriers and wells. Importantly, the model requires only four relatively easily determined parameters: the bulk Seebeck coefficients of the two materials that form the superlattice, the energy relaxation length of carriers in the wells, and the length of the wells. We validate the model against advanced NEGF simulations, and we find very good agreement for a range of structural and material physical properties (see attached Figure). The model would prove useful in the identification of material combinations and the estimation of ideal sizes of nano-engineered materials with enhanced power factors. As we show, only when energy relaxation is taken into account, significant power factor improvements can be achieved.

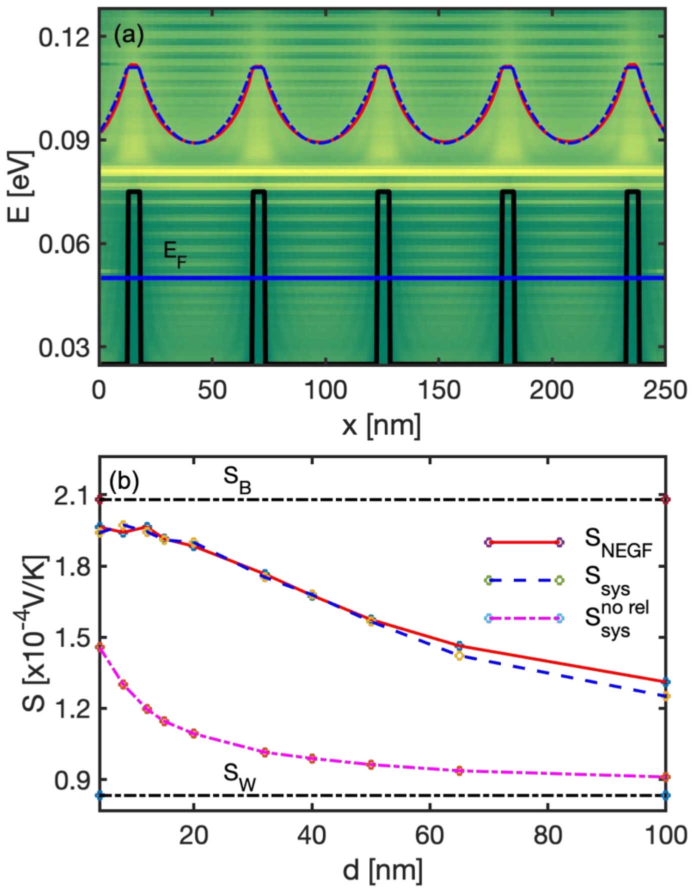

Figure 1: (a) Average energy of the current flow $\langle E(x) \rangle$ along the channel with five barriers calculated from NEGF (solid, red line) and from the analytical model (dashed, blue line) for which d = 50nm and λ_E = 16.5nm. (b) Seebeck coefficient vs well size d calculated from (i) NEGF (solid, red line), (ii) model with energy relaxation (dashed, blue line), and (iii) model without energy relaxation (dashed-dotted, magenta line). S_B and S_W are the individual (bulk) Seebeck coefficients of the barrier and well regions, respectively.