

A5_19: Engineering the Thermoelectric Power Factor of Si and Ge Ultra Narrow 1D Nanowires and 2D Thin Layers Using Atomistic Modeling

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Low-dimensional materials such as ultra-narrow nanowires (NWs) and ultra-thin layers (UTLs) have attracted significant attention as efficient thermoelectric materials because these structures have exhibited extremely low thermal conductivity [1, 2]. On the other hand, it was suggested that low dimensionality can improve the Seebeck coefficient [3]. Boukai et al. [1], and Hochbaum et al. [2] have recently shown that due to strong reduction in thermal conductivity it is indeed possible to achieve $ZT \sim 0.5$ at room temperature even in Si NWs of diameters less than 50nm (compared to bulk Si $ZT_{\text{bulk}} \sim 0.01$). The benefits from thermal conductivity reduction, however, seem to be reaching their limits. To achieve further ZT improvements one will need to increase the power factor. For this, proper modeling tools that account for all important features of the electronic structure of low dimensional systems are necessary.

In this work we calculate the electrical conductivity and Seebeck coefficient of 1D ultra-narrow NWs and 2D ultra-thin layers (UTLs) of Si and Ge. We address structures of up to 12nm in NW diameter or layer thickness (up to ~ 5500 atoms in the simulation domain). We use the atomistic sp³d⁵s* tight-binding model coupled to linearized Boltzmann transport theory. We investigate the effect of feature size, and several combinations of transport and confinement orientations. We show that the bandstructure and electronic properties of low-dimensional channels are geometry dependent. They can thus be engineered to achieve optimal thermoelectric power factor. We show that proper choice of geometry can in some cases yield even up to $\sim 4X$ power factor improvements. We identify the physical reasons behind this behavior and provide engineering guidelines relevant to other materials with similar bandstructures. Our results suggest that most of the improvement at low dimensionality originates from conductivity improvements, rather than the improvement of the Seebeck coefficient.