A5_31: Nanograin effects on the thermoelectric properties of poly-Si nanowiress

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Silicon nanowires (NWs) have attracted significant attention as efficient thermoelectric materials mostly due to significant reduction in the thermal conductivity, whereas no benefits were observed to the power factor. Due to enhanced electron scattering [1], the electrical conductivity degrades – although e.g. in NWs modulated by interconnected dots an improvement of power factor was predicted [2-3]. Polycrystalline NWs structures might offer an alternative approach to achieve simultaneous thermal conductivity reduction and power factor improvements through improvements in the Seebeck coefficient. In polycrystalline silicon it has been reported an unexpected increase of the power factor with respect to single crystals that was related to the precipitation of a second phase around grain boundaries [4-5]. Here, we perform a theoretical analysis of the thermoelectric performance of polycrystalline Si NWs by considering both electron and phonon transport. We extract the relevant parameters from atomistic simulations, and use them in macroscopic transport models. The simulations are calibrated with experiments for bulk and NW polycrystalline structures. We perform an analysis involving all relevant geometrical and structural features such as grain and grain boundary sizes, density, barrier heights, roughness. We find that any increase in the disorder of the channel, or any reduction in the diameter provides strong reduction in the thermal conductivity. Interestingly, we show that the Seebeck coefficient and consequently the power factor can be improved significantly once the polycrystalline geometry is properly optimized, while avoiding strong reduction in the electrical conductivity. In such a way, even larger ZT improvements can be achieved compared to monocrystalline NWs, also in agreement with our recent experimental observations.

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