Journal of ELECTRONIC MATERIALS, Vol. 42, No. 7, 2013
DOI: 10.1007/s11664-012-2424-8

Nanograin Effects on the Thermoelectric Properties of Poly-Si Nanowires

N. NEOPHYTOU,[1] X. ZIANNI,[2,3,7,8] M. FERRI,[4] A. RONCAGLIA,[4]
G.F. CEROFOLINI,[5] and D. NARDUCCI[5,6]

1.—Institute for Microelectronics, Technical University of Vienna, Vienna, Austria. 2.—Department of Applied Sciences, Technological Educational Institution of Chalkida, 34 400 Psachna, Greece. 3.—Institute of Microelectronics, NCSR 'Demokritos', 153 10 Athens, Greece. 4.—IMM-CNR, Bologna, Italy. 5.—Department of Materials Science, University of Milano–Bicocca, via R. Cozzi 53, 20125 Milan, Italy. 6.—Consorzio DeltaTi Research, Milan, Italy. 7.—e-mail: xzianni@gmail.com. 8.—e-mail: xzianni@teihal.gr

In this work we perform a theoretical analysis of the thermoelectric performance of polycrystalline Si nanowires (NWs) by considering both electron and phonon transport. The simulations are calibrated with experimental data from monocrystalline and polycrystalline structures. We show that heavily doped polycrystalline NW structures with grain size below 100 nm might offer an alternative approach to achieve simultaneous thermal conductivity reduction and power factor improvements through improvements in the Seebeck coefficient. We find that deviations from the homogeneity of the channel and/or reduction in the diameter may provide strong reduction in the thermal conductivity. Interestingly, our calculations 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, *ZT* values even higher than the ones reported for monocrystalline Si NWs can be achieved.

Key words: Polycrystalline, silicon, thermoelectrics, Seebeck, power factor, thermal conductivity

INTRODUCTION

Silicon nanowires (NWs) have attracted significant attention as efficient thermoelectric materials mostly due to significant reduction in their thermal conductivity. Recent experimental measurements reported thermal conductivity values as low as κ_l = 1 W/mK to 2 W/mK in Si NWs with diameters below 50 nm, which resulted in an impressive *ZT* of ~1, compared with the Si bulk value of $ZT_{\text{bulk}} \approx 0.01$.[1,2] As of now, however, no benefits were observed through the power factor. Moreover, experimental efforts were not able to achieve significant relaxation of the adverse interdependence between the electrical conductivity and Seebeck coefficient. To achieve higher performance, efforts need to be directed towards power factor improvements as well, since the thermal conductivity of nanostructures is reaching the amorphous limit.[3,4] Unfortunately, improvements to the power factor from the sharp features of the low-dimensional density of states as suggested in Ref. 5 were not observed because small feature sizes enhance electron scattering and significantly reduce the electrical conductivity.[6] It was theoretically shown, however, that in NWs modulated by interconnected dots,[7–9] or nanocomposite materials,[10] an improvement in the power factor could be achieved. In those cases, the Seebeck coefficient increases in certain regions of the channel where filtering is more effective. Such effects can also exist in polycrystalline NW structures, which might offer an alternative approach in achieving simultaneous thermal conductivity reduction and power factor improvements through improvements in the Seebeck

---

(Received July 7, 2012; accepted December 27, 2012;