Modeling power factor enhancement by inhomogeneous distribution of impurities in two-phase Si-B nanocrystalline systems

Xanthippi Zianni[1,2], Neophytos Neophytou[3], Bruno Lorenzi[4], Stefano Frabboni[5] and Dario Narducci[4]
[1]Dept. of Applied Sciences, Technological Educational Institution of Chalkida, Psachna, Greece
[2]IAMPPNM, Dept. of Microelectronics, NCSR Demokritos, Athens, Greece
[3]Institute for Microelectronics, Technical University of Vienna, Vienna Austria
[4]Dept. of Materials Science, University of Milano Bicocca, Milan, Italy
[5]Dept. of Physics, University of Modena and Reggio Emilia, Modena, Italy

An unexpected concurrent increase of the electrical conductivity sigma and the Seebeck coefficient S and a consequent increase of the power factor have been previously observed in heavily boron-doped polycrystalline silicon [1-4]. Based on this evidence, it was proposed that the precipitation of silicon boride around grain boundaries may lead to considerable increase of the power factor in poly-crystalline silicon. Theoretical modeling has indeed shown [5] that the formation of a two-phase material consisting of grains and grain boundaries can actually lead to a concurrent increase of sigma and S. Additional recent experimental evidence confirmed that the concurrent increase of sigma and S with the carrier density is found only upon formation of such two-phase material with grain sizes <100nm. Here, we discuss the dependence of this behavior on the microscopic characteristics of the material. Our theoretical investigation, involving both electron and phonon transport in nanocrystalline Si materials reveals that: i) The improvement in the Seebeck coefficient can be attributed to the increase in carrier filtering due to the energy barriers at the grain boundaries, and due to the non-uniformity of the lattice thermal conductivity between the grains and grain boundaries. ii) The improvement in the electrical conductivity is a result of a higher Fermi level in the grain compared to bulk material at the same carrier concentration. This allows high energy carriers contributing to transport, increases the mean-free-path due to impurity scattering, and thus increases the conductivity in the grain. Our conclusions provide insight that may be useful towards achieving enhanced power factor in bulk nanocrystalline materials.

1.D. Narducci, E. Selezneva, G.F. Cerofolini, E. Romano, R. Tonini, and G. Ottaviani, 8th European Conference on Thermoelectrics, Como, (2010), 141.
2.D. Narducci, E. Selezneva, A. Arcari, G.F. Cerofolini, E. Romano, R. Tonini, and G. Ottaviani, MRS Proceedings, 1314, mrsf10-1314-ll05-16.
3.D. Narducci, E. Selezneva, G.F. Cerofolini, S. Frabboni, and G. Ottaviani, Journal of Solid State Chemistry, 193 (2012) 19.
4.D. Narducci, E. Selezneva, G.F. Cerofolini, S. Frabboni, and G. Ottaviani, AIP Conference Proceedings, 1449 (2012) 311.
5.N.Neophytou, X.Zianni, M.Ferri, A.Roncaglia, C.F. Cerofolini and D.Narducci, Journal of Electronic Materials, DOI: 10.1007/s11664-012-2424-8.