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

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An unexpected concurrent increase of the electrical conductivity σ 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 polycrystalline 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 σ and S. Additional recent experimental evidence confirmed that the concurrent increase of σ and S with the carrier density is found only upon formation of such two-phase material with grain sizes \( <100\text{nm} \). 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.