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Thermal conductivity of disordered porous Silicon GIUSEPPE ROMANO, MIT, JEFFREY GROSSMAN, Department of Materials Science and Engineering, MIT — Nanostructuring bulk materials is a promising approach for engineering high-efficiency thermoelectric devices thanks to its ability to decoupling the thermal and electrical transport. Among different approaches, porous Silicon has been attracting much attention due to its ability of strongly suppressing heat transport. Recent experimental works show that classical size effects of phonons can be further enhanced by having staggered pores, as opposed to the aligned pores case. Motivated by these results, we solve the phonon Boltzmann Transport Equation to compute heat transport across an arbitrary pores arrangement. The model has been discretized by means of the Discontinuous Galerkin method, which allows complex simulation domains. We focus on triangular, circle and square pores where the orientation is allowed to change stochastically. In order to compute the ZT, the electrical conductivity and the Seebeck coefficients are computed by means of diffusive theory. Our main finding is that pore disorder can play a crucial rule in optimizing thermoelectric materials. Indeed, in the special case of triangular pores we predict an increasing in ZT of up to ten times the value found for the aligned case.

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