Abstract Submitted
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Lattice thermal conductivity of nanostructured semiconductors from atomistic simulations[1] YUPING HE, DAVIDE DONADIO, University of California Davis, JOO-HYOUNG LEE, JEFFREY C. GROSSMAN, Universtiy of California Berkeley, GIULIA GALLI, University of California Davis — We present an atomistic analysis of the thermal conductivity (k) of nanoporous silicon (np-Si) [1, 2], and we compare our results with those obtained for bulk crystalline (c-Si) and amorphous Si. We computed k using equilibrium molecular dynamics and Green Kubo relations; we then analyzed our results by solving the Boltzmann Transport Equation in the single mode relaxation time approximation, and by using an approach devised [3] to describe thermal transport in disordered semiconductors. We observe that in np-Si the phonon mean free path is reduced by up to a factor of 10 with respect to c-Si, yielding a reduction of the k of about 2 orders of magnitude. The predominant phonon scattering processes contributing to k can be modeled by the same non-perturbative [3] approach that describes thermal transport in a-Si.
[1] J-H. Lee, et al. Appl. Phys. Lett, 91, 223110 (2007)
[2] J-H. Lee, et al., Nano. Lett., 8(11), 3750 (2008)
[3] P, B. Allen and J. L. Feldman, Phys. Rev. B 48, 12581 (1993)

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