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A comparative study of thermal transport in crystalline,amorphous and nano-porous silicon

Y.P. HE, D. DONADIO, G. GALLI — Recent theoretical predictions [1] suggest that nanoporous Silicon(np-Si) is a promising material for thermoelectric applications, with a figure of merit(ZT) close to 1. One of the reasons for the increased ZT with respect to crystalline Si is a smaller thermal conductivity k. By using a combination of techniques (equilibrium and non-equilibrium molecular dynamics, and the Boltzman transport equation),we analyze the origin of the predicted small k in np-Si, and the interplay between disorder at the mesoscopic scale(the presence of nanometer sized pores) and at the atomic scale(the presence of amorphized pore surfaces). We find that for pores with ordered surfaces, the reduction in k– observed only in the plane perpendicular to the pores– is due to a reduction of both phonon group velocities and lifetimes. Upon amorphization of the pore surfaces, k is dominated by contributions from diffusive modes and it may decrease to values close to that of amorphous Si even for modest sizes of the amorphized regions. The decrease is observed both in the direction parallel and perpendicular to the pores. Our results are compared to those obtained for Si nanowires[2] with similar surface structures. [1]J-H.Lee, et al., Appl.Phys.Lett. 91, 223110(2007);J-H.Lee,et al., Nano.Lett., 8(11), 3750(2008) [2]D.Donodio and G.Galli, Phys.Rev.Lett. 102, 195901(2009), Work supported by DOE/SciDAC-DE-FC02-06ER25794

Y.P. He

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