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Thermal transport in Si-based disordered systems: amorphous silicon and silicon germanium alloys YUPING HE, IVANA SAVIC, GIULIA GALLI, UC Davis, DAVIDE DONADIO, MPI for Polymer Research — Understanding and modeling heat transport in structurally and mass disordered semiconductors (e.g. amorphous silicon–a-Si and SiGe alloys) have long been a challenging problem in solid state physics. Using a combination of techniques (equilibrium and non-equilibrium molecular dynamics and lattice dynamics), we analyze the nature of vibrations and compute the thermal conductivities (k) of a-Si, bulk and nanoporous SiGe. We find that in amorphous and mass disordered systems, two types of modes are present, phonons and diffusive modes. In a-Si, phonons (who are only 3 % of the total vibrations) contribute to approximately half of k [1]. The value of k critically depends on the morphology of the system [2], for example it considerably dereases if thin films or samples with nano-holes are considered. A discussion of how mean free paths and lifetimes change as a function of morphology and disorder will be presented, together with results showing the effect,on k, of disorder at pores or film surfaces.Work supported by grant DOE DE-FC02-06ER25777.

[1] Y.He, D.Donadio and G.Galli (submitted, 2010).
[2] Y. He, D. Donadio, Joo-H. Lee, J. C. Grossman and G. Galli (submitted, 2010)

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