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Crossover in Thermal Transport Mechanism in Nanocrystalline Silicon ARUN BODAPATI, PAWEL KEBLINSKI, Rensselaer Polytechnic Institute, PATRICK SCHELLING, University of Central Florida, SIMON PHILLPOT, University of Florida — Using vibrational mode analysis of model structures we demonstrate that lattice vibrations in small grain (< 3 nm) structurally inhomogeneous nanocrystalline silicon are almost identical to those of homogeneous amorphous structures. In particular, the majority of the vibrations are delocalized and unpolarized. As a consequence the principal thermal conductivity mechanism in such nanocrystalline materials is essentially the same as in the amorphous material. With increasing grain size the ability of vibrations to "homogenize" over the nanocrystalline structure is gradually lost and the phonon spectra and polarization become progressively more like that of a crystalline material; this is reflected in a crossover in the mechanism of thermal transport. Interestingly, a few of the vibrational modes are localized either on the grain boundary and the grain interiors.

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