

Heat Transport in Silicon Nanowires within Full-band Phonon Monte Carlo Approach

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Abstract: In order to investigate the heat transport at the nanoscale, a Full Band Monte Carlo (MC) algorithm has been used to solve the Boltzmann Transport Equation (BTE) for phonons [1]. In this approach, the dispersion of phonons is computed over the Full Brillouin [2] zone to accurately describe the properties of the material and in particular to capture the orientation effects. Interfaces are currently a major issue in nanotechnology and the phonon reflection/transmission across interfaces [3] have been implemented in an original way. By using our simulator, phonon transport in Silicon and Germanium nanostructures such as nanowires including heterostructures are investigated from diffusive to ballistic regime, i.e. beyond the Fourier heat equation validity.

References

- [1] D. Lacroix, K. Joulain, and D. Lemonnier, Phys. Rev. B 72, 064305 (2005).
- [2] J. Larroque, B. Davier, P. Dollfus and J. Saint-Martin, Full-band modeling of phonon transport in polytype cubic/hexagonal Ge and Si structure, EDISON 20, Buffalo, N.Y. USA, July 16-21 2017, J. Phys.: Conf. Ser., To be published.
- [3] J. Larroque, P. Dollfus and J. Saint-Martin, Phonon transmission at Si/Ge and polytypic Ge interfaces using Full-Band mismatch based models, J. Appl. Physics, Submitted

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