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Scalable, Composable Operators for Defect Analysis and Design

ROSE WEISBURGH, PETER CHUNG, University of Maryland — Defect structures in semiconductors can profoundly affect electronic properties through electron-phonon interactions. Knowledge of the changes to phonon properties induced by defects is vital for understanding phonon effects on electronic behavior. Defects can cause the dominant phonon peaks in the spectrum to split and shift resulting in carriers that can scatter in energy levels not foreseen in the bulk. We have developed a novel mathematical and computational framework for estimating the phonon spectra in the harmonic approximation for lattices containing arbitrary defect structures. Linear operators are used to calculate defective phonon spectra directly from the spectrum of a pristine reference lattice. The primary benefit is that the full eigensolve must only be performed once for the reference defect-free crystal. The operators can be adjusted to vary the defect concentration, defective mass ratio, and/or defective potential subsequently without having to re-evaluate the eigensystem. In the talk, we will present the theory behind our methodology and initial results about the sensitivity of electro-thermal properties of semiconductors to various point defects.

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