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Suppression of phonon heat conduction in cross-section modulated nanowires

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Materials with low thermal conductivity are prospective for thermoelectric applications, while enhanced thermal transport is necessary for the efficient heat removal at nanoscale. In this work we have theoretically investigated phonon heat flux in cross-section modulated Si/Ge segmented nanowires, employing the Born-von Karman type and Face-centered cubic cell models of lattice vibrations and the Boltzmann transport equation within the relaxation time approximation. It has been demonstrated that thermal flux decreases significantly in such nanowires in comparison with generic homogeneous Si or Ge nanowires due to redistribution of phonon energy spectra and localizations of phonon modes in nanowire segments. As a result, three- to five-fold drop of the phonon heat flux in the 50 K to 400 K temperature range is predicted for cross-section modulated Si/Ge segmented nanowires in comparison with generic nanowires. The obtained results indicate that cross-section modulated segmented nanowires are promising candidates for thermoelectric applications.