Optimal Geometric Parameters to Maximize or Minimize Phonon Boundary Scattering in Periodic Coaxial Cylindrical Nanowires

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The thermal conductivity (k) of semiconducting nanomaterials is determined by the geometry-dependent phonon boundary scattering mean free path (*L*). Although prior work has investigated phonon transport in periodically corrugated nanowires, the detailed relationship between geometric parameters and *L* in recently fabricated diameter-modulated cylindrical nanowires is not known. For example, it is not clear whether enhancing the larger cylinder diameter would reduce *L* due to the phonon backscattering effect, or enhance *L* due to the larger average distance between phonon collisions. Here, we use phonon ray tracing simulations to comprehensively study the effect of geometric parameters on *L* in cylindrical nanowires. We find that for a fixed smaller cylinder diameter, *L* can be maximized or minimized via geometric control of the pitch, length, and diameter ratios. Our simulations show that the phonon backscattering framework is appropriate for small-pitch nanowires, while a resistors-in-series expression is required to model long-pitch nanowires. Combining our calculations with analytical phonon dispersion and bulk scattering model, we predict that of periodic silicon nanowires with a fixed smaller diameter of 50 nm can be tuned by up to 27% at 300 K via geometric control. Our results provide insight into the mechanisms of suppression and enhancement in periodically modulated nanowires, and can be used by experimentalists to explore boundary scattering in complicated nanostructure geometries.