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Thermally-Active Screw Dislocations in Si Nanowires and Nanotubes TRAIAN DUMITRICA, University of Minnesota, SHIYUN XIONG, École Centrale du Paris, France, JIHONG MA, University of Minnesota, SEBASTIAN VOLZ, École Centrale du Paris, France — New properties appear when nanomaterials contain dislocations. Understanding whether these features, which arise naturally during growth, are beneficial or problematic becomes essential for developing applications. Here we investigate 110 Si nanowire and nanotube structures containing an axial screw dislocation, as described by objective molecular dynamics coupled with the classical Tersoff potential. By means of direct nonequilibrium molecular dynamics simulations, we uncover significant reductions in thermal conductivity when nanostructures contain axial screw dislocations with closed and open cores. Analysis based on the atomistic Green function method reveals that in nanowires, the effect originates largely in the phonon-phonon scattering due to the enhanced anharmonicity introduced by highly distorted core region of the dislocation. In nanotubes, the inner surface compensates effectively for the missing core region. The uncovered effect can act in combination with other already known thermal conductivity limiting mechanisms, and thus can enable the further optimization of the figure of merit for a new family of complex thermoelectric nanomaterials.

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