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Thermally Active Screw Dislocations in Si, SiC, PbSe, and SiGe Nanowires. JIHONG AL-GHALITH, YUXIANG NI, University of Minnesota, Twin Cities, SHIYUN XIONG, Max Planck Institute for Polymer Research, SEBASTIAN VOLZ, Ecole Centrale Paris, TRAIAN DUMITRICA, University of Minnesota, Twin Cities — We elucidate thermal conductivity along the screw dislocation line, which represents a transport direction inaccessible to classical theories. By using equilibrium and non-equilibrium molecular dynamics simulations, and the atomistic Green function method, we uncover a Burgers vector dependent thermal conductivity reduction in Si, SiC, PbSe, and SiGe nanowires. The effect is uncorrelated with the classical theory of Klemens. The influence of dislocations on thermal transport originates in the highly deformed core region, which represents a significant source of anharmonic phonon-phonon scattering. High strain reduces the phonon relaxation time, especially in the longitudinal acoustic branches, and creates an effective internal thermal resistance around the dislocation axis. The effect can be distinguished from the thermal transport reduction caused by the nanowire surface imperfections and vacancies. Our results have implications for designing materials useful for high-temperature electronics and thermoelectric applications.

Jihong Al-Ghalith
University of Minnesota, Twin Cities

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