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Defect induced carrier transport in semiconductor junctions¹ SANGHAMITRA NEOGI, VITALY PROSHCHENKO, Univ of Colorado - Boulder — Thermal management technologies are of critical importance to maintain the temperatures of myriad devices within the required temperature limits, regardless of the external environment or thermal loads imposed from operations. As opposed to conventional bulky passive heat exchanger mechanisms, thermoelectric (TE) devices have the potential to provide targeted localized cooling, and thereby, drastically reduce the thermal budget of a system. Significant progress has been made to enhance ZT with the development of nanostructured TE materials, and thin-film superlattice structures are often reported to have improved performance over bulk materials. However, understanding the mechanism of thermal transport across various dissimilar materials is critical to the development of TE devices with predictable, robust and optimal performance. We combine atomistic and first-principle methods to analyze both phononic and electronic transport across Si/Ge interfaces by solving Boltzmann transport equations. We investigate the change in spectral properties of heat carriers near the interface under imperfect conditions. Our results will establish a relationship between interfacial thermal transport and nanoscale interfacial structures, dictated by methods of fabrication and processing.

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