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Phonon thermal transport in 2H, 4H and 6H silicon carbide from first principles NAKIB PROTIK, Boston College, ANKITA KATRE, CEA-Grenoble, LUCAS LINDSAY, Oak Ridge National Laboratory, JESUS CARRETE, CEA-Grenoble, B. DONGRE, G.K.H. MADSEN, Technical University of Vienna, NATALIO MINGO, CEA-Grenoble, DAVID BROIDO, Boston College — Silicon carbide (SiC) is widely used in electronic devices, in part because its high thermal conductivity helps prevent 'hot spots' to maintain uniform device operating temperatures. Here we present *ab initio* calculations of the in-plane and cross-plane thermal conductivities, k_{in} and k_{out}, of the hexagonal SiC polytypes, 2H, 4H and 6H. These calculations combine a full solution of the phonon Boltzmann equation with accurate determination of interatomic force constants from density functional theory. Generally, k_{out} values are found to be smaller than k_{in} values for a given polytype. Both k_{in} and k_{out} decrease with increasing n in nH SiC. This finding is contrary to previous measurements, which showed 4H SiC having lower k than 6H SiC [1]. Specific comparisons will be made to existing measured and calculated results. We will also discuss the formation of defects, and their effect on thermal conductivity. [1] D. T. Morelli, J. P. Heremans, C. P. Beetz, W. S. Yoo, and H. Matsunami, Appl. Phys. Lett. 63, 3143 (1993); Rusheng Wei, et al., J. Appl. Phys. 113, 053503 (2013).

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