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Molecular Dynamics Simulations of the Thermal Conductivities of Group IV Bulk Materials and Nanowires JOHN REED, ANDREW WILLIAMSON, Lawrence Livermore National Laboratory, GIULIA GALLI, University of California, Davis — We present the results of equilibrium molecular dynamics simulations of the thermal conductivities of bulk C, Si, Ge, and SiC using the Green-Kubo formalism. We use an empirical interatomic potential developed by Tersoff [1] and investigate the effects of modifications to this potential suggested by Porter et al [2]. We also investigate the effects of choosing a symmetric versus nonsymmetric definition of the local heat. A generalization of this approach to study the dependence of the thermal conductivity of SiGe nanowires on their size and composition will also be presented. [1] J. Tersoff, PRB 39 (8), 5566-5568 [2] L. Porter, J. Li, S. Yip, J. Nuc. Matl. 246 (1997) 53-59 This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

John Reed
Lawrence Livermore National Laboratory

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