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Optimized thermal conductivities of Silicon Germanium nanowires JOHN REED, ANDREW WILLIAMSOM, GIULIA GALLI, Lawrence Livermore National Laboratory, YING MENG, MUELLER TIM, CEDER GERBRAND, Massachusetts Institute of Technology — The measure of the thermoelectric efficiency of a material is given by its "Figure of merit" (Z), which is inversely proportional to its thermal conductivity, and directly proportional to its electrical conductivity. Alloys of Si and Ge are promising thermoelectric materials, since they can be engineered so as to have a low thermal conductivity relative to their electrical conductivity. We present molecular dynamics simulations of the thermal conductivities of Si_xGe_{1-x} nanowires, and an optimization strategy to obtain maximal values of ZT for these systems. We found that Si-Ge alloy nanowires have a significantly lower thermal conductivity than pure Si or Ge nanowires of the same diameter. Furthermore the alloy ordering is found to significantly effect thermal conductivities, and hence is a key parameter to control and vary in order to optimize thermal conductivities and eventually Z values. Towards this end optimal orderings of Si and Ge for low thermal conductivities have been predicted. 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.

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