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Thermal conductivity and thermal rectification in graphene nanoribbons: a molecular dynamics study JIUNING HU, School of Electrical and Computer Engineering and Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana 47907, XIULIN RUAN, School of Mechanical Engineering and Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana 47907, ZHIGANG JIANG, School of physics, Georgia Institute of Technology, Atlanta, Georgia 30332, YONG CHEN, Department of physics, School of Electrical and Computer Engineering and Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana 47907 — We have used molecular dynamics based on the Brenner potential to calculate the thermal conductivity of graphene nanoribbons. For symmetrical nanoribbons, the calculated thermal conductivity is the similar order of magnitude of the experimentally measured value for graphene. We have investigated the effects of edge chirality and found that nanoribbons with zigzag edges have considerable larger thermal conductivity than that of nanoribbons with armchair edges. For asymmetric nanoribbons, we have found considerable thermal rectification. For example, for a 6nm-long triangular shaped nanoribbon, the thermal conductivity from the wider to the narrower end is nearly 2.5 times that from the narrower to the wider end. Furthermore, the thermal rectification can be significantly enhanced by increasing the size of the asymmetrical nanoribbon. Such rectification effects can be useful in nanoscale thermal management.

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