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Micrometer-scale molecular dynamics simulations on the lattice thermal conductivities of graphene and silicon MINKYU PARK, KRISS-University of Science & Technology, SUN-CHUL LEE, KRISS, YONG-SUNG KIM, KRISS-University of Science & Technology — We calculated lattice thermal conductivity of graphene and silicon by using large-scale molecular dynamics simulations. In the molecular dynamics simulations, whether the non-equilibrium systems reach the steady states is rigorously investigated, and the times to reach the steady states are found to drastically increase with the lengths of the system. From the ballistic to the diffusive regime, the lattice thermal conductivities are explicitly calculated and found to keep increasing in a wide range of lengths with finally showing a converging behavior at 16 micrometer for graphene and 8 micrometer for silicon. That obtained macroscopic values of the lattice thermal conductivity of graphene and silicon are 3200 and 210 W/mK respectively.

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