Atomistic Study of Heat Conduction in Silicon Carbide Ceramics

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Abstract

Molecular dynamic simulation is a powerful computational technique to simulate the atomic-scale dynamics of materials over short nanosecond time scales, in order to predict macroscopic physical and mechanical properties under extreme conditions that are not directly accessible experimentally. This poster will present a molecular dynamics simulation study of thermal conductivity in silicon-carbide ceramic materials at ultrahigh temperature, which is important for the performance of thermal protection systems in hypersonic space re-entry vehicles currently in development at NASA. In this study, the Large-scale Atomic/Molecular Massively Parallel Simulator software was deployed using supercomputers to compute lattice thermal conductivities in different silicon-carbide crystal polytypes (2H, 3C, 4H, 6H, 8H) at temperatures ranging from 1200 K to 2200 K. It is found that heat conduction in silicon-carbide ceramics decreases with increasing temperature, and strongly depends on the crystal structure.