

# **Engineering Lattice Thermal Transport in Nanomesh Metastructures Towards Improved Radioisotope thermoelectric generators for NASA's Space Missions**

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Radioisotope thermoelectric generators (RTGs) have been utilized in multiple NASA space missions to convert the heat released by the decay of a suitable radioactive material into electricity using the Seebeck effect. To enhance the performance of RTGs, researchers aim to reduce lattice thermal conductivity by suppressing phonon contributions. Nanomesh structures, which are thin films containing densely arranged nanoholes, show promise in efficiently modulating lattice thermal conductivity and improving RTGs performance. In this work, we present a comprehensive investigation of phonon thermal transport in silicon nanomeshes with varying hole sizes, shapes, surface roughness, and periodicity/aperiodicity using nonequilibrium molecular dynamics simulations. Our results indicate that surface roughness hinders phonon coherence in nanomeshes and that aperiodicity affects the transport of both coherent and incoherent phonons. We found that incoherent phonon backscattering and coherent phonon localization are the primary reasons for reduced thermal conductivity in aperiodic nanomeshes. Furthermore, we determined a critical hole size below which coherent phonons significantly contribute to thermal conductivity, and above which they can be ignored as they do not dominate thermal transport.