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

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## Introduction

- Understanding thermal transport in nanoscale structures is crucial for designing energy-efficient electronics and energy conversion/storage systems such as the radioisotope thermoelectric generator (RTG) shown in Fig.1 used in multiple space missions in NASA like the Mars rover Curiosity in Fig.2.

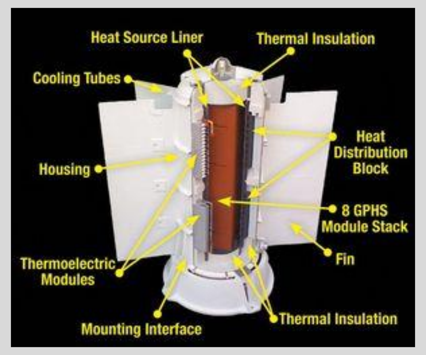



Fig.1. Radioisotope thermoelectric generator (RTG)

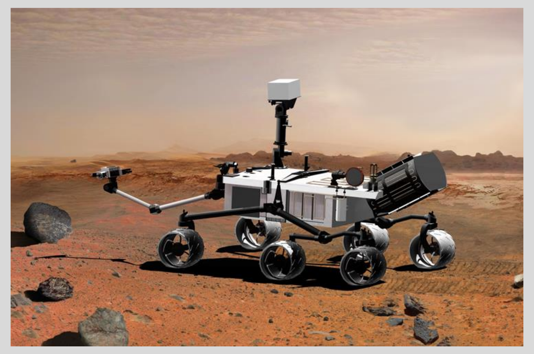


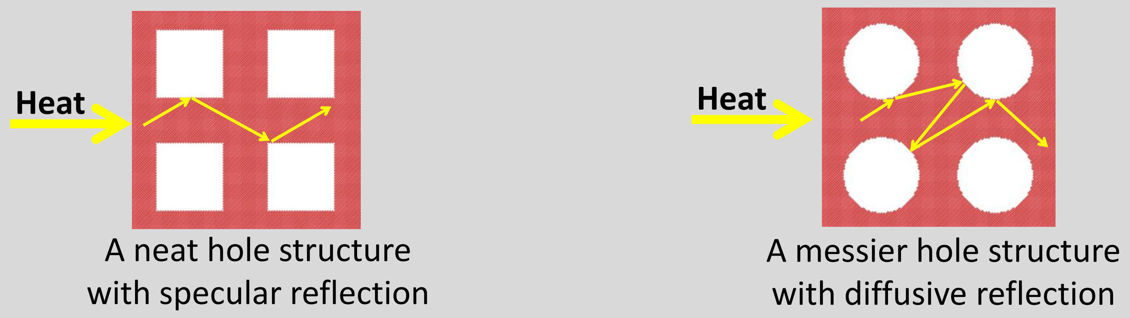
Fig.2. NASA's Mars rover Curiosity

- Nanomesh (NM) shown in Fig.1, also referred to as phononic crystal, is one of the promising nanostructures to efficiently modulate thermal transport.
- Phonon, a quantum description of collective atom vibrations, dominates heat transfer in semiconductors.
- Types of phonons: coherent (wave-like) and incoherent (particle-like) phonons as illustrated in Fig.2.

## Problem Statement

**Potential factors influencing thermal conductivity**

- Temperature:
  More intense anharmonic phonon scattering at higher *T*.
- Nanohole geometries:
  (1) square holes (2) circular holes

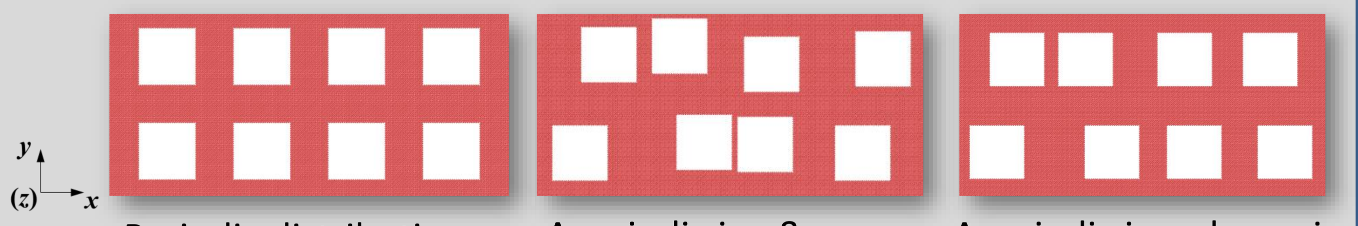



A neat hole structure with specular reflection — A messier hole structure with diffusive reflection

- Boundary roughness:
  (1) rough boundary (2) smooth boundary


More diffusive scattering of phonons — More specular scattering of phonons

- Periodicity:
  (1) periodic (2) aperiodic (3) ap-x

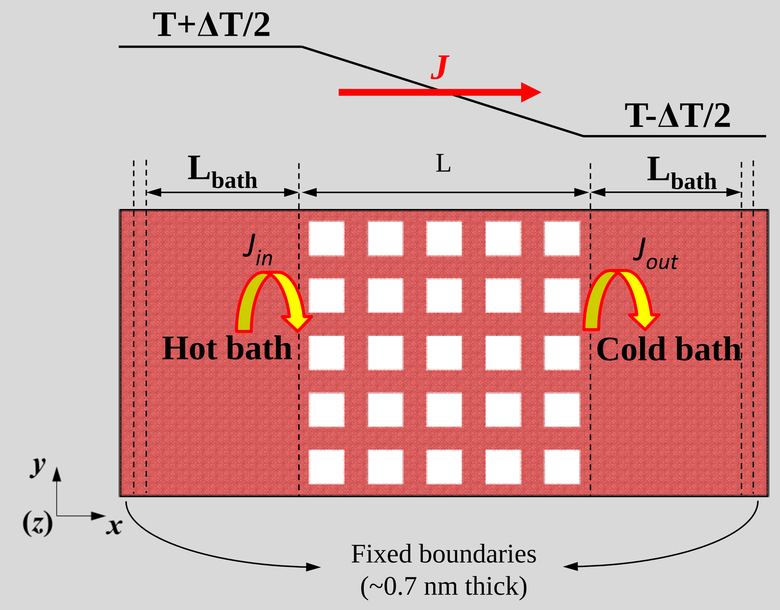



Periodic distribution — Aperiodic in x&y axes — Aperiodic in only x axis

## Methodology

**Non-equilibrium molecular dynamic simulations**

Model system: silicon nanomesh




$$q'' = -\kappa \nabla T$$

$$J = \frac{(J_{out}+J_{in})}{2} \qquad \kappa = \frac{J}{(\Delta T/L)}$$

$q''$ : local heat flux density

$J$ : steady state heat current

Fig.3. NEMD simulation model

## Results and Discussions

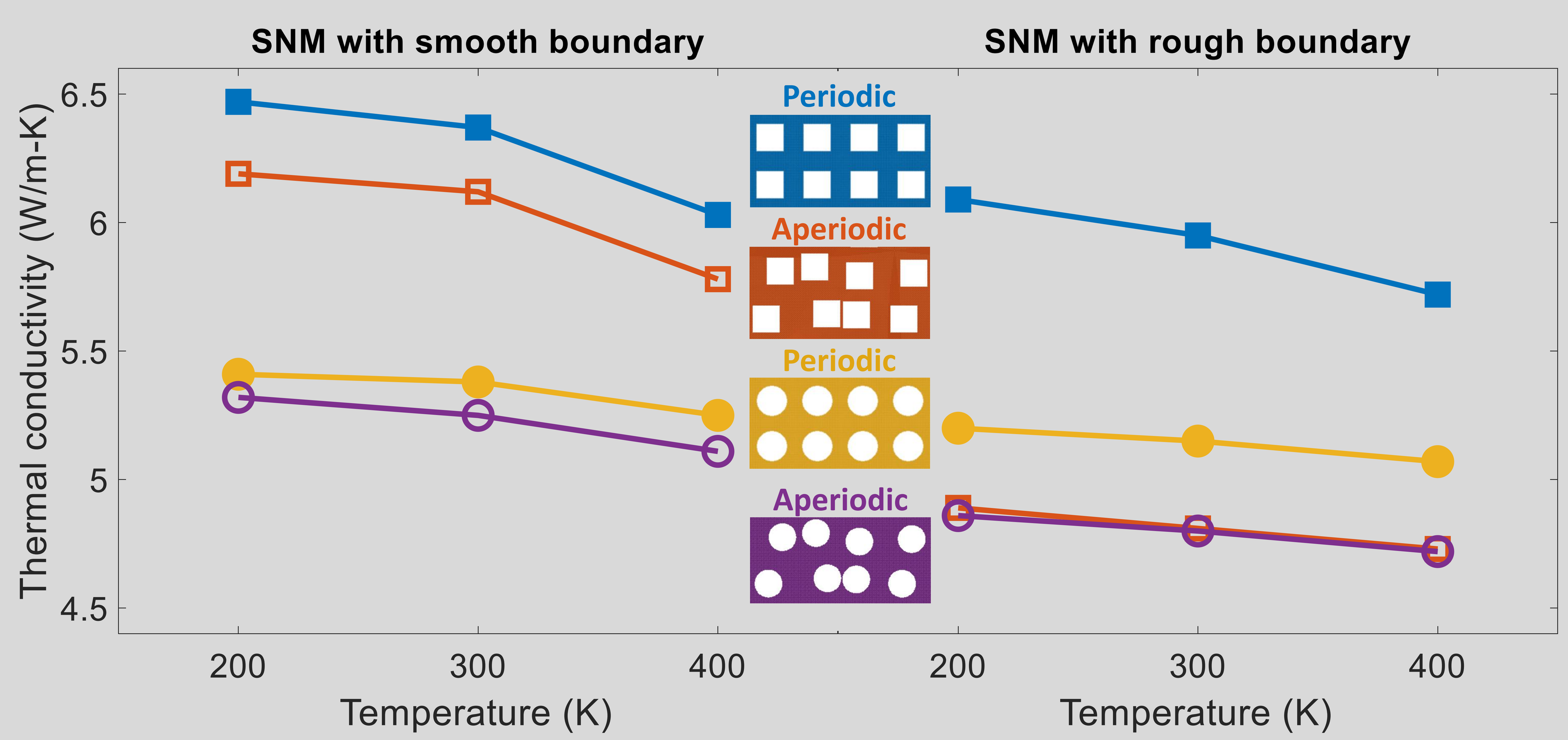



Fig.4. Thermal conductivity of SNM at different temperatures

- κ(square holes)>κ(circular holes):

Phonons are scattered more diffusively by circular holes than square holes.

- κ(200K)>κ(300K)>κ(400K):

More intense anharmonic phonon scattering at higher temperature results in the reduction of thermal conductivity.

- κ(smooth)>κ(rough):

(1) Rough boundary with diffusive scattering of phonons suppresses thermal transport, indicating that roughness could kill coherent phonons.

(2) Smooth boundary with specular scattering of phonons enhances thermal transport, suggesting that there might be coherent phonons.

- κ(periodic)>κ(aperiodic)

Random localization of holes significantly suppresses phonon transport.

**Additional verification of coherent phonons**

- The comparison of thermal conductivity between SNM with periodic and aperiodic holes could not rigorously validate the existence of coherent phonons because fully aperiodic holes would directly block the straight propagation of phonons, whether they are coherent or incoherent, making it hard to find out the origin of reduction of thermal conductivity.
- SNM with aperiodic holes in only *x* direction (ap-x), the same direction of heat flux, would be a complementary case to quantify the contribution of coherent and incoherent phonons to thermal transport because it has a similar straight propagation channel as SNM with periodic distributed holes, while the random localization in *x* direction would suppress coherent phonons.
- We find κ(ap-x)≅κ(periodic) even for longer structures considering length effect shown in Fig.5, because there might not be coherent phonons in SNM with period=12nm, where period is defined as the center-to-center distance between two neighboring nanoholes.

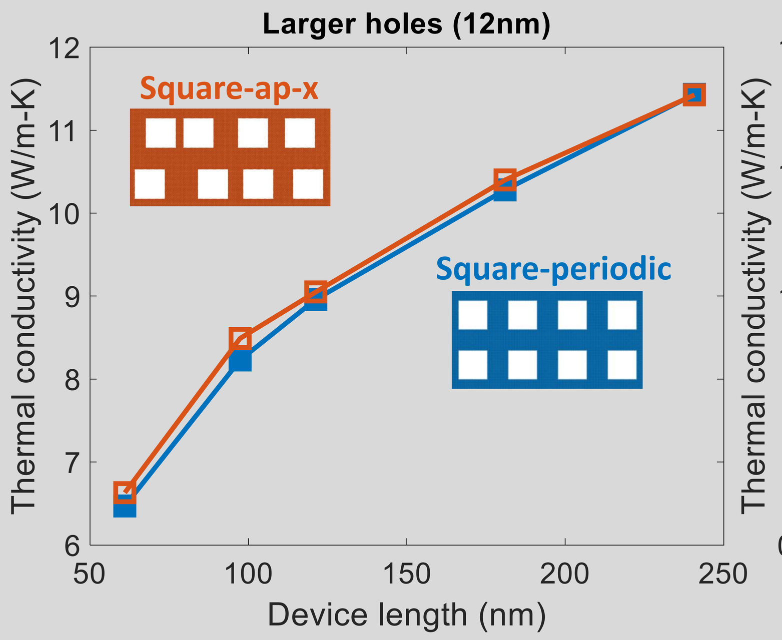



Fig.5. κ of SNM with smooth square larger holes at 200K

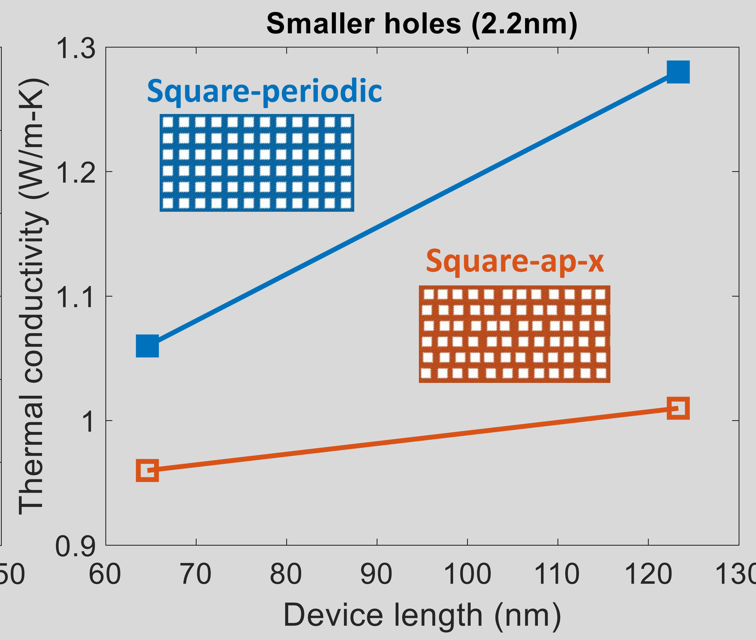



Fig.6. κ of SNM with smooth square smaller holes at 200K

- For SNM with period=2.2nm, possessing the same porosity as the one with period=12nm, the finding of κ(period)>κ(ap-x), shown in Fig.6, is a direct evidence to verify the existence of coherent phonons.
- κ(SNM with 12nm period)>κ(SNM with 2.2nm period), indicating significant boundary scattering in the latter one due to increasing number of holes, more boundaries and higher possibility for phonons to be scattered.

## Acknowledgement

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