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Thermal Rectification using Asymmetrically Perforated Graphene

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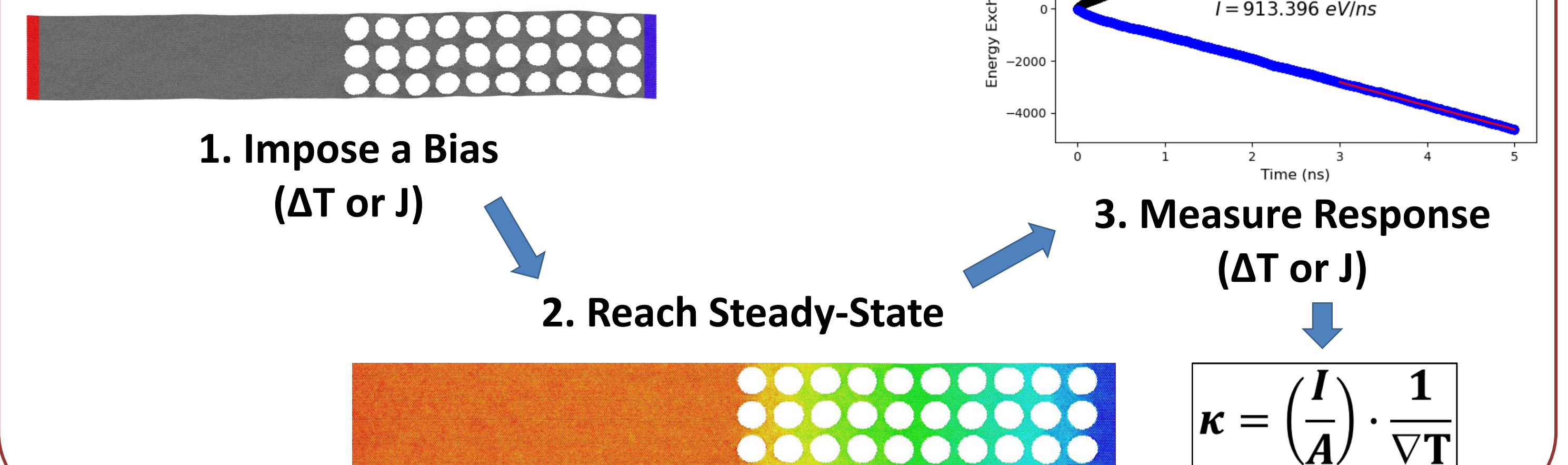
Abstract: Non-Equilibrium Molecular Dynamics simulations were performed to study thermal rectification effects in perforated graphene monolayers with various geometrical pore parameters. Circular and triangular pores have been used. The Thermal Rectification (TR) ratios found are of the order of 6.5%. Phonon overlap mismatch and directional scattering have been proposed as possible mechanisms of thermal rectification in these systems.

Introduction/Context:

- Continuous **miniaturization** of devices leads to **hotspots** that limit their **efficiency**; need efficient **heat management** at the nanoscale
- Still, efficient **thermal diodes** at the nanoscale are not yet fully developed. Systems studied for **thermal rectification** include: *TMDC lateral heterostructures¹, hBN-graphene VdW heterostructures², trapezoidal and T-shaped graphene nanoribbons³, thickness asymmetric graphene nanoribbons⁴, etc.*
- In this work we studied the thermal rectification performance of **asymmetrically perforated graphene monolayers**

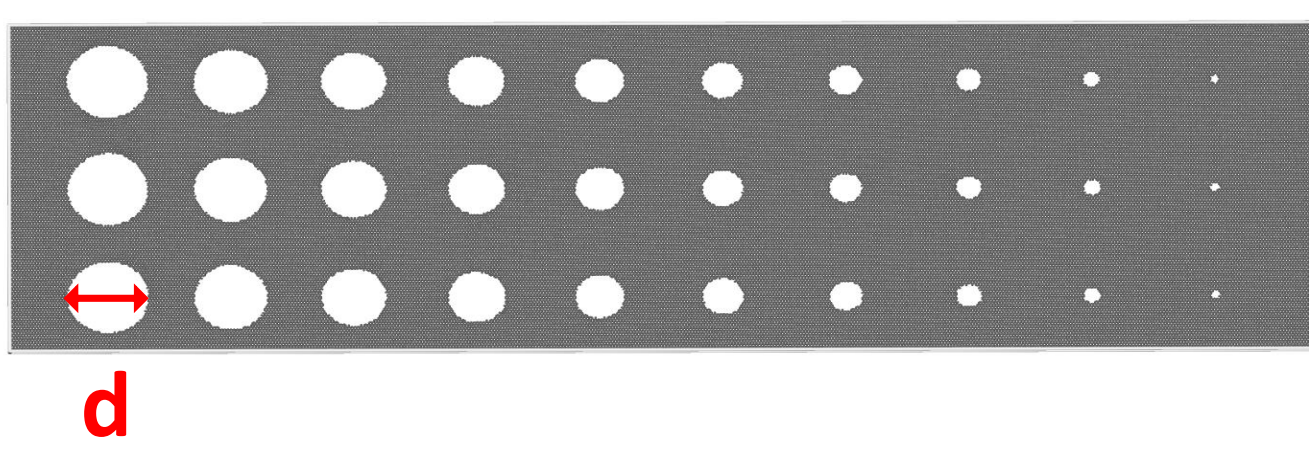
Methodology:

Non-Equilibrium Molecular Dynamics (NEMD)

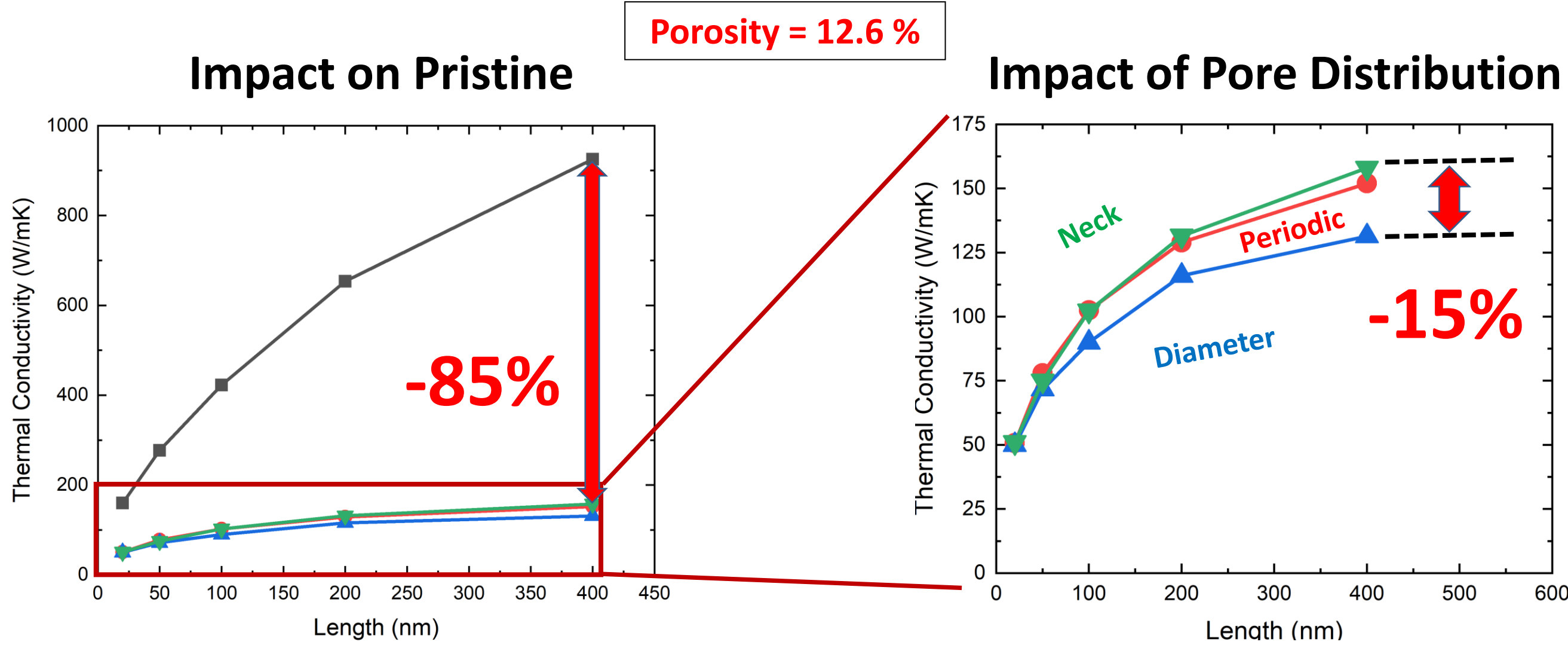
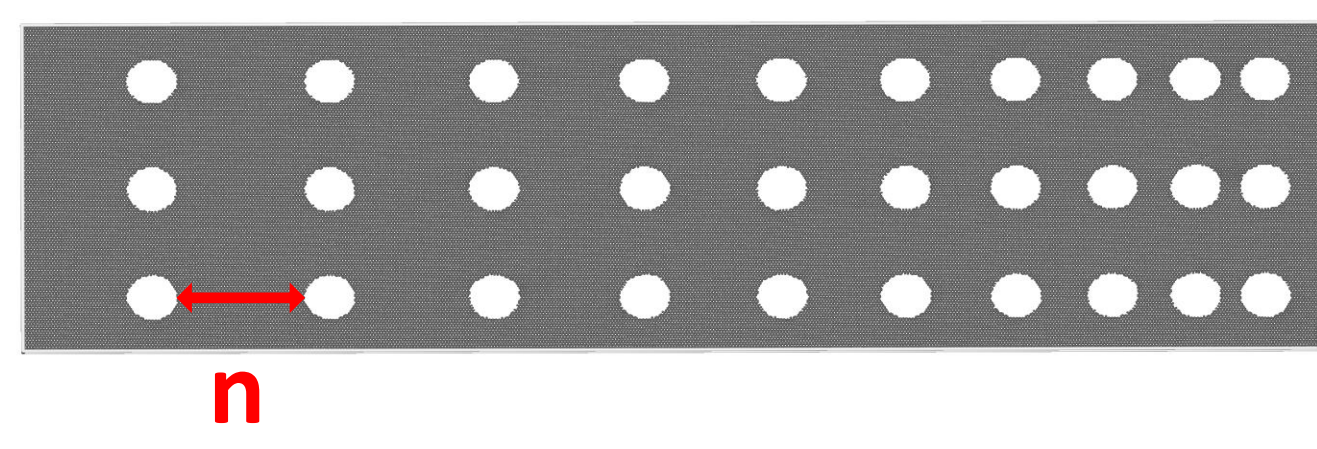


Impact of Pore Distribution on Thermal Conductivity

Distribution of Diameters



Distribution of Neck Sizes

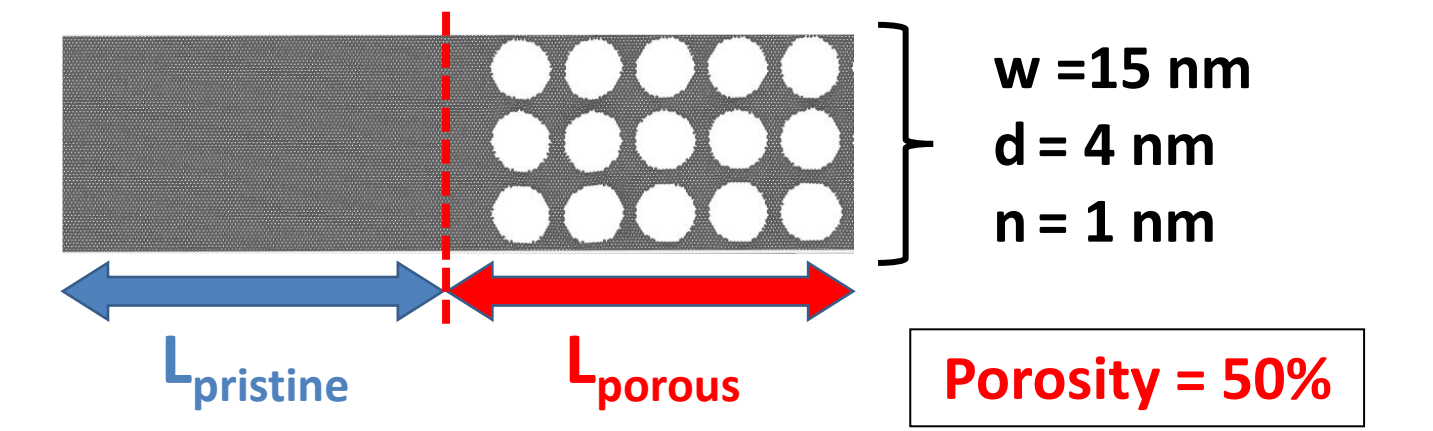
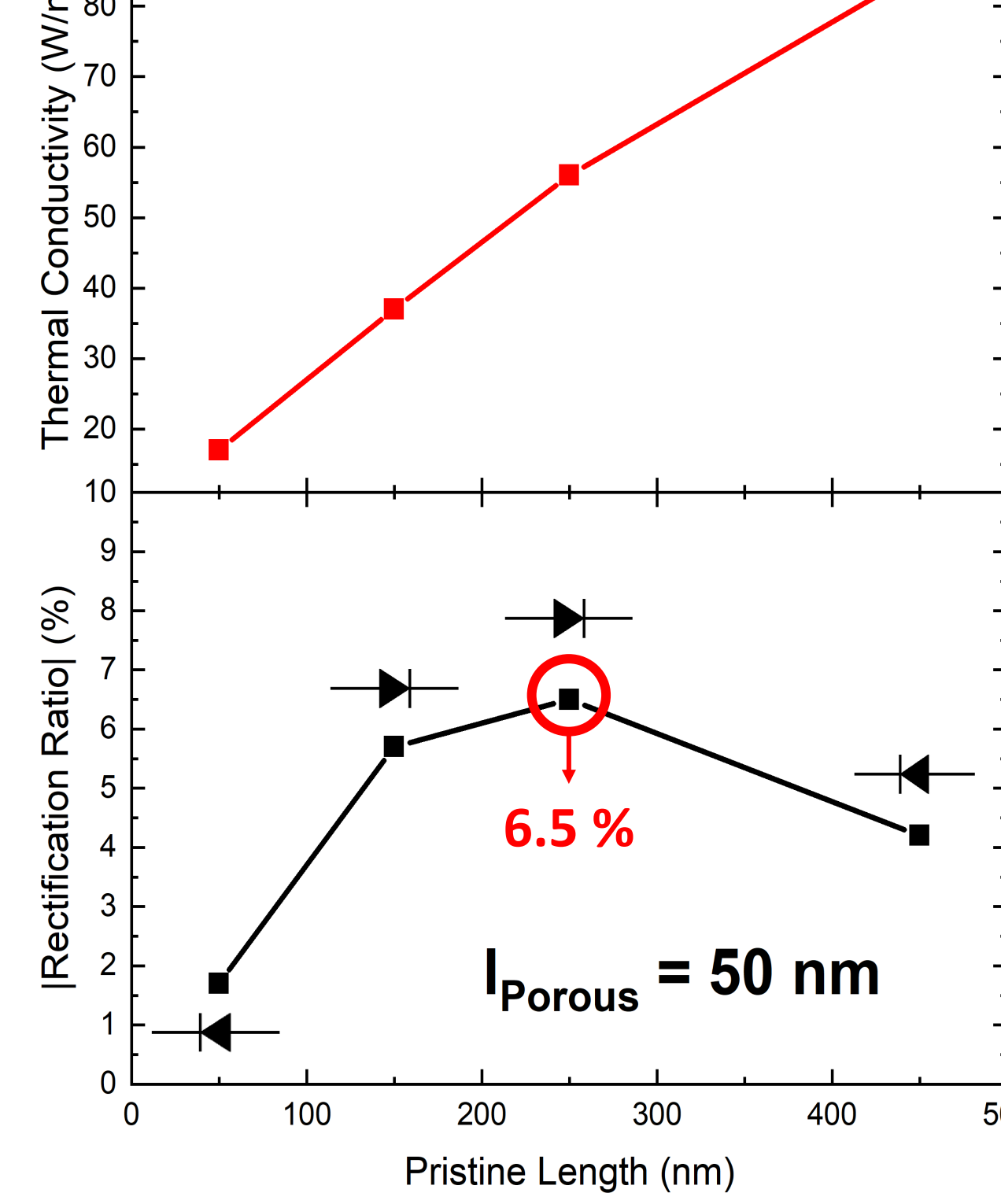


Huge suppression of κ even for a very small porosity

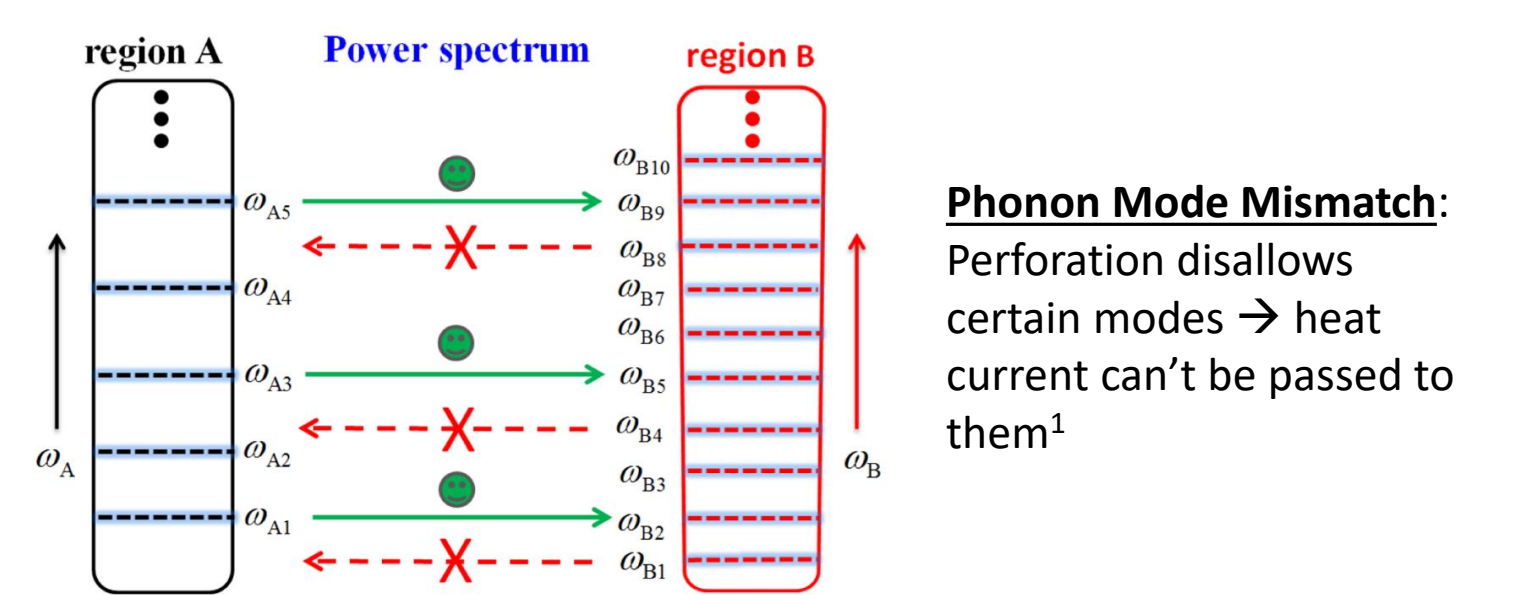
Lower κ despite same porosity: smaller available "phonon pathways" for diameter-modulated case

Rectification: Circular Pores + Pristine

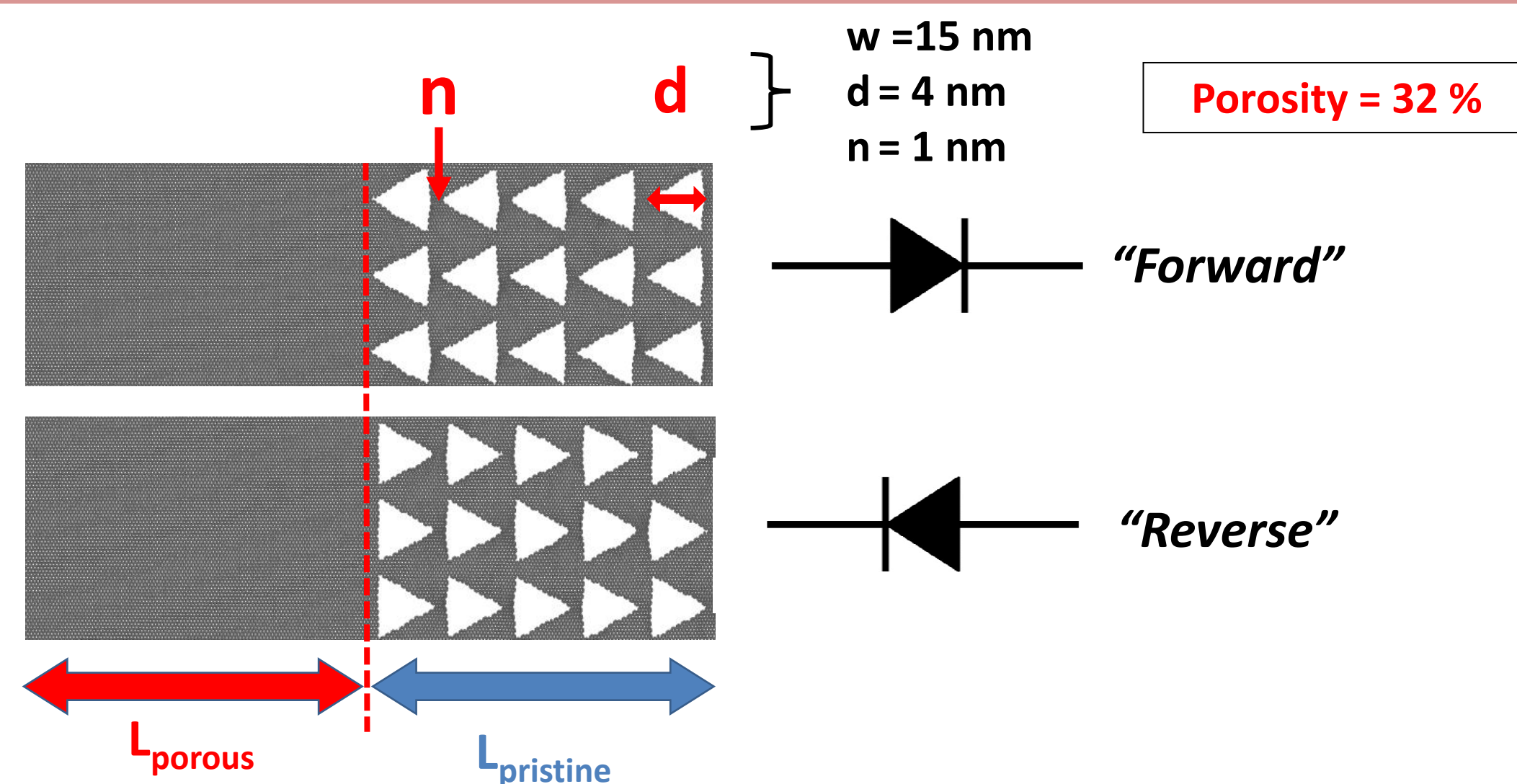
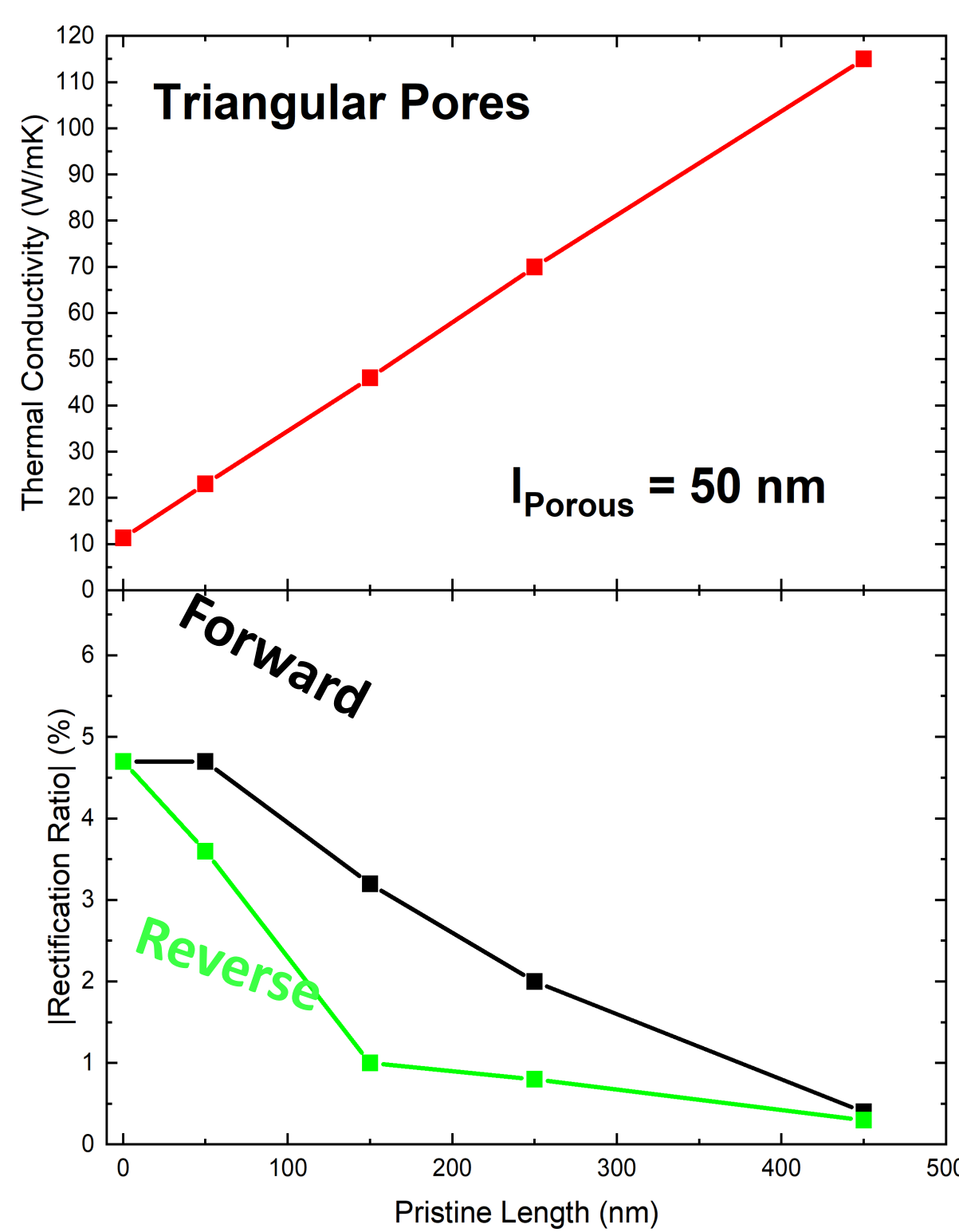
Circular Pores



- Diode **directionality changes** with changing the **length** of the pristine side
- Possible **TR mechanism: phonon mode mismatch** in pristine/perforated sides due to perforation



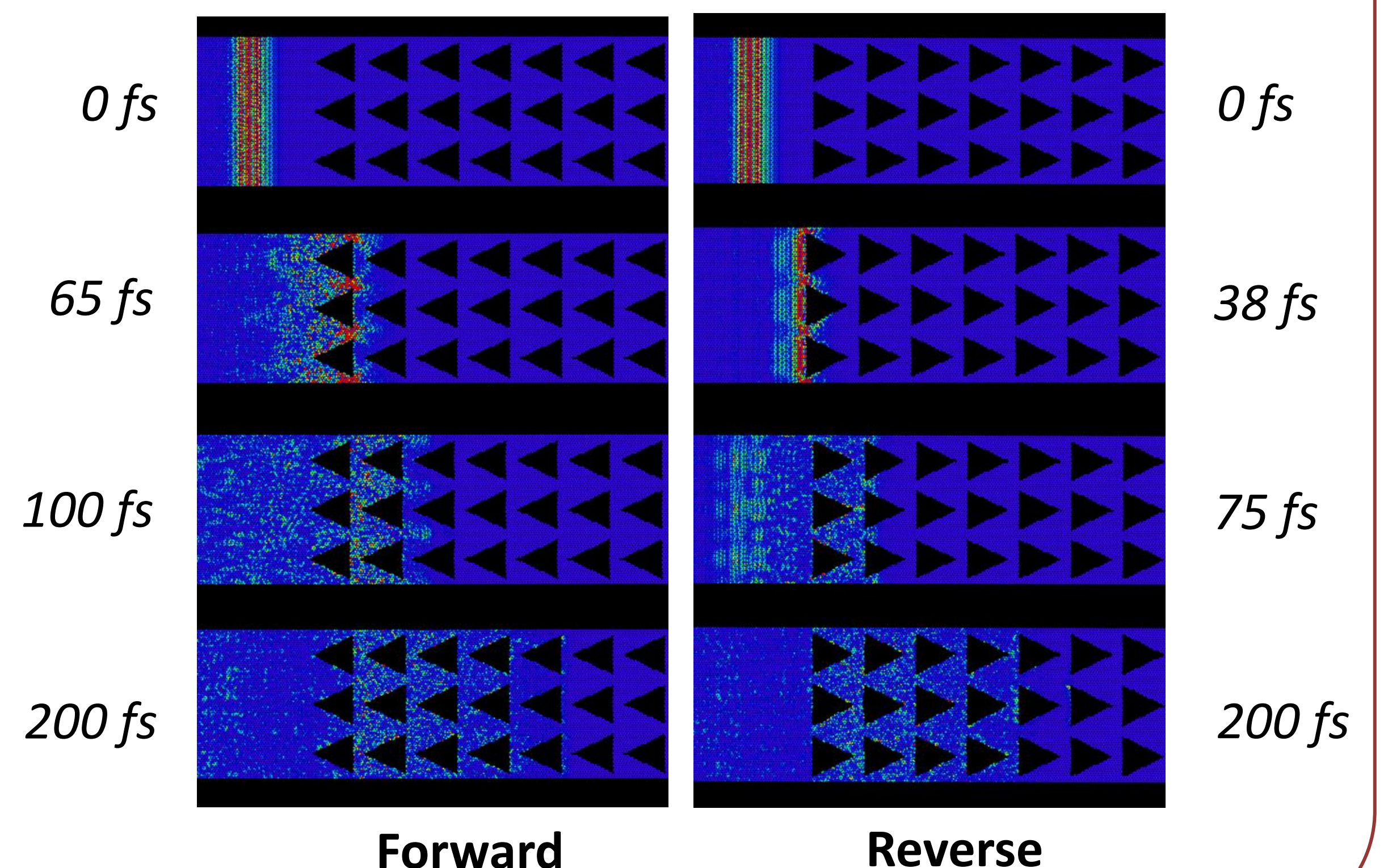
Rectification: Triangular Pores + Pristine



- Diode **directionality changes** with the **orientation** of the triangles
- The **easy direction** is due to **directional scattering** by the triangles
- For larger sizes, **larger λ -modes** dominate heat flow; they "see" the pores as **point defects** → **no directional scattering!**
- For larger sizes phonon mismatch probably dominates
- Lower TR than circular due to **smaller porosity (max limit: 50%)**

Phonon Wavepacket Propagation

ZA Polarization, $\omega=200 \text{ cm}^{-1}$



Conclusions

- **Perforation** lowers **dramatically** the **thermal conductivity** of pristine graphene, even for **small porosities**
- Thermal rectification can be a result of different **mechanisms**, such as phonon mode mismatch and directional phonon scattering; all arise due to some **asymmetry**
- Triangular pores with **different orientation** scatter phonons differently; this is a source of **directional scattering** that potentially leads to **thermal rectification**

Perspectives

- Different perforation patterns, shapes, etc.
- Explore the effects of more perforation parameters (diameter, neck, porosity, etc.)
- Apply to different 2D materials (hBN, TMDC's, etc.) and heterostructures thereof
- Implement experimentally

References:

[1] Zhang et al., *Science* **378**, 169-175 (2022)
 [2] Chen et al., *ACS Appl. Mater Interfaces* **12**, 15517-15526 (2020)
 [3] Wang et al., *Nano Lett.* **378**, 169-175 (2013)
 [4] Zhong et al., *Appl. Phys. Lett.* **99**, 193104 (2011)