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Thermal Rectification using Transition Metal Dichalcogenide Heterostructures

Markos Poulos, Konstantinos Termentzidis

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Abstract: Non-Equilibrium Molecular Dynamics simulations were performed to study thermal rectification effects in monolayer MoS₂/WS₂ lateral heterostructures. The parameters studied were the system length and the temperature bias ΔT . The maximum Thermal Rectification (TR) ratios found are of the order of 30%. The phonon Densities of States (pDOS) in the out-of-equilibrium steady state conditions were also probed, as well as the transmission of acoustic Phonon Wavepackets across the interface. We have found that non-linearities induced by large temperature biases ΔT are necessary for significant rectification ratios η .

Introduction/Context:

- Continuous **miniaturization** of devices leads to **hotspots** that limit their **efficiency**; need efficient **heat management** at the nanoscale
- Still, efficient nanoscale **thermal diodes** are not yet developed. Systems studied for **thermal rectification** include: *TMDC lateral heterostructures*¹, *hBN-graphene vdW heterostructures*², *trapezoidal and T-shaped graphene nanoribbons*³, *thickness asymmetric graphene nanoribbons*⁴, etc.
- In this work we studied the thermal rectification performance of **MoS₂/WS₂ monolayer lateral heterostructures**.

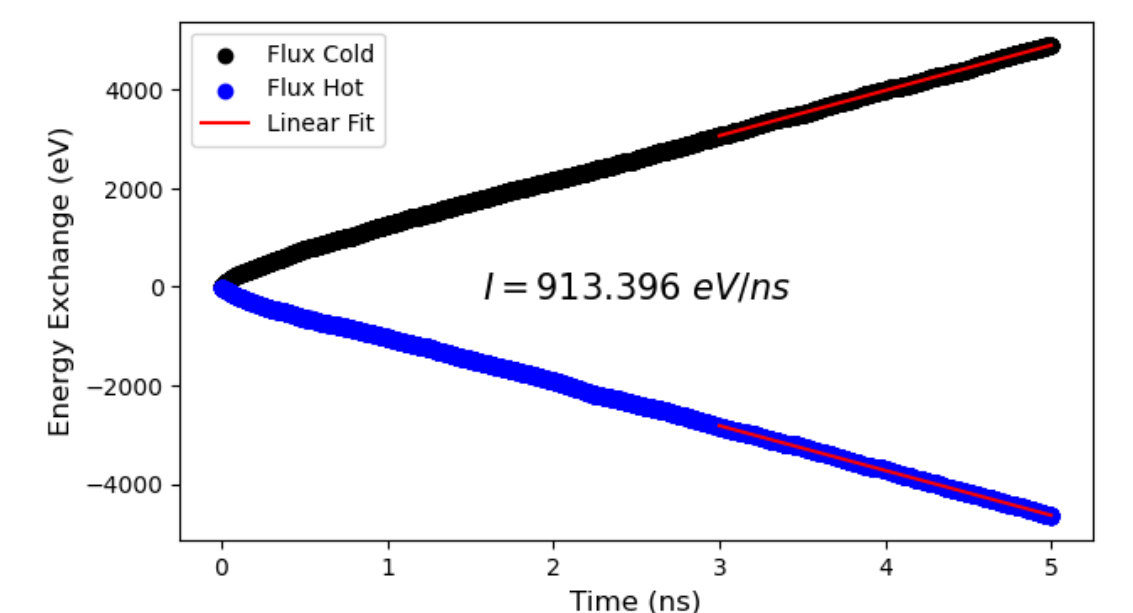
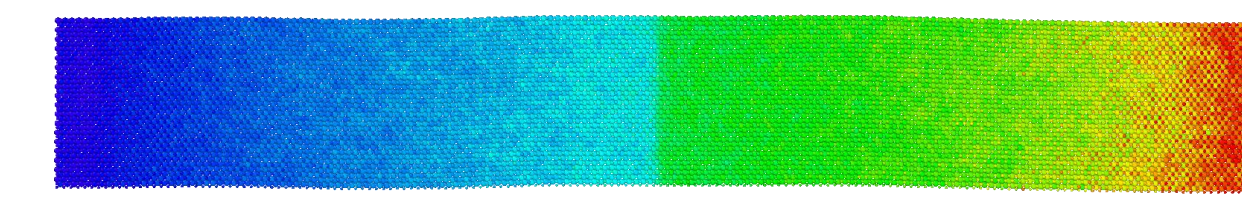
Methodology:

Non-Equilibrium Molecular Dynamics (NEMD)



1. Impose a Bias (ΔT or J)

2. Reach Steady-State



3. Measure Response (ΔT or J)

$$\kappa = \left(\frac{I}{A}\right) \cdot \frac{1}{\Delta T}$$

Conditions: Asymmetry + Non-linearity

$$q = \sum_s \int \frac{dk}{(2\pi)^3} \hbar \omega_{ks} n_{ks} v_{ks}$$

$$n_{ks} \approx n_{ks}^0 - \frac{\partial n_{ks}^0}{\partial (\hbar \omega_{ks})} \Theta_{ks} = n_{ks}^0 + \frac{n_{ks}^0 (n_{ks}^0 + 1)}{k_B T} \Theta_{ks}$$

$$\Theta_{ks} = -\Psi_{ks} \cdot \nabla T$$

$$q = \sum_s \int \frac{dk}{(2\pi)^3} \hbar \omega_{ks} v_{ks} \left(-\frac{n_{ks}^0 (n_{ks}^0 + 1)}{k_B T} \Psi_{ks} \cdot \nabla T \right)$$

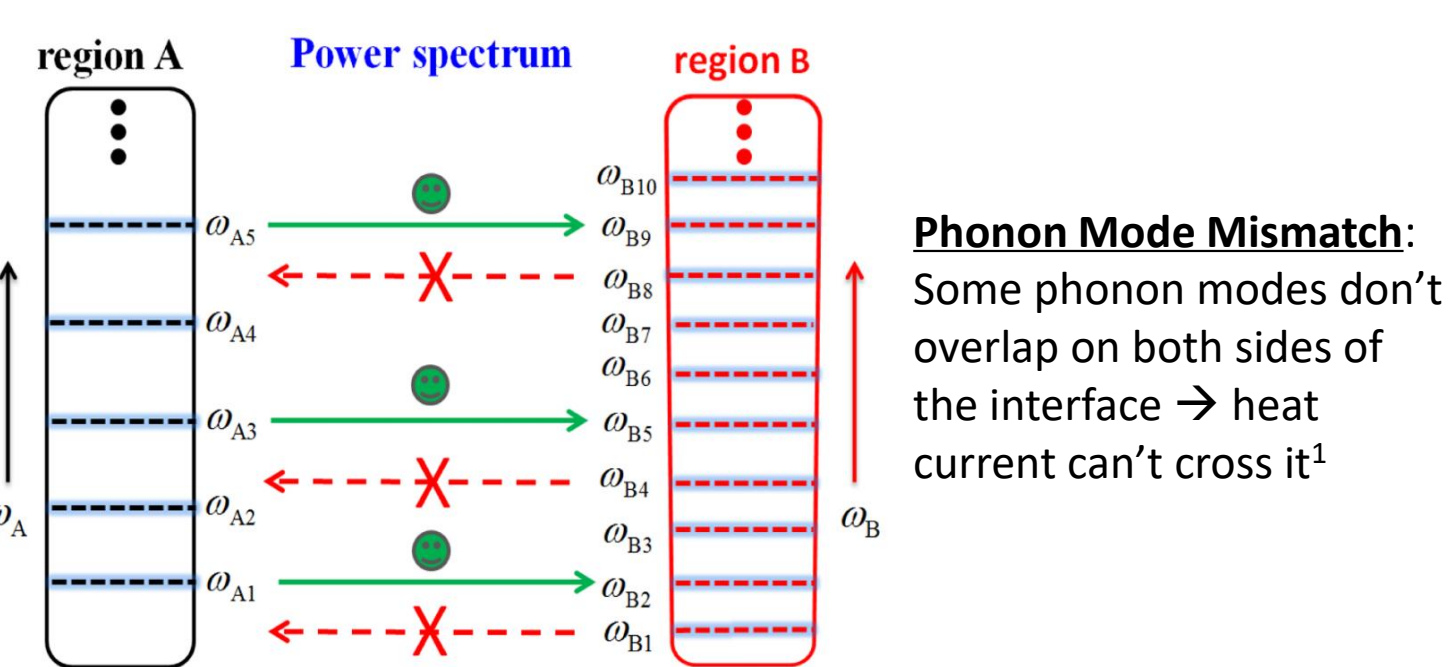
Thermal Conductivity

Limit $\Delta T \rightarrow 0$

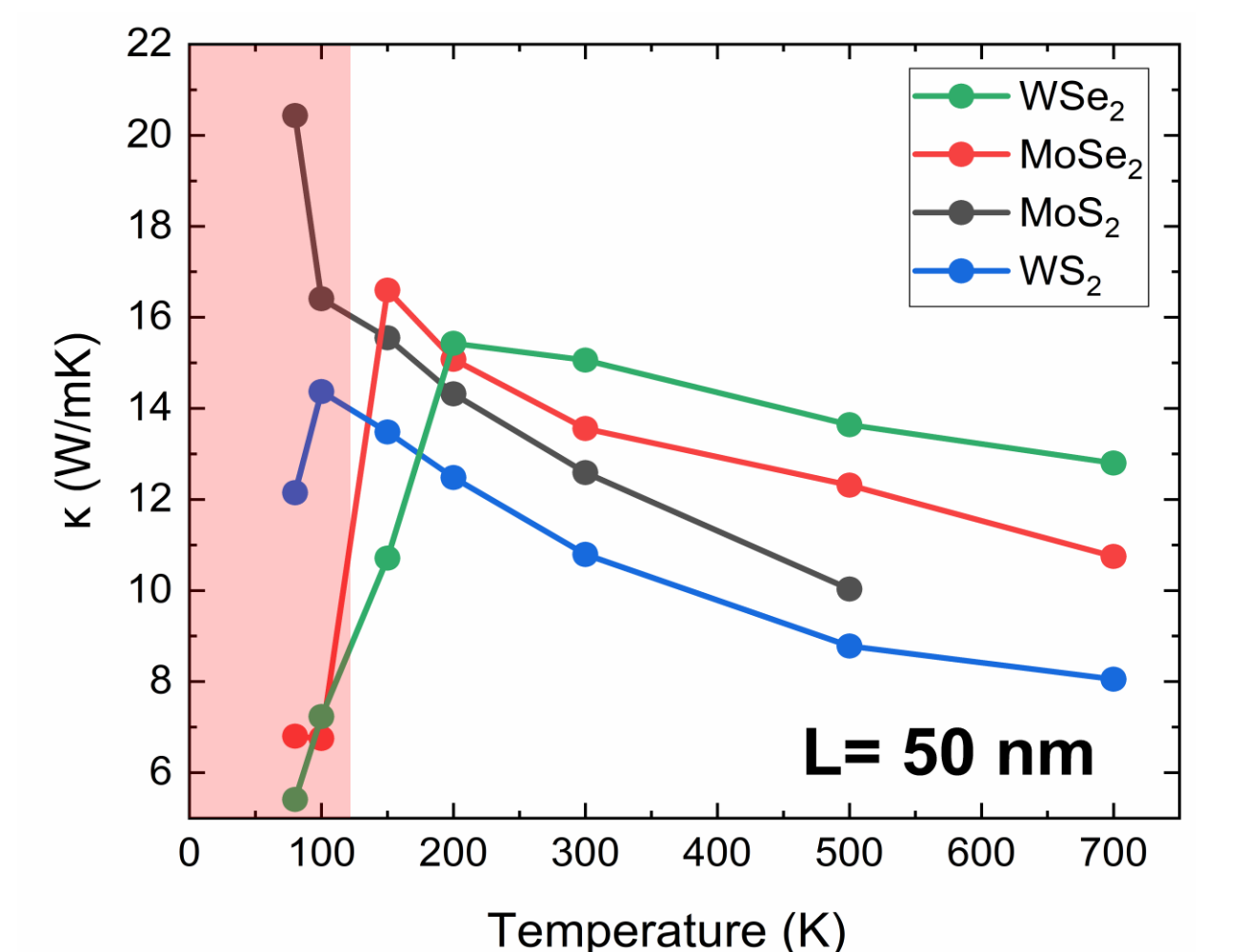
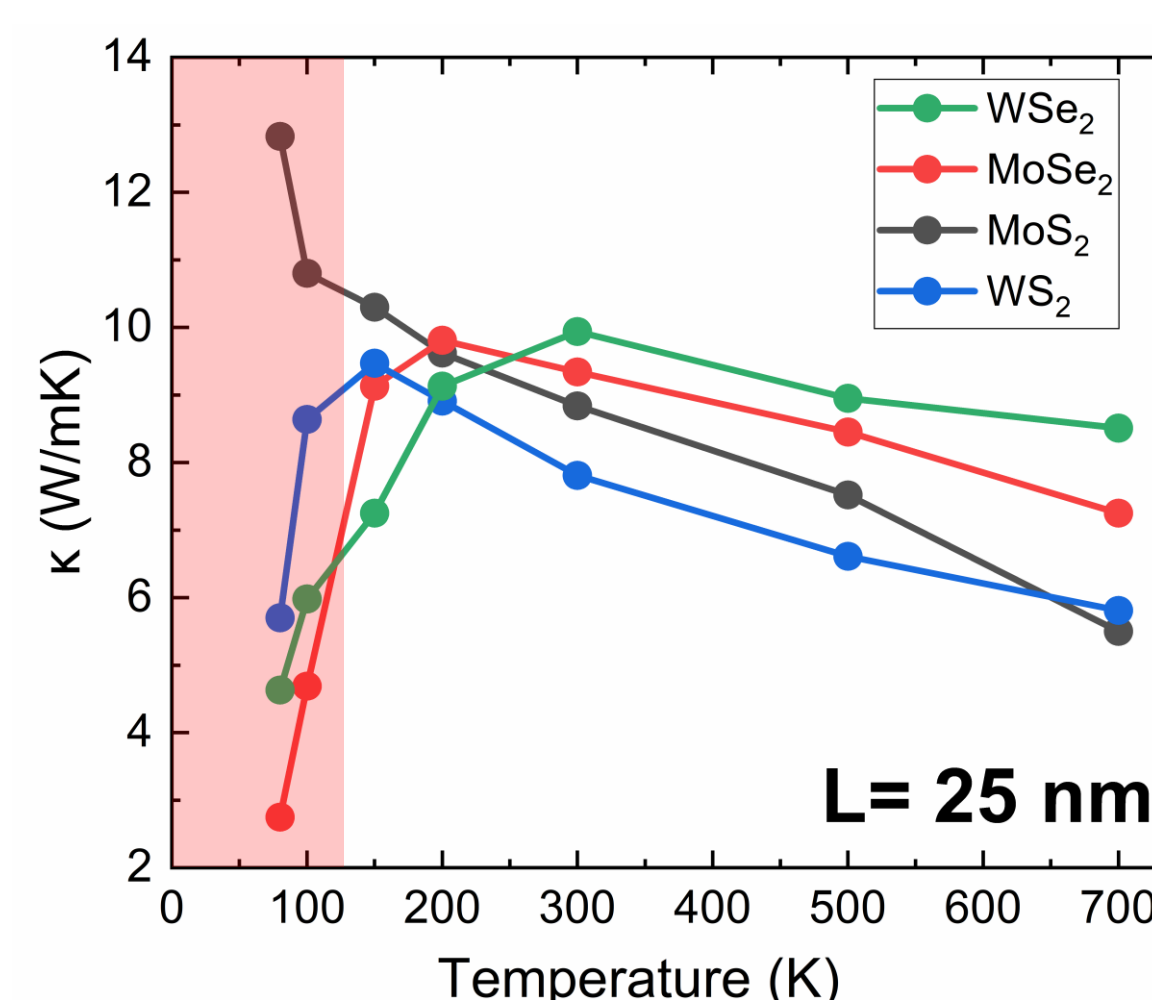
➤ **Higher ΔT** induces higher-order terms in n_{ks} , which is a **necessary condition** for non-reciprocity

➤ For systems symmetric along the gradient, even terms in ∇T vanish \rightarrow **asymmetry** is also a **necessary condition** for non-reciprocity

➤ Large $|\Delta T|$ induces a **mismatch in pDOS** that is **non-reciprocal** with inversion of the direction of $\Delta T \rightarrow$ reflected in the temperature dependence of $\kappa(T)$



Temperature Dependence of Thermal Conductivities



➤ At low $T \leq 150$ K, the heterostructures cannot reach proper steady state!

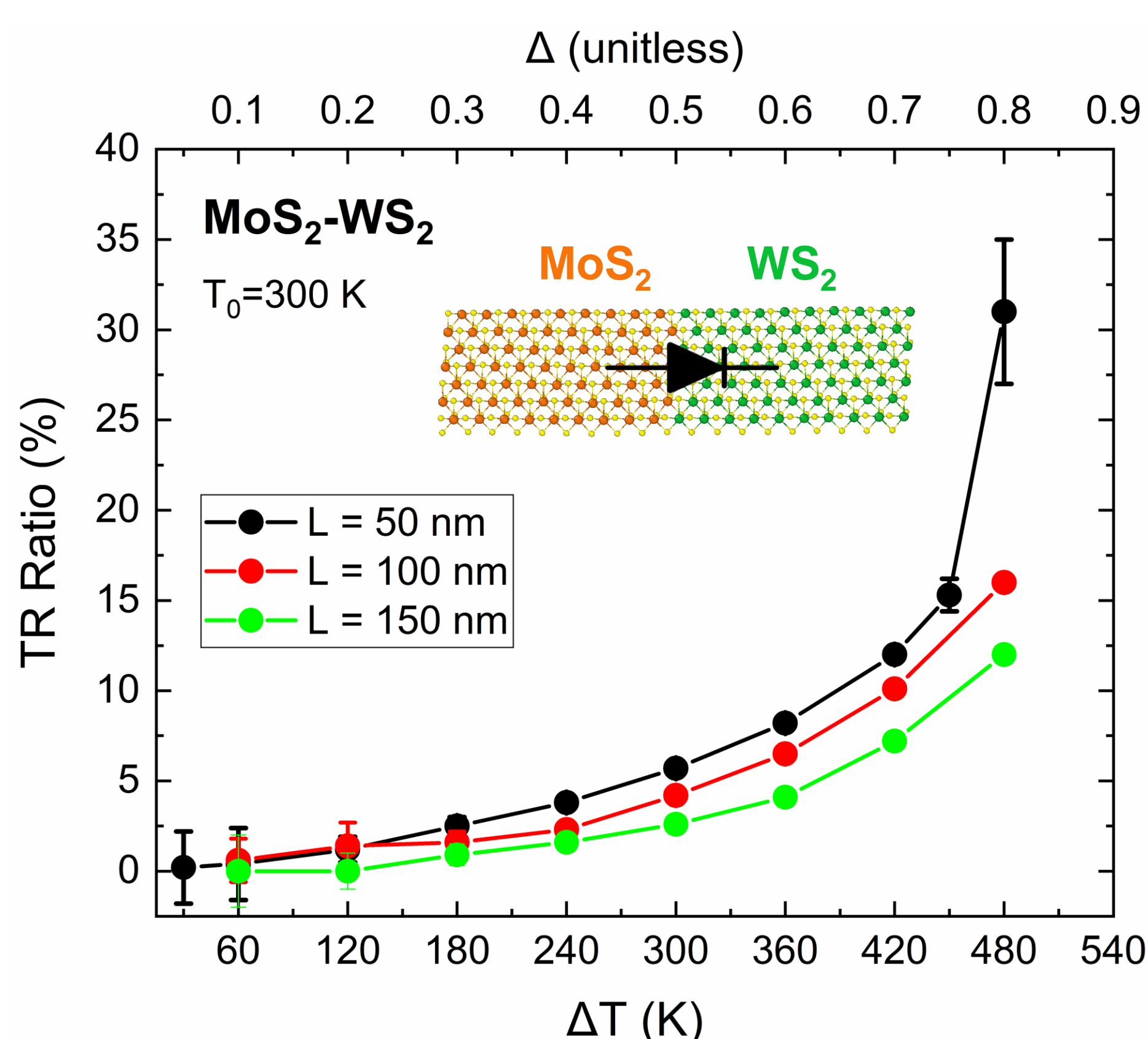
➤ At high $T \geq 700$ K the materials **decompose**

➤ Thermal conductivity κ of TMD's follows a **monotonous trend**: WS₂ \rightarrow MoS₂ \rightarrow MoSe₂ \rightarrow WSe₂

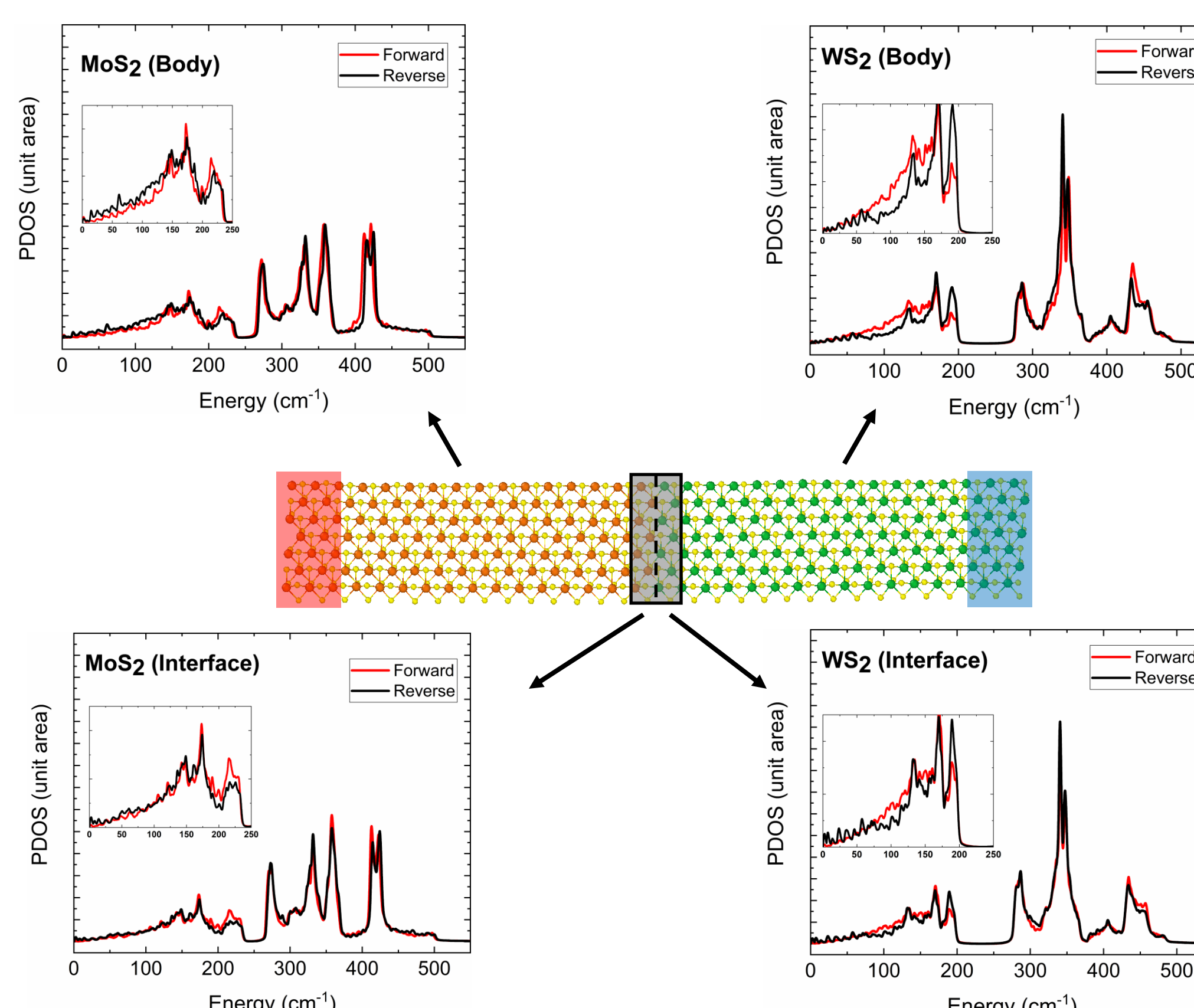
➤ Thermal conductivity **increases with length**

➤ Temperature dependence of $\kappa(T)$ **non-monotonous trend**; inflection point depending on material and length!

Rectification: Larger Temperature Bias ΔT enhances the Rectification Ratio η

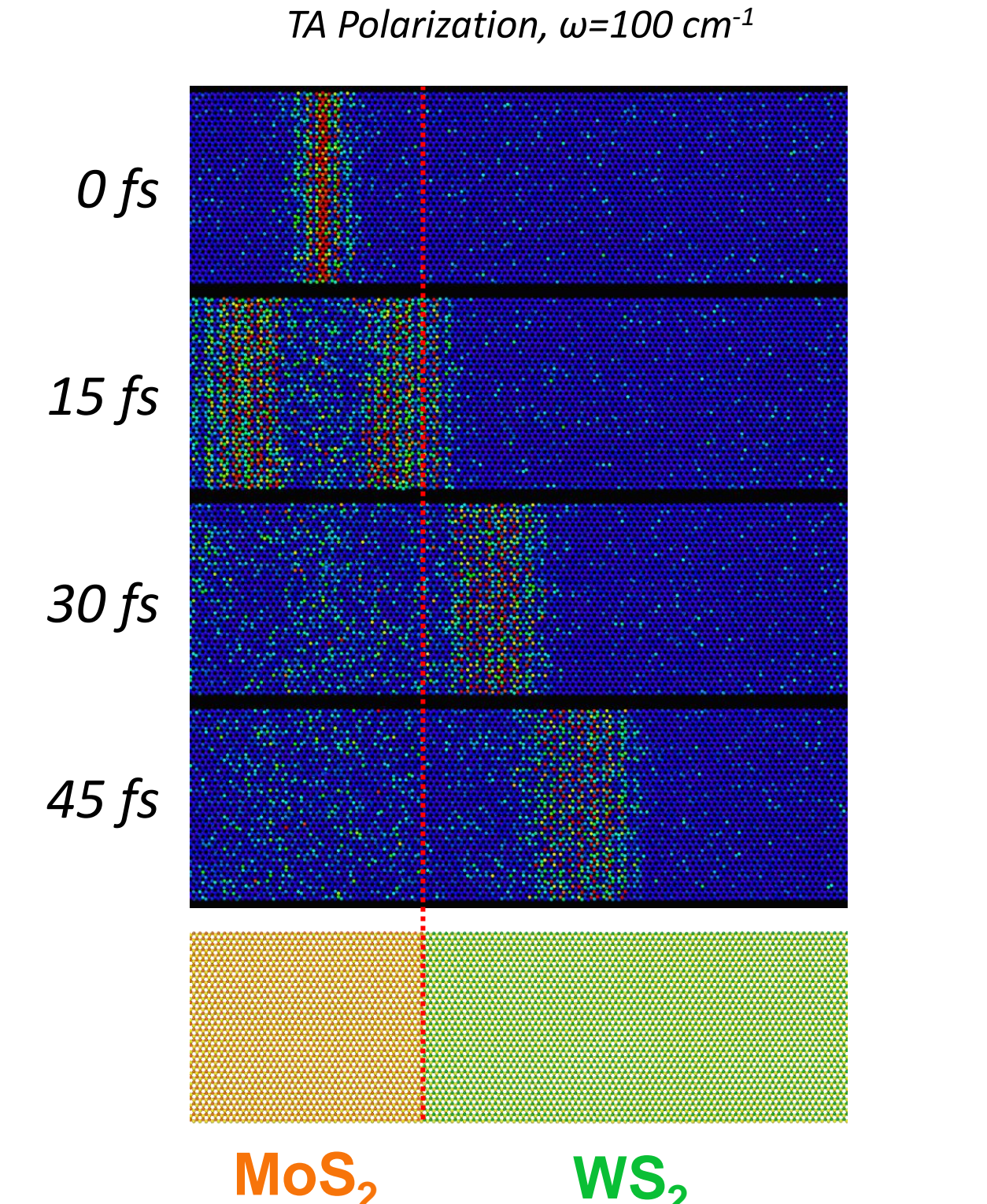


Rectification Ratio η increases with ΔT



Non-Equilibrium pDOS depends on ∇T (direction + magnitude)

Phonon Wavepacket Propagation



Acoustic phonons don't "see" the interface!

Conclusions

- **Large temperature biases ΔT** necessary for significant rectification ratios η
- Under **non-equilibrium** conditions the pDOS are **non-constant**: **acoustic phonons are affected the most**
- The **acoustic phonons** responsible for thermal transport are **poorly scattered by the interface**:

Perspectives

- Find correlations of pDOS overlaps with η for different T-biases ΔT (Phonon Mismatch model)
- Explore the effects of the average temperature T_0 of the heterostructure on η
- Apply to different combinations of TMD's (with potential lattice mismatch strain)
- 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)