



## GeTe/a-C Superlattices : Thermal Conductivity and Wave-Propagation

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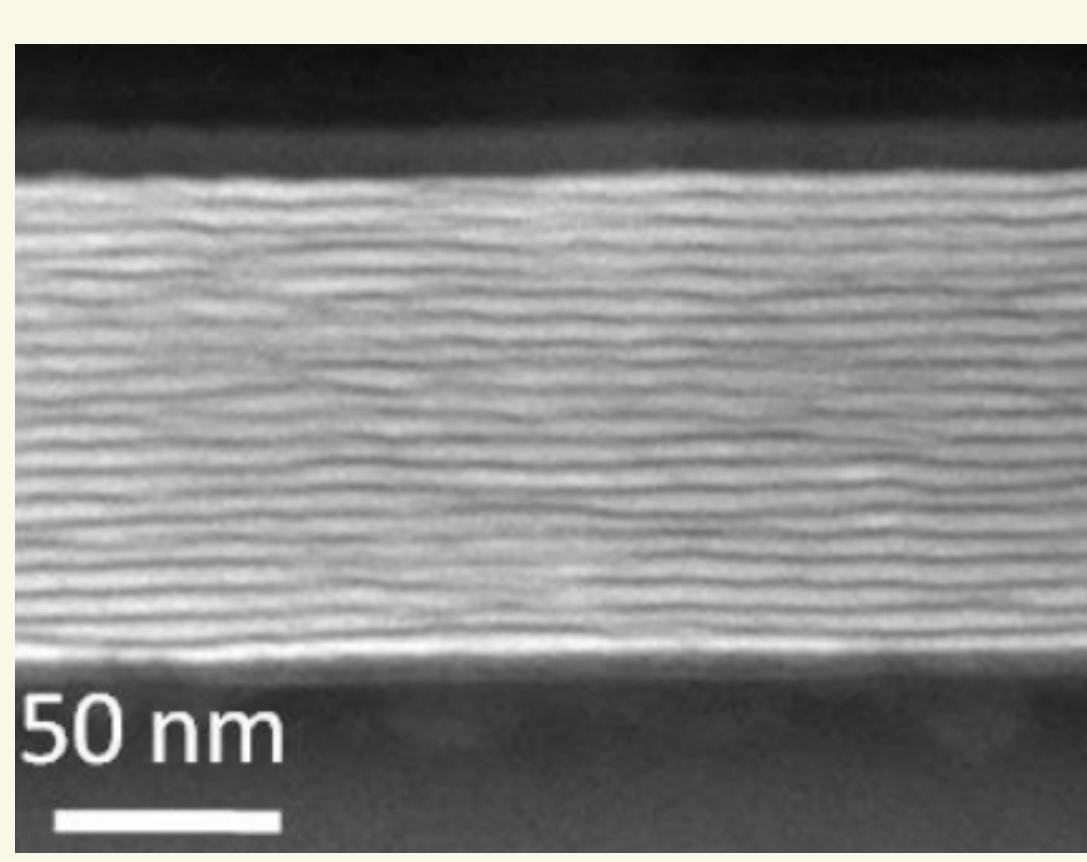
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## 1. c-GeTe/a-C Superlattice

GeTe has promising properties for both phase change memory and thermoelectric generation applications. One of them is its low thermal conductivity, the nanostructuration in superlattice can further decrease it. Here, we study the impact of the structure on thermal properties.



[Chahine, Thesis, 2020]

## 3. Modelisation: Molecular Dynamics

- Simplified approach with a 3 body potential used for Si
  - GeTe as a single atom
- Tuning of the impedance  $Z = \rho v$ 
  - $v$  via Intensity the interaction
  - $\rho$  via Atomic Masses

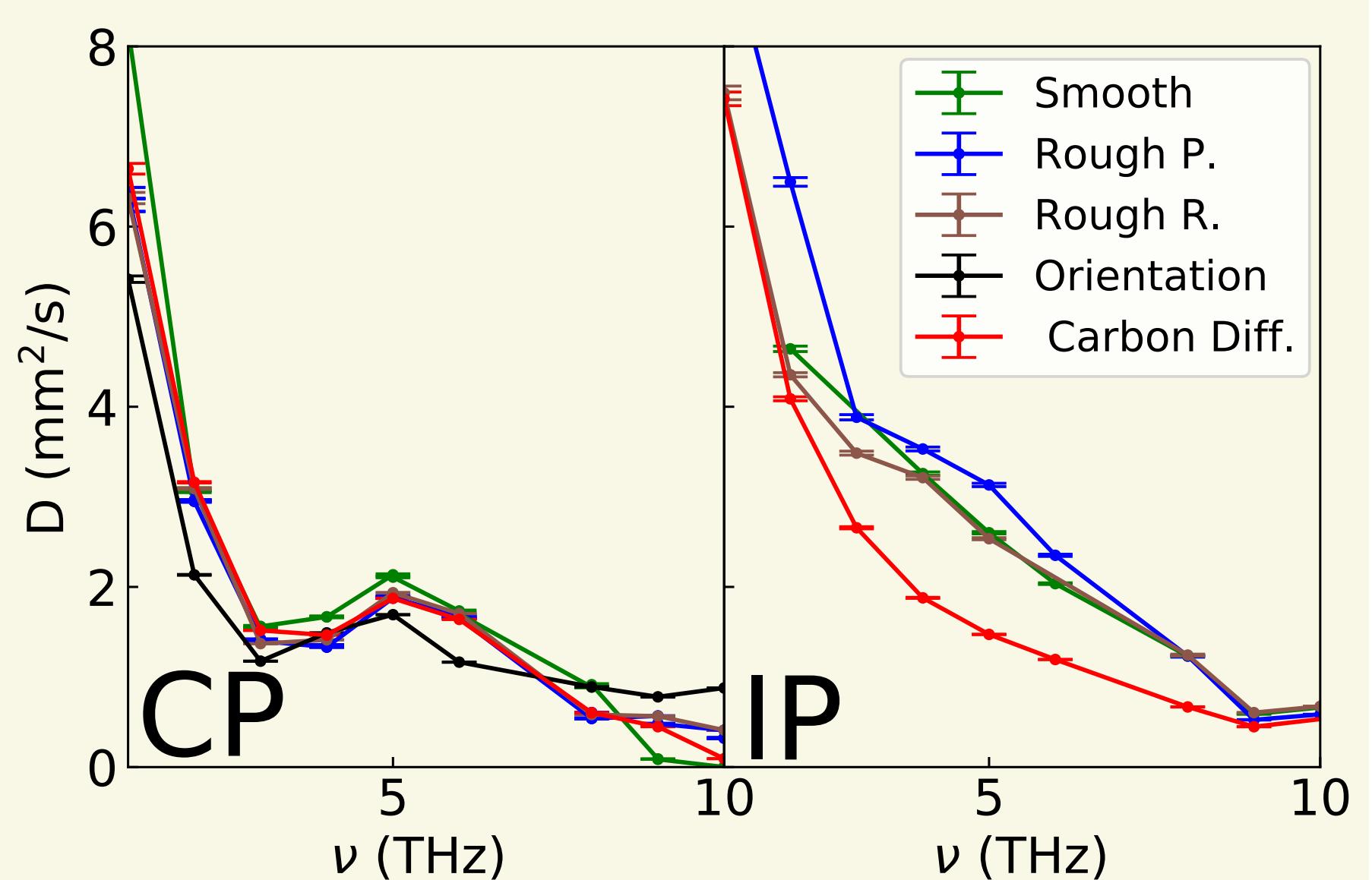
	SW	Ref.
$v_{\text{sound}}$ ( $\text{km s}^{-1}$ )	a-C	9 14.5
	GeTe	4 1.9
$\kappa$ ( $\text{W m}^{-1} \text{K}^{-1}$ )	a-C	.93 $\approx 1^1$
	GeTe	44 $\approx 3.3$

<sup>1</sup>[Bullen et al., JAP, 2000]

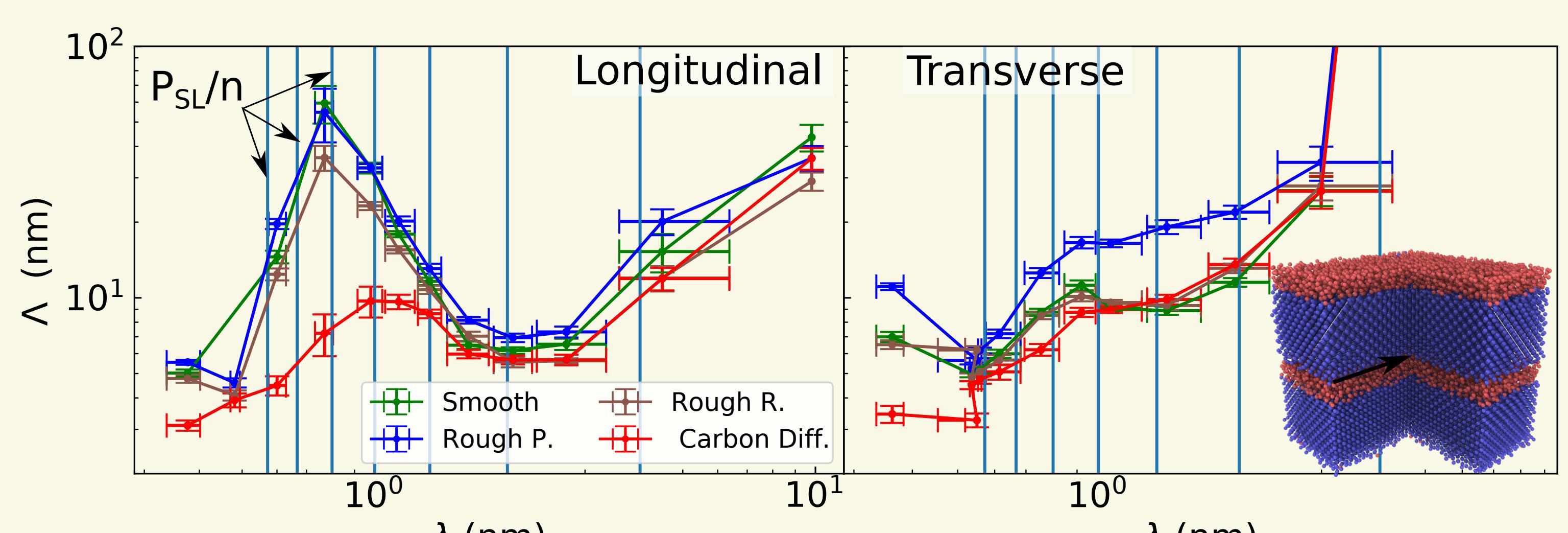
Reproduction of a high impedance mismatch crystalline amorphous superlattice.

## 6. Diffusivity

- Energy diffusivity ( $D$ ) after a non coherent excitation
- Orientation change and interdiffusion create obstacles
  - decrease of  $D_{CP}$  and  $D_{IP}$
- Roughness periodicity also increases  $D_{IP}$



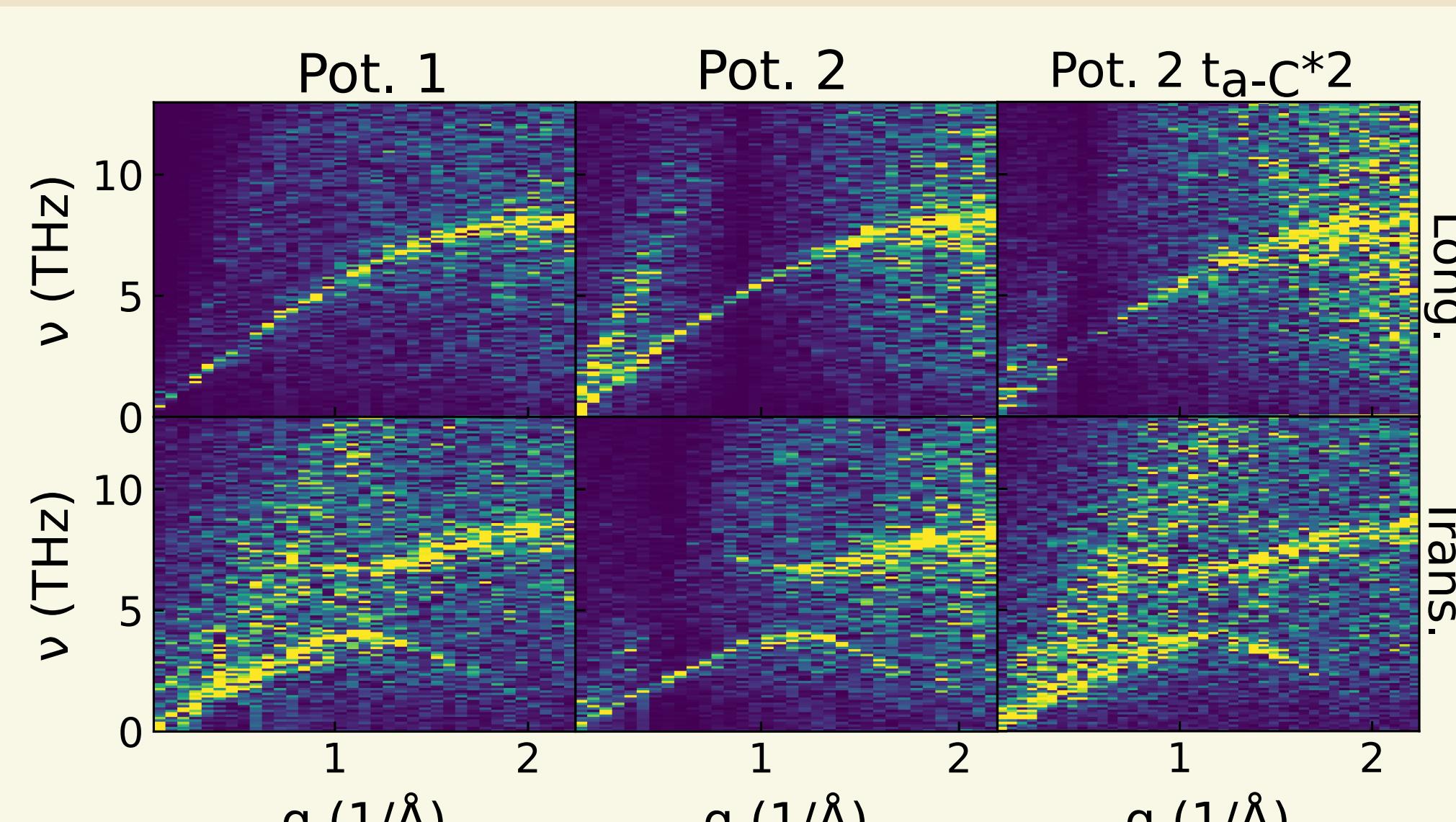
## 7. Transmission in the In-Plane Direction



- Interdiffusion of C decrease  $\Lambda_L$  at high frequency
- Periodicity increases  $\Lambda_T$  on a large spectrum

## A. q-Bandgap and Interaction Potential

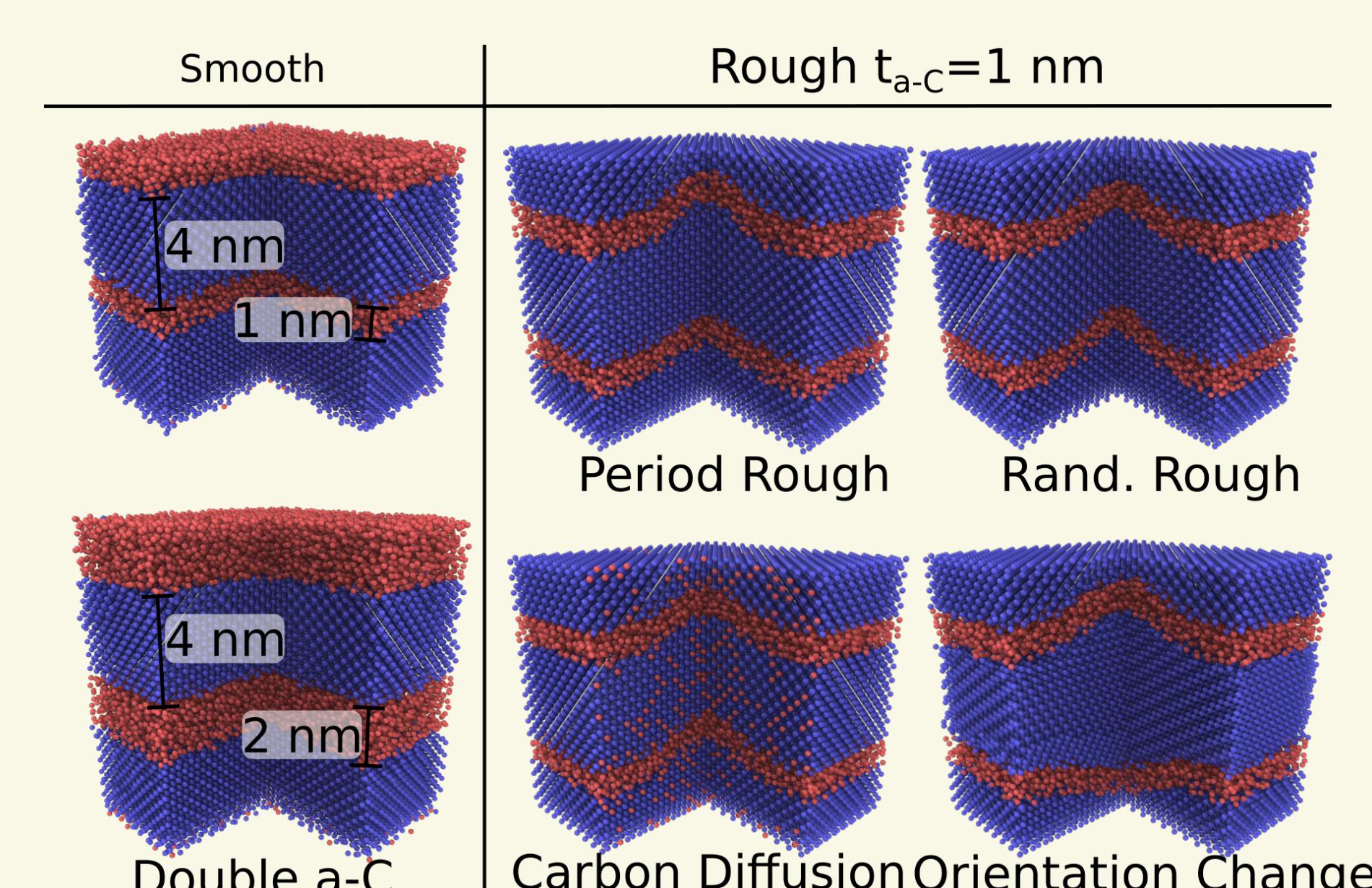
- Variation of GeTe-C interaction
  - Pot. 1 (this study): GeTe-C = averaged
  - Pot. 2: GeTe-C = GeTe-GeTe
- With Pot. 2 bandgap opening in the IP dir.



## 2. Studied Geometries

Study the effects:

- of a-C thickness on dispersion (1-2 nm)
- of a-C layer roughness (via shape)
- Periodicity of the roughness
- Diffusion of a-C in the GeTe



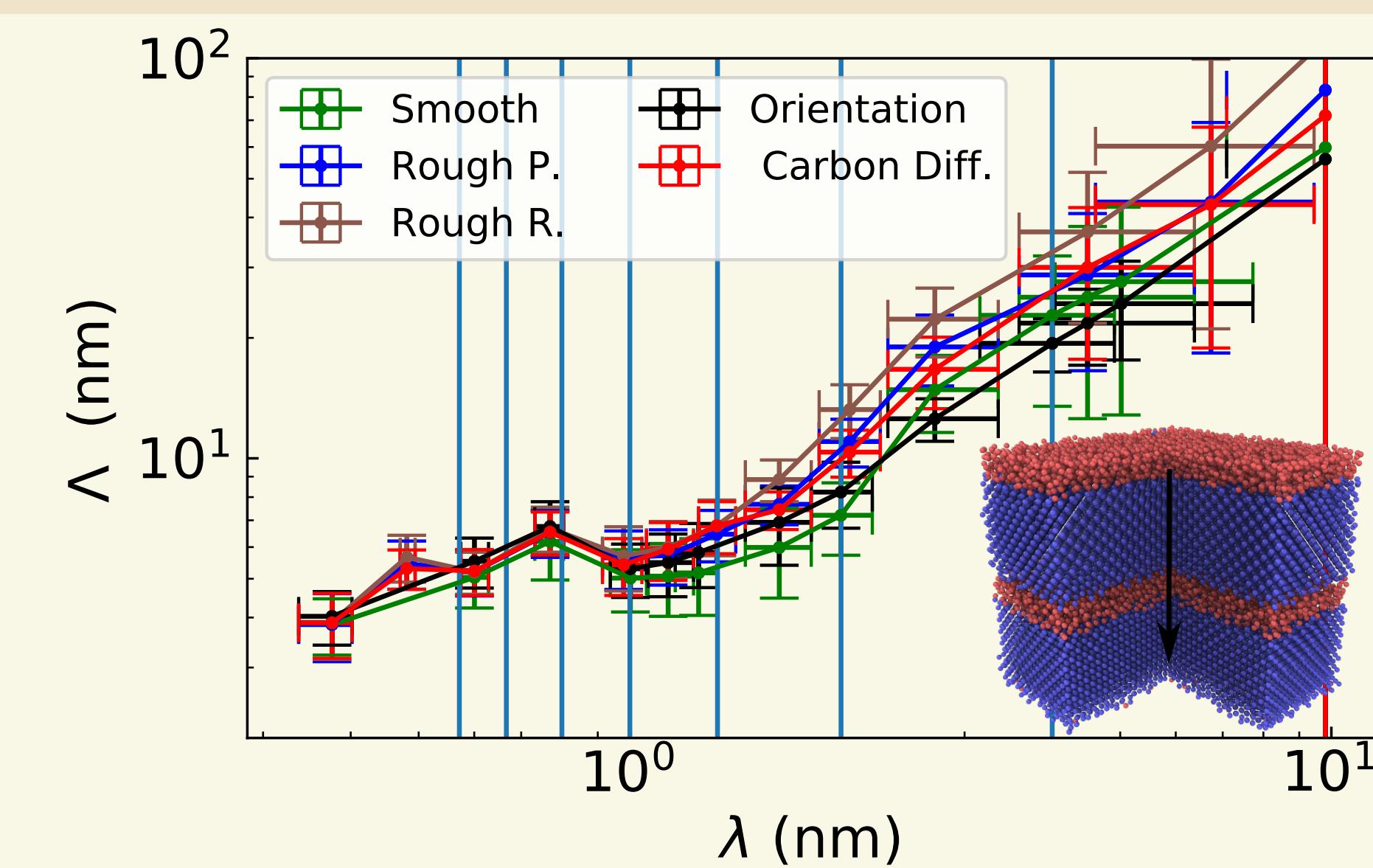
## 4. Thermal Conductivity (Equilibrium MD)

( $\text{W m}^{-1} \text{K}^{-1}$ )	Smooth	Double $t_{a-C}$	Period Rough	Rand. Rough	Orientation Change	Carbon Diffusion
$\kappa_{IP}$	<b>3.4±.6</b>	<b>2.0±.5</b>	4.2±.4	3.7±.5	4.3±.5	3.4±.3
$\kappa_{CP}$	<b>1.3±.2</b>	<b>0.5±.3</b>	1.7±.1	0.94±.1	1.2±.2	1.1±.2
$\kappa_{Total}$	2.6±.2	1.5±.4	3.4±.1	2.8±.1	3.3±.1	2.6±.2
$\frac{\kappa_{IP}}{\kappa_{CP}}$	2.6	3.7	2.5	4	3.6	3.2

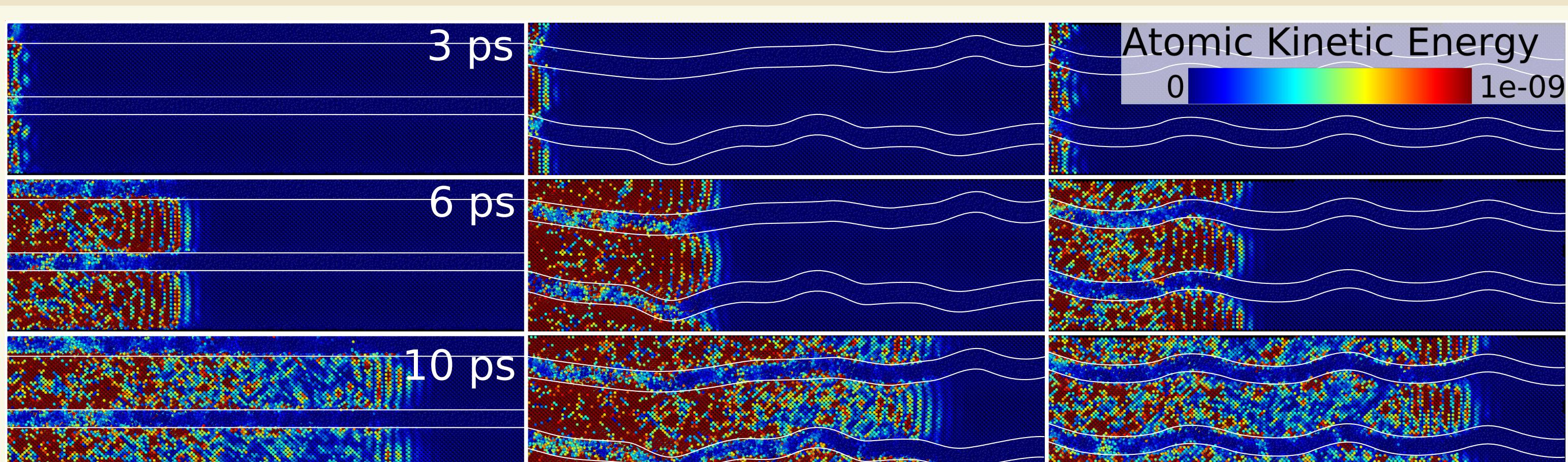
- Impact a-C thickness ( $t_{a-C}$ ) on  $\kappa_{IP}$  and  $\kappa_{CP}$
- At constant  $t_{a-C}$ 
  - Little impact of the geometry on  $\kappa_{IP}$
  - Impact of the roughness periodicity on  $\kappa_{CP}$

## 6. Transmission in the Cross-Plane direction

- MFP ( $\Lambda$ ) via the attenuation of wave-packet amplitude at low temperature
- Little difference between the configurations
  - Smoothness marginally decreases  $\Lambda$



## 8. Transverse IP Propagation at 2 THz



- Periodic roughness increases the coherent transmission
- Random roughness increases the diffusivity

## 9. Conclusion and Perspectives

- Low impact of geometry on  $\kappa_{IP}$
  - The roughness periodicity
    - Increases  $D$  and  $\Lambda_{IP}$
    - Increases  $\kappa_{CP}$
  - Orientation and interdiffusion affect  $D$  and  $\Lambda$  but not  $\kappa$ 
    - Importance of phonon scattering
- However, there is a dependence on the C-GeTe interactions: study with a more realistic potential on-going.

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