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

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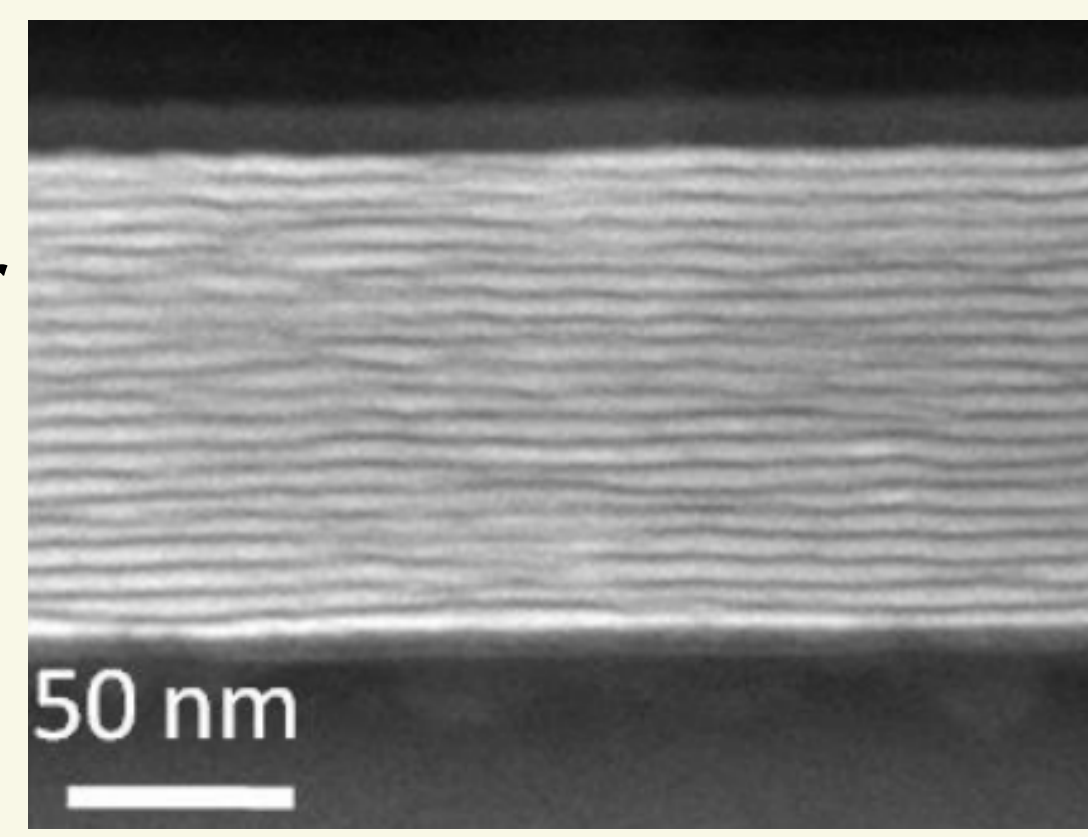
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1. c-GeTe/a-C Superlattice

GeTe has promising properties for both phase change memory and thermoelectric generation applications. One of them is its low thermal conductivity, the nanostructuring 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
 - ρ via Atomic Masses

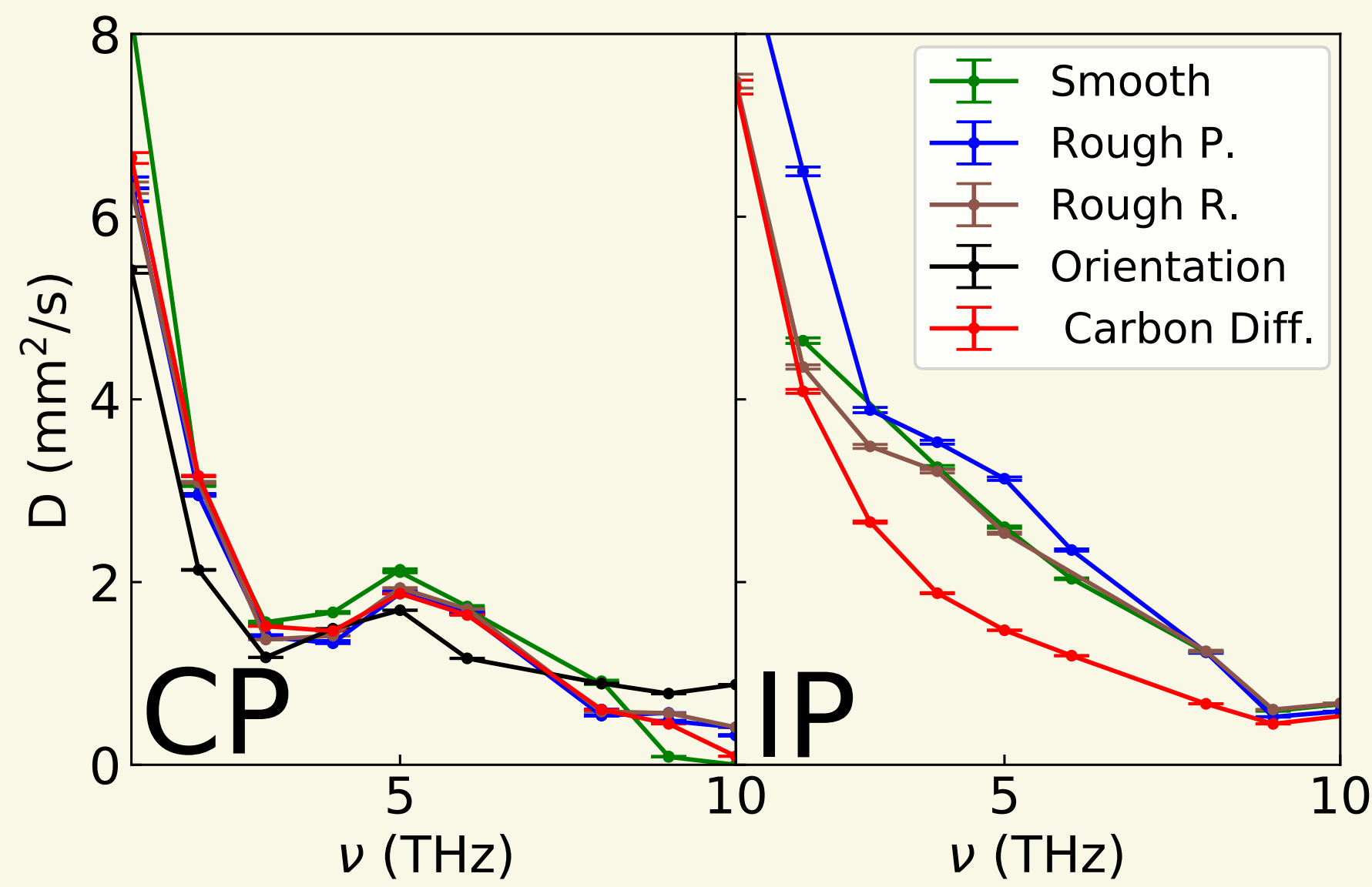
Reproduction of a high impedance mismatch crystalline amorphous superlattice.

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

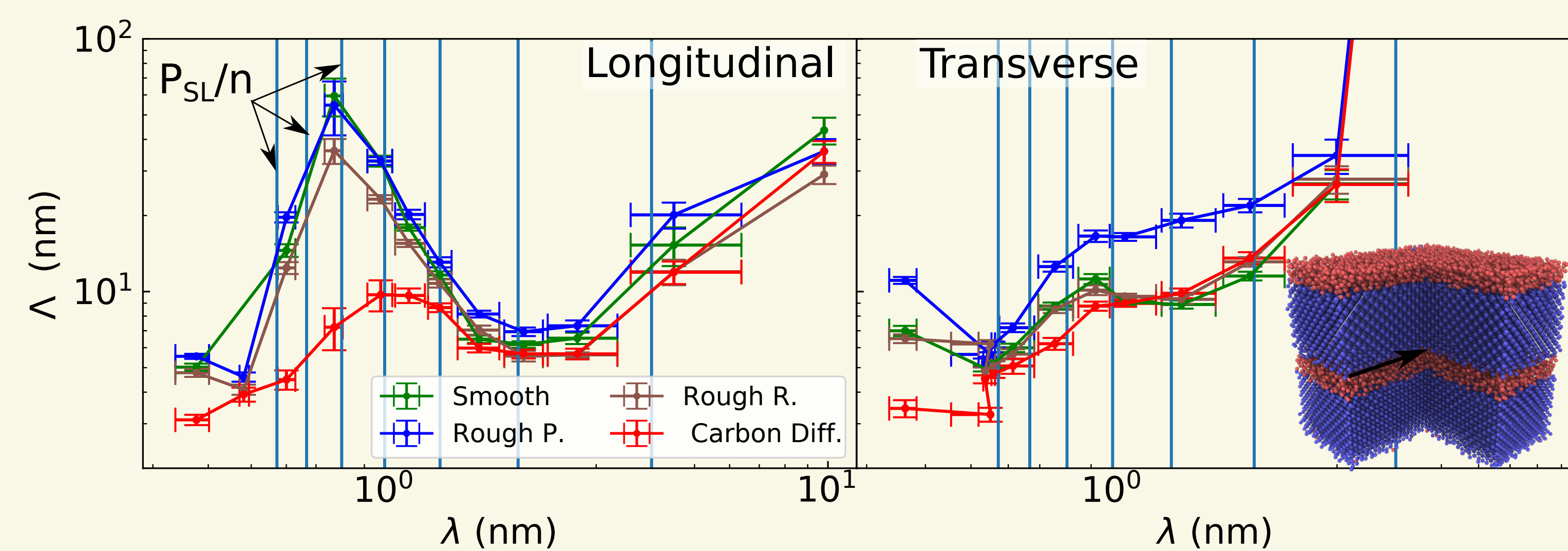
¹[Bullen et al., JAP, 2000]

6. Diffusivity

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



7. Transmission in the In-Plane Direction



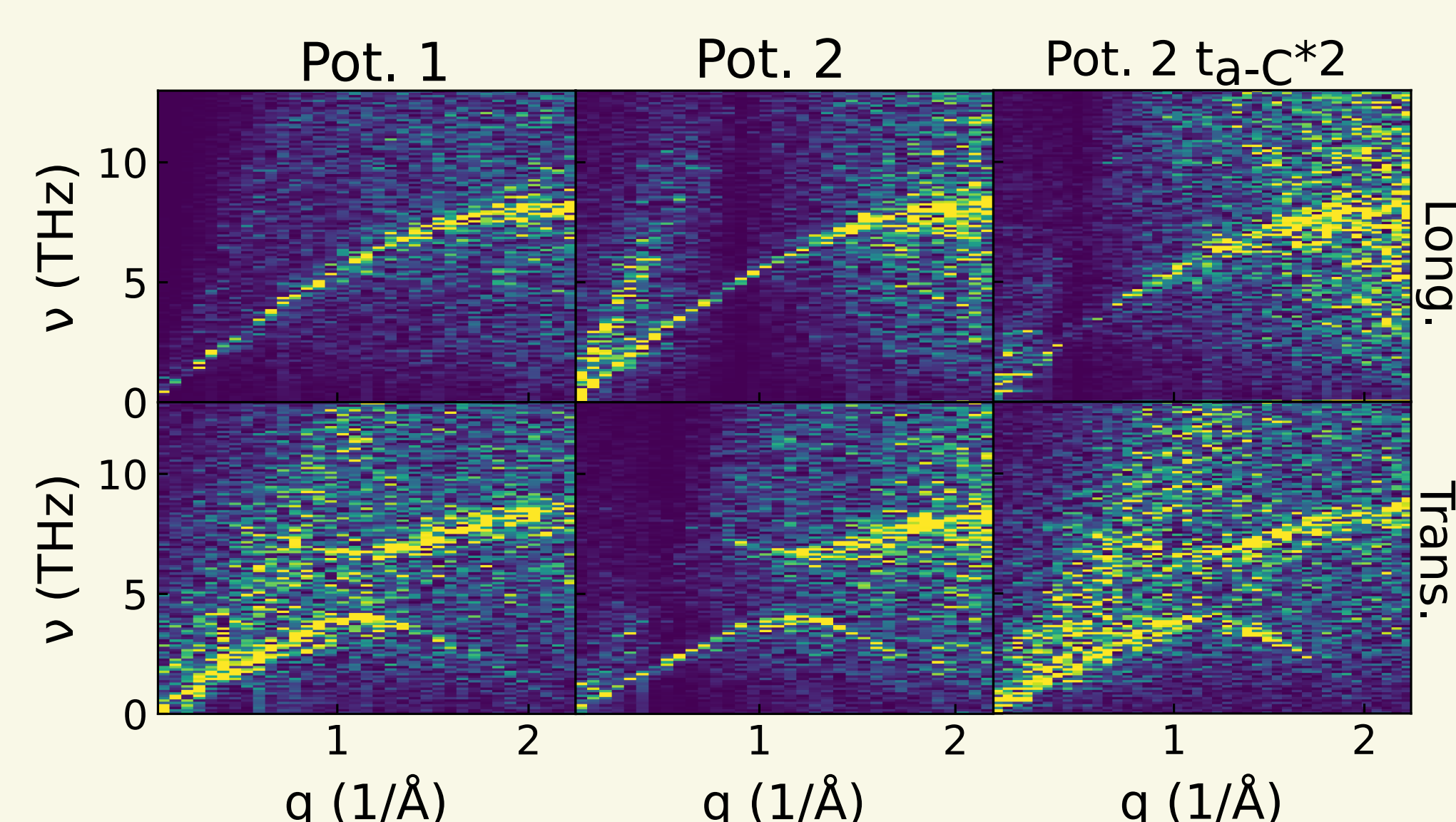
- Interdiffusion of C decrease Λ_L at high frequency
- Periodicity increases Λ_T on a large spectrum

A. q-Bandgap and Interaction Potential

Variation of GeTe-C interaction

- Pot. 1 (this study): GeTe-C = averaged
- Pot. 2: GeTe-C = GeTe-GeTe

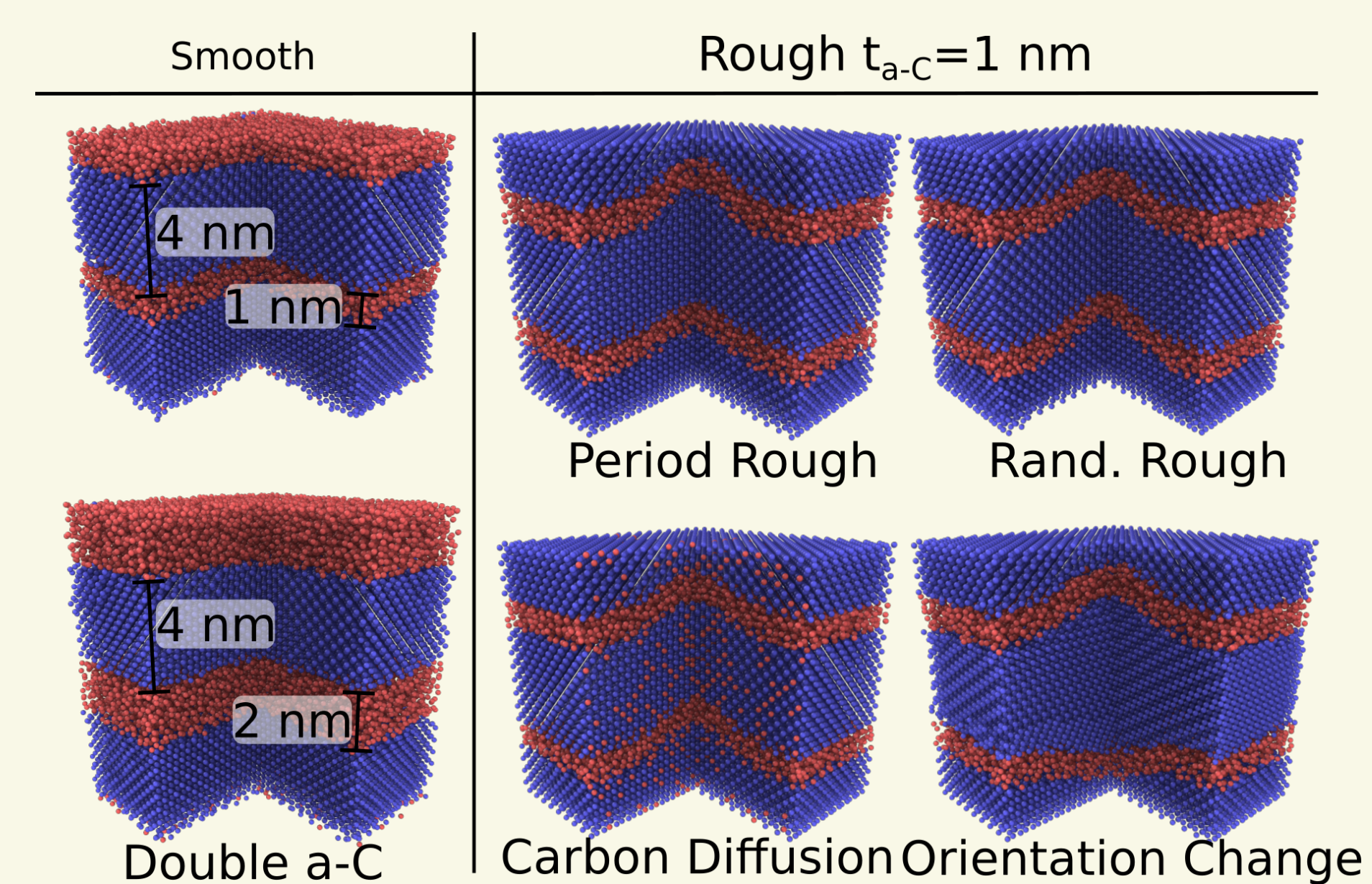
With Pot. 2 bandgap opening in the IP dir.



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



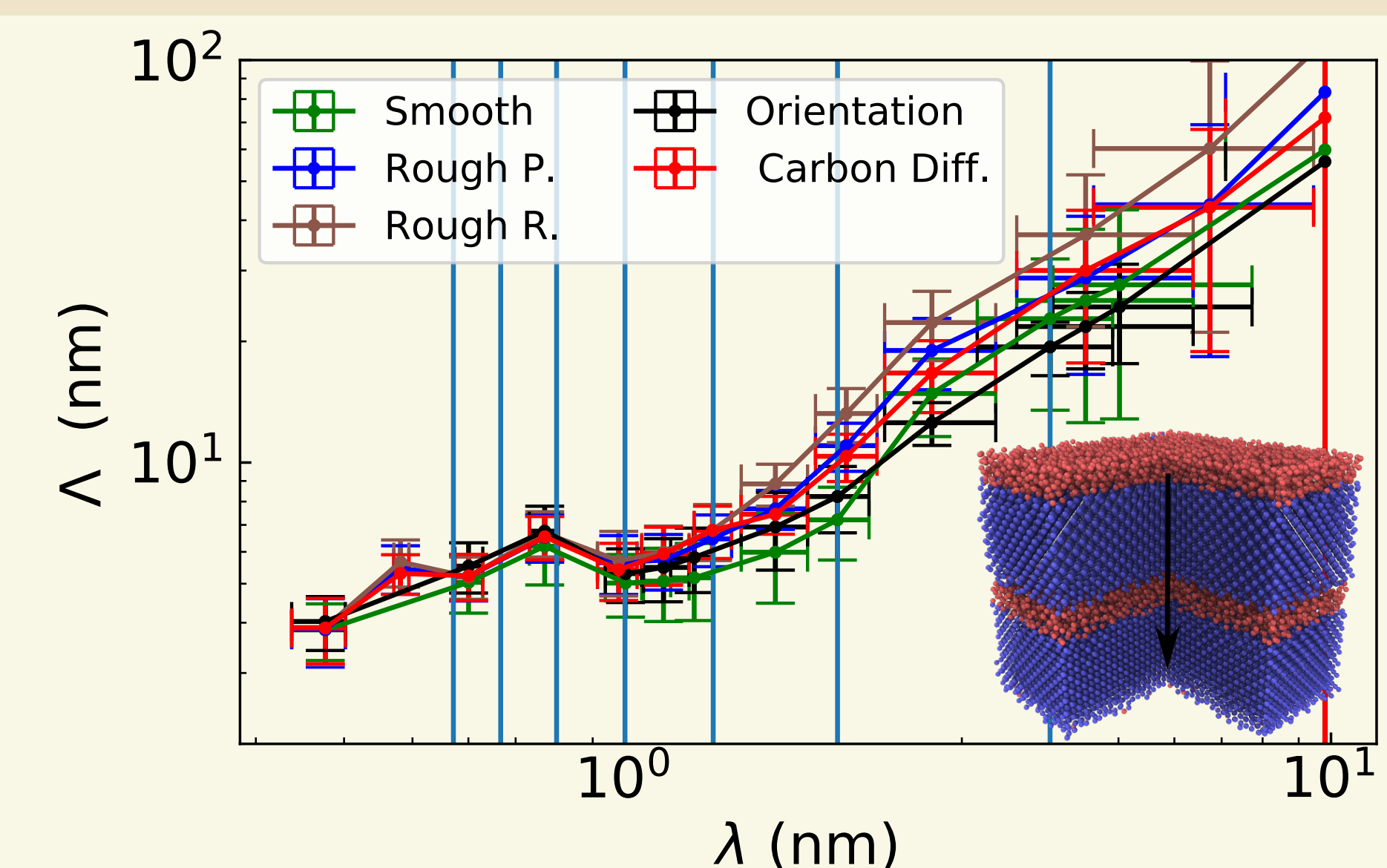
4. Thermal Conductivity (Equilibrium MD)

(W m ⁻¹ K ⁻¹)	Smooth	Double t _{a-C}	Period Rough	Rand. Rough	Orientation Change	Carbon Diffusion
κ_{IP}	3.4±.6	2.0±.5	4.2±.4	3.7±.5	4.3±.5	3.4±.3
κ_{CP}	1.3±.2	0.5±.3	1.7±.1	0.94±.1	1.2±.2	1.1±.2
κ_{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

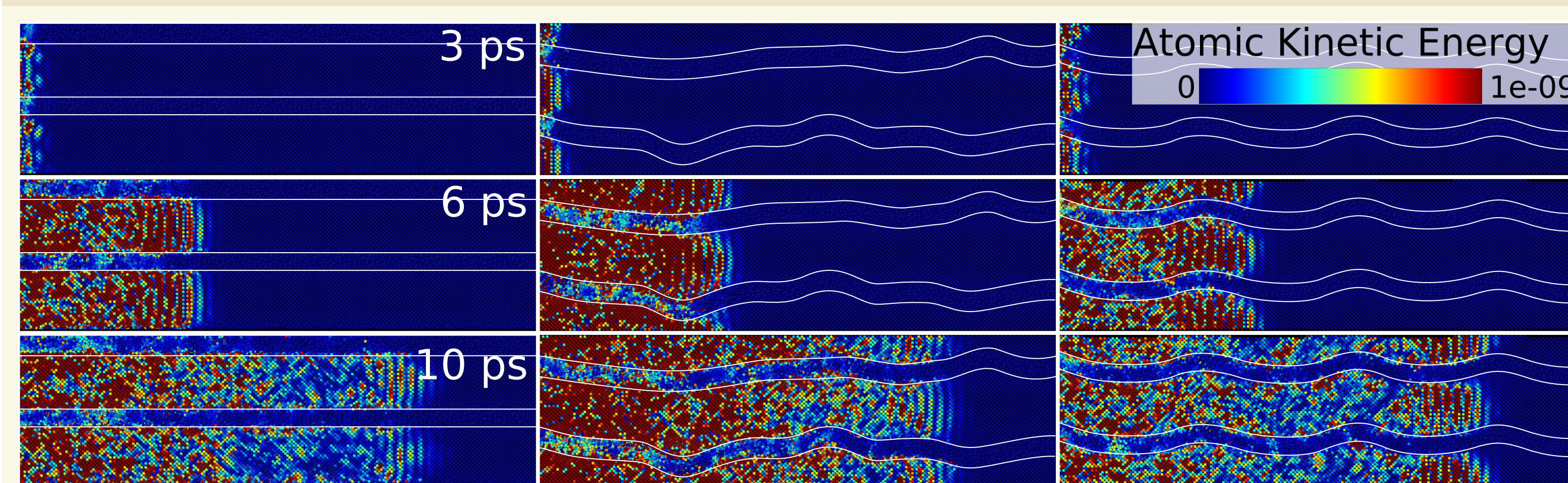
- Impact a-C thickness (t_{a-C}) on κ_{IP} and κ_{CP}
- At constant t_{a-C}
 - Little impact of the geometry on κ_{IP}
 - Impact of the roughness periodicity on κ_{CP}

6. Transmission in the Cross-Plane direction

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



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 κ_{IP}
 - The roughness periodicity
 - Increases D and Λ_{IP}
 - Increases κ_{CP}
 - Orientation and interdiffusion affect D and Λ but not κ
 - 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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