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Wave-Packet Propagation in Silicon Nano-Composite

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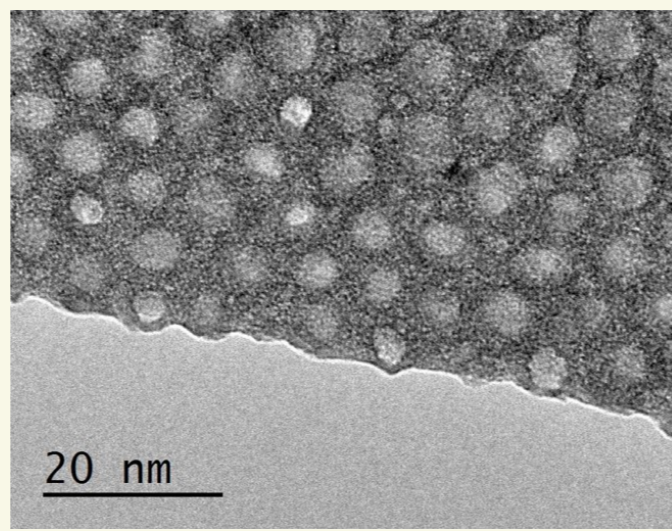
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Desmarchelier Paul^{1,2}, Giordano Valentina⁴, Beltukov Yaroslav³, Termendzidis Konstantinos², Tanguy Anne¹

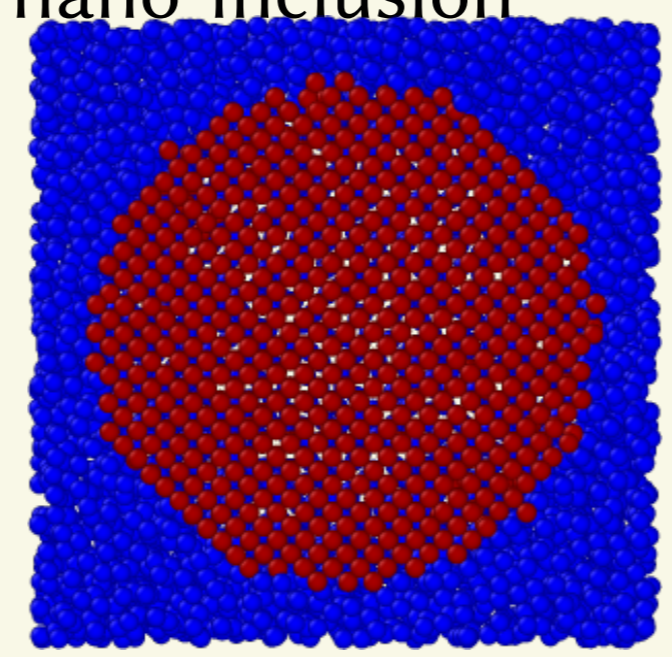
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1 Introduction and Configurations

Thermal management becomes more and more important in decreasing the sizes of devices and increasing their density. The evolution of fabrication allows to avoid hot spots using isolating and heat dissipative materials.



Crystalline nano-inclusion⁶



Unit Cell⁵

► Effect of crystalline inclusion rigidity and comparison with bulk amorphous silicon

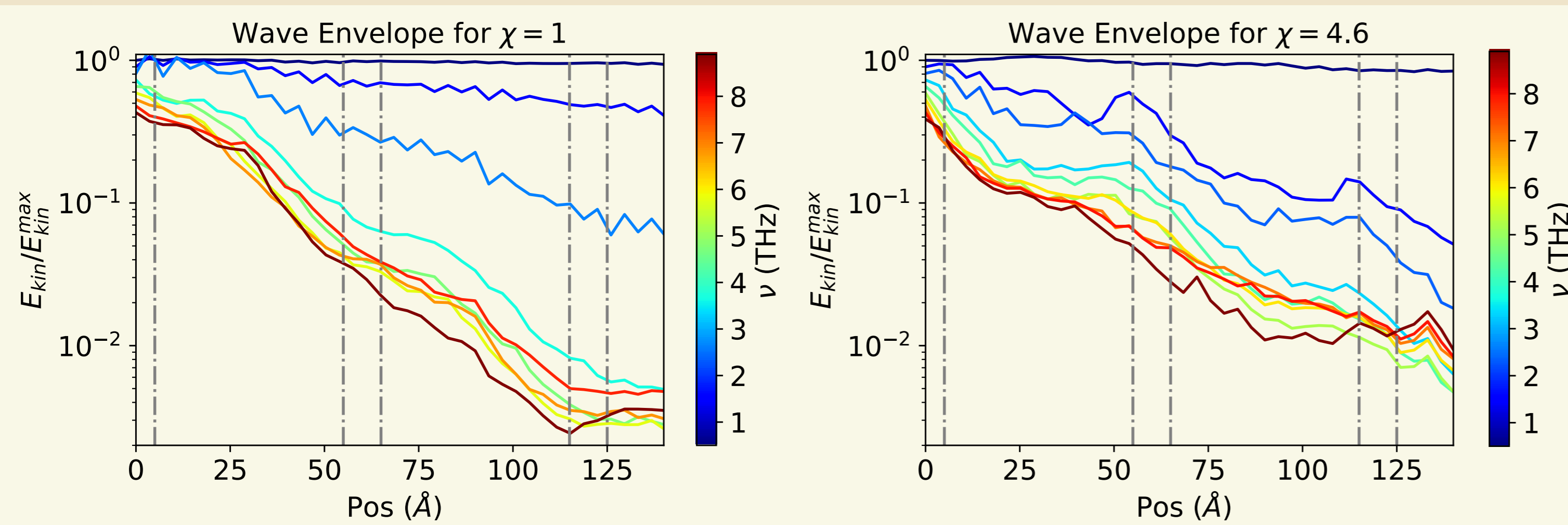
- On propagation/diffusion of excitation

► Varying rigidity

- Variation of the 3 body interaction

- $\chi = \frac{E_{Incl}}{E_{Mat}} = 1$ or 4.6

4 Propagation



Maximum value of E_k along the propagation direction: nano-composite

► Nano-composite

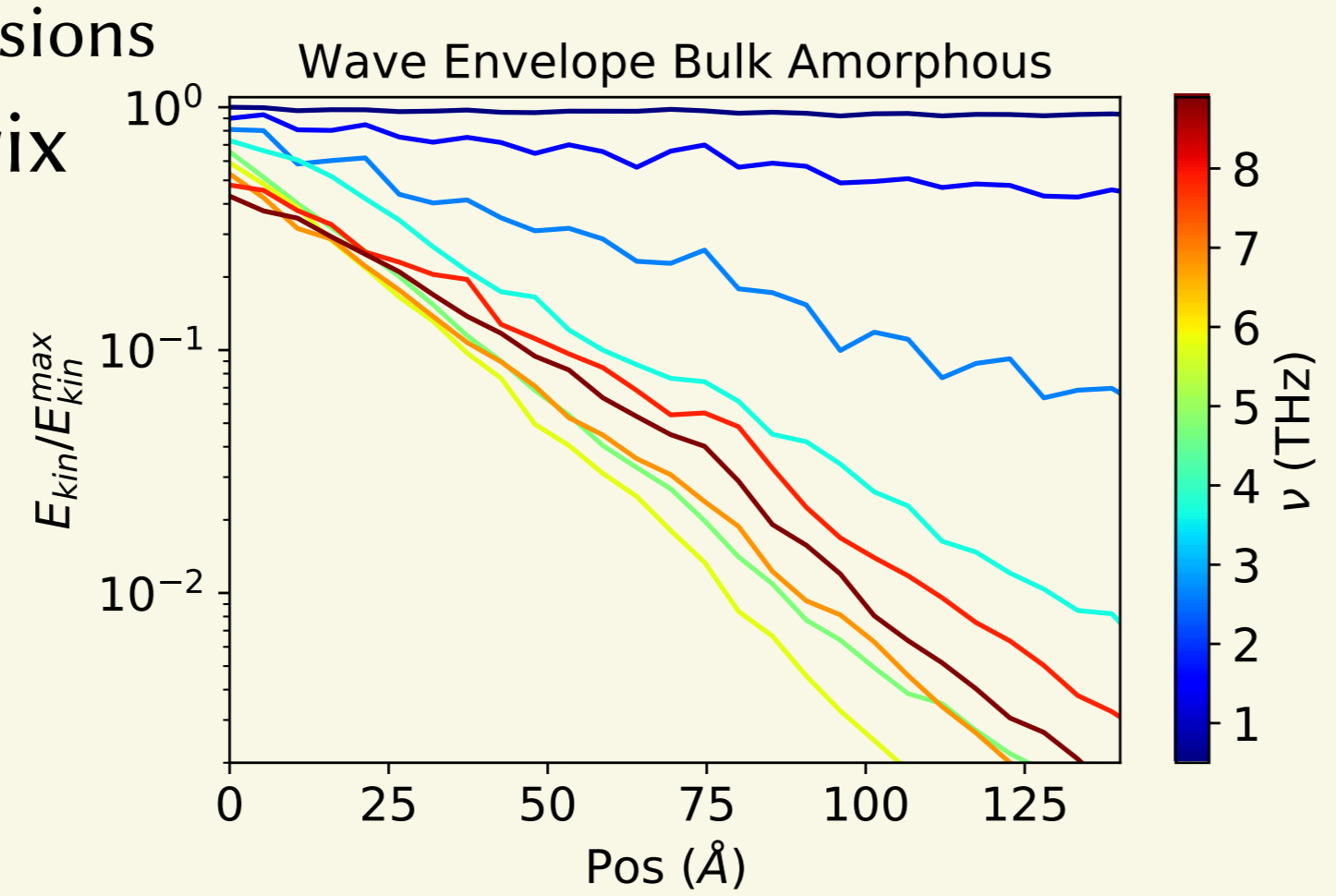
- Increasing acoustic mismatch intensifies attenuation

- Most important at low frequencies
- Local maximum of E_k between inclusions

- Stronger attenuation in the matrix
- Ballistic at low frequencies/diffusive at higher frequencies

► Amorphous

- Stronger propagation at low frequencies
- Higher attenuation at higher frequencies



Bulk amorphous

6 Consequences on the thermal conductivity

► For phonons below the Ioffe-Regel criterium the thermal conductivity is defined by

$$\kappa_{prop} = \int_0^{\omega_{IR}} C(\omega, T) v(\omega) l(\omega) g(\omega) d\omega$$

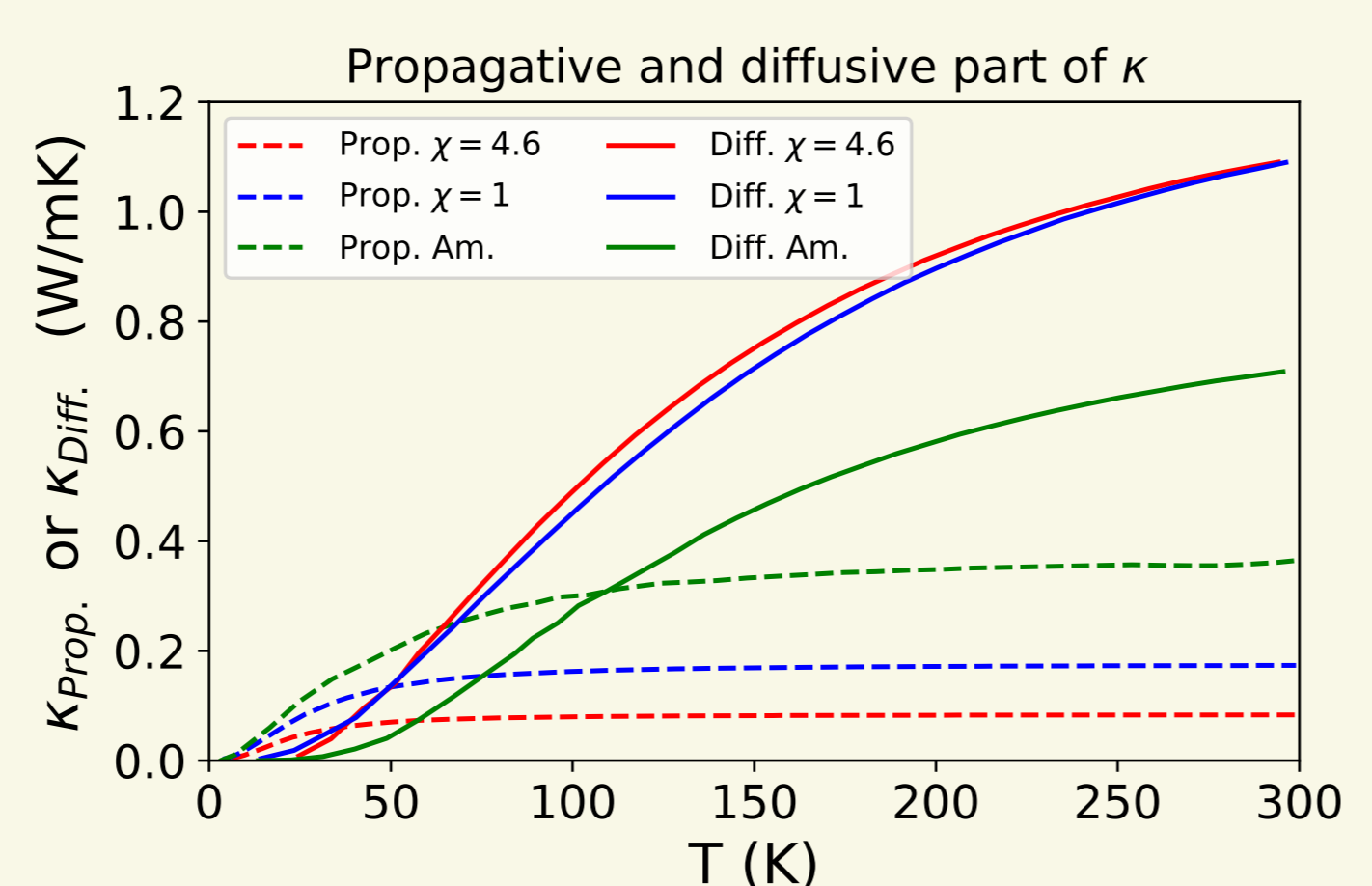
► For phonons above the Ioffe-Regel we have

$$\kappa_{diff} = \int_{\omega_{IR}}^{\infty} D(\omega) C(\omega, T) g(\omega) d\omega$$

► The higher the mismatch, the stronger the reduction of κ

► Inclusion effect mostly sensible on κ_{prop} ⁷

► Small effect on the conductivity at 300K



At 300K	$\chi = 1$	$\chi = 4.6$	Am.
κ_{tot} W/mK	1.43	1.23	1.48

2 Simulation Methods

► MD simulation

- SW⁴ interaction potential for Si
- LAMMPS³

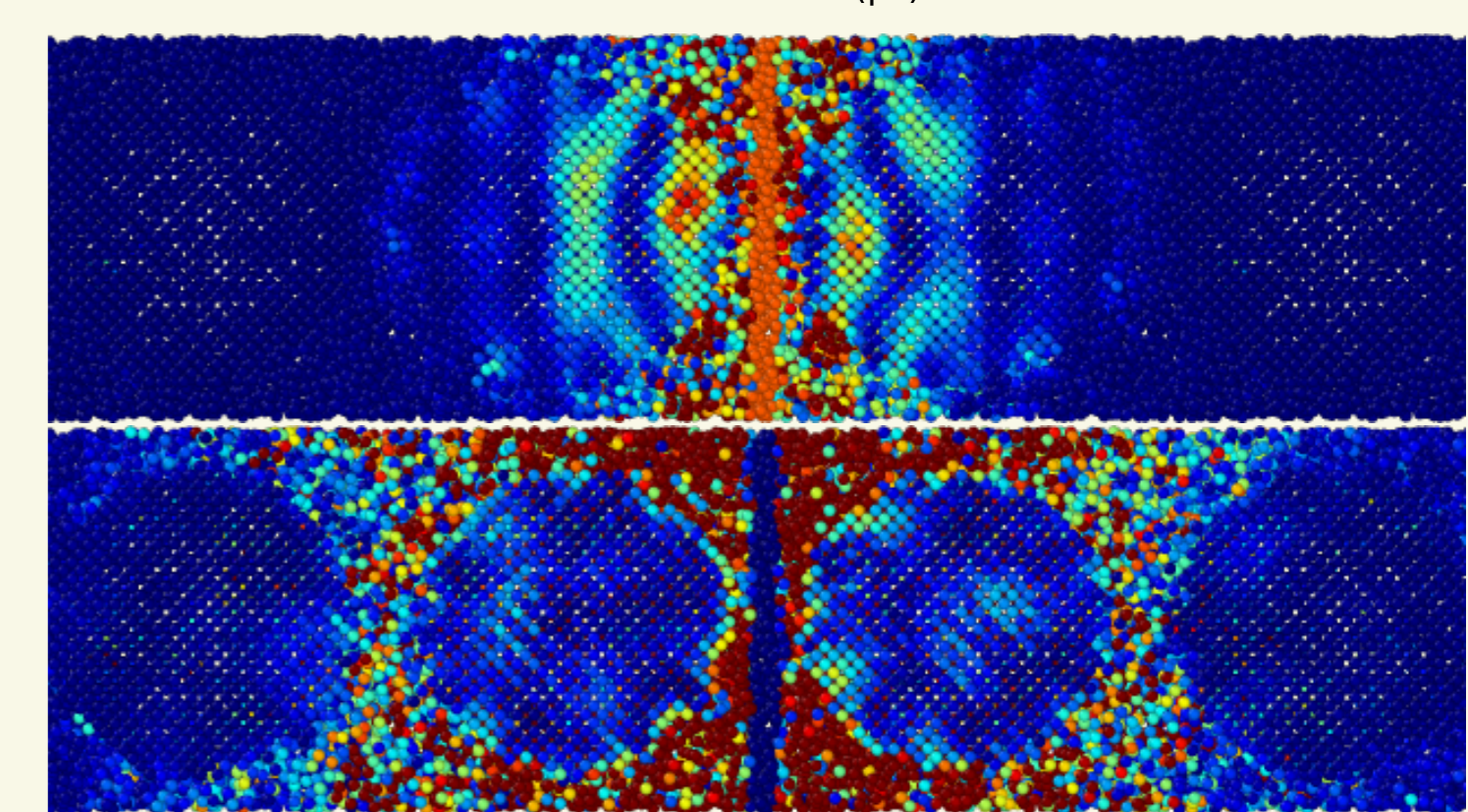
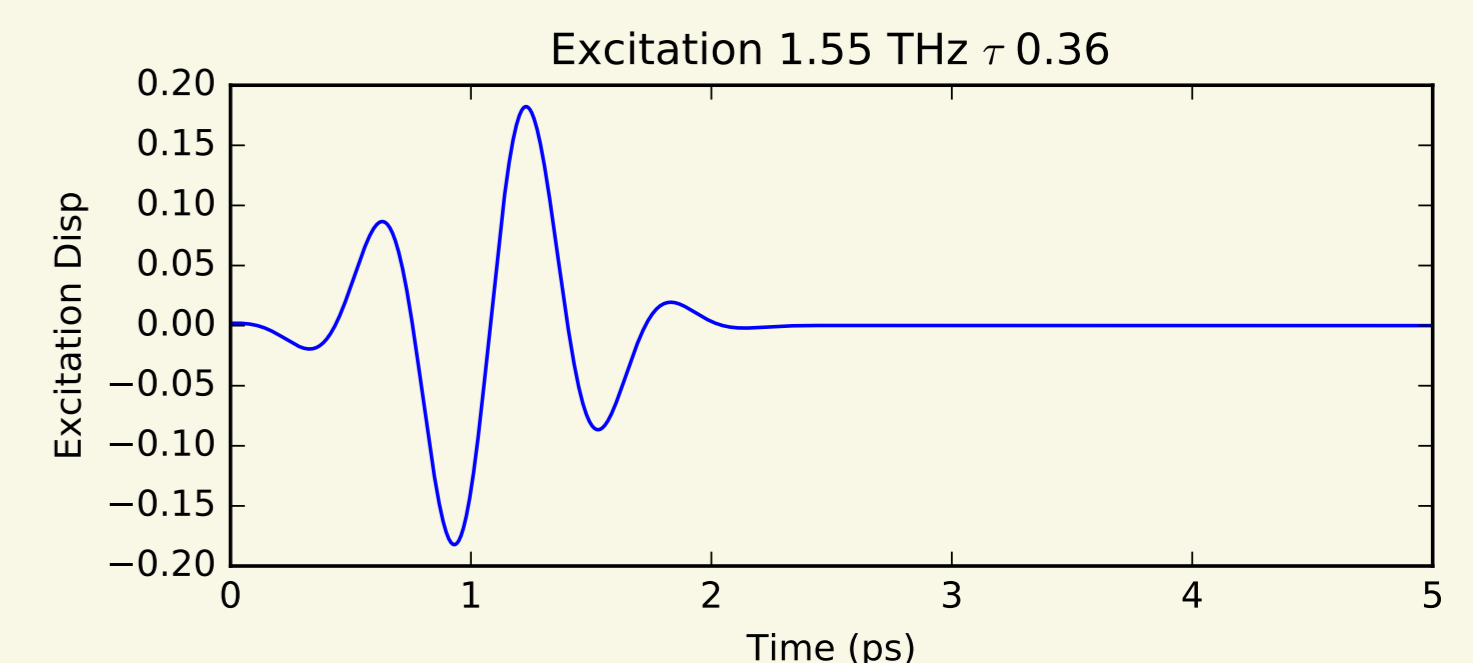
► Wave-Packet excitation²

- Displacement imposed on central atoms between inclusions

$$u_i = \frac{A}{\omega} \sin(\omega(t - 3\tau)) e^{-\frac{(t-3\tau)^2}{2\tau^2}}$$

► Polarization

- Longitudinal
 - Propagation analysis
- Random
 - Diffusivity computation



Evolution of a wave-packet with $\omega = 3.65$ THz and $\chi = 4.6$

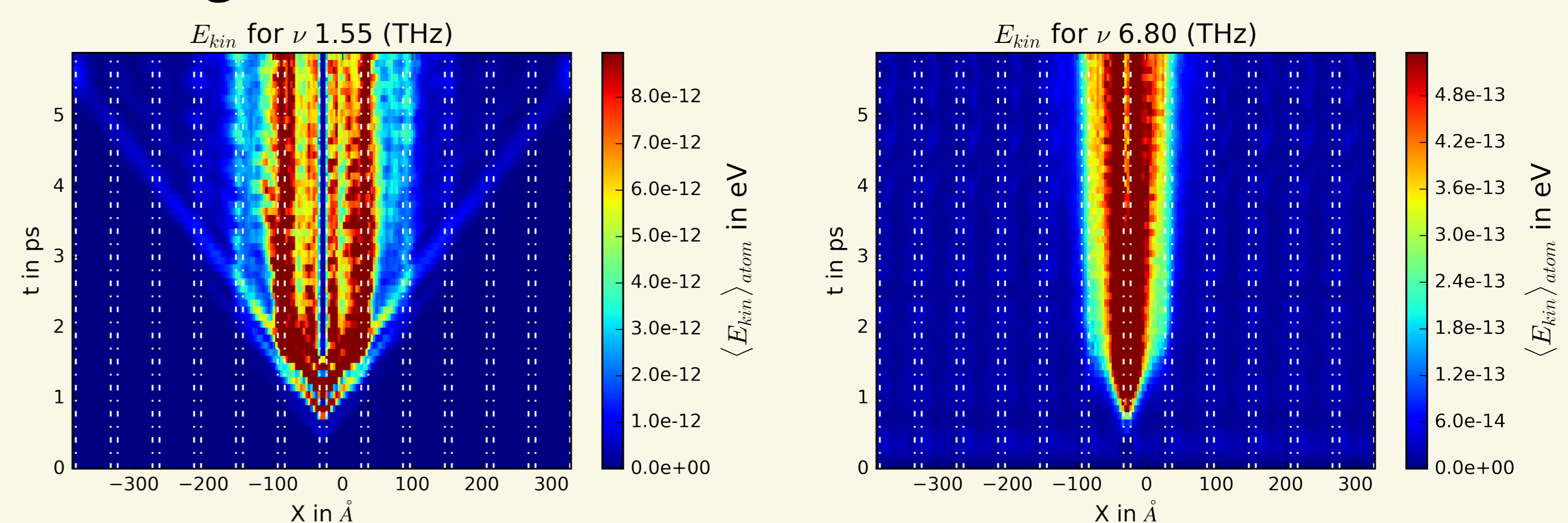
3 Kinetic Energy Distribution

► Kinetic energy maps as a function of time and position

- For frequencies between 0.5 and 11 THz
 - lower limit due to resolution
 - higher limit due to energy propagation limitation

► Propagation/Diffusion

► Pinning between inclusions



Time evolution of kinetic energy distribution for different frequencies

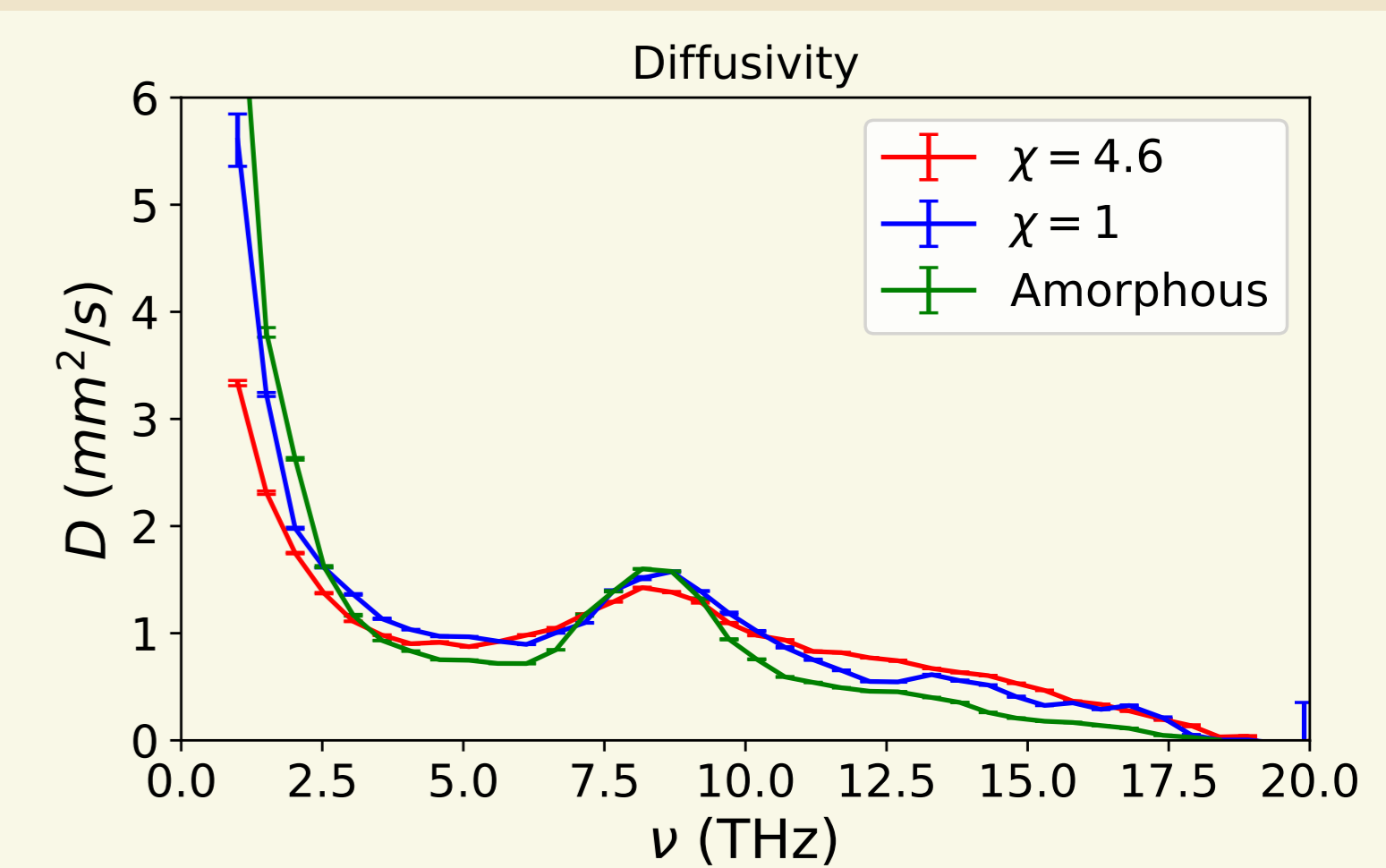
5 Diffusivity

► Randomly polarized excitations allows the computation of the diffusivity¹

- From the MSD of the energy front $R^2(t) = \frac{1}{E_{tot}} \sum_{i=1}^N x_i^2 E_i(t)$
- Diffusivity defined by the slope $R^2(t) = 2D(\omega)t$

► Small discrepancies between $\chi=1,4.6$ or bulk amorphous

► Highly dependent on the glass structure



7 Conclusion

Through wave packets excitation simulations we have separately computed the propagative and diffusive parts of heat conduction. Though propagation is lowered by the rigid inclusions, the diffusion tends to be increased. This work can be continued with the study of different nano-composites.

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