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## Study of anomalous effects in thermal conductivity in c-GaN/a-SiO<sub>2</sub> nano-composites

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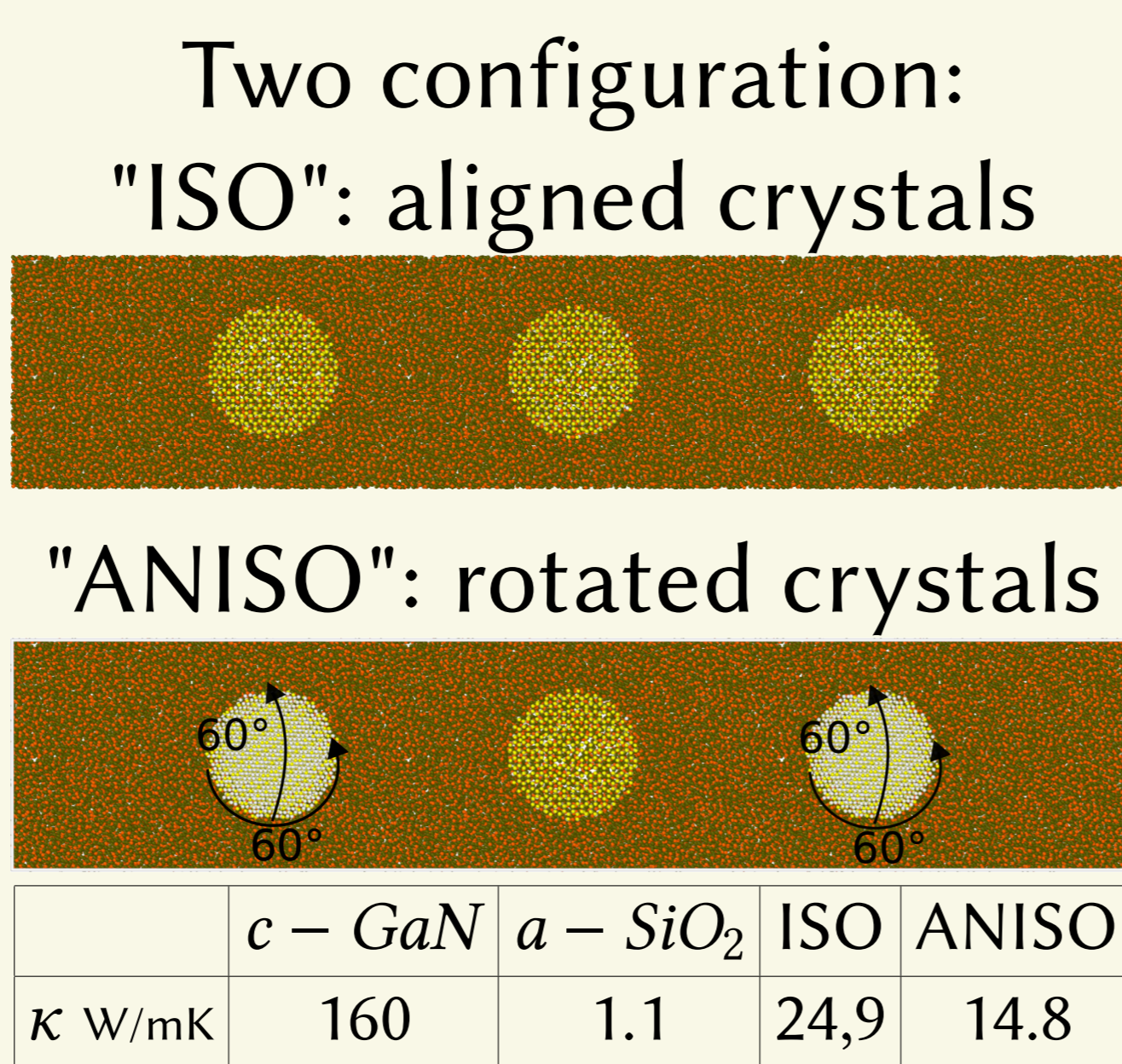
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## 1 Introduction and Configurations

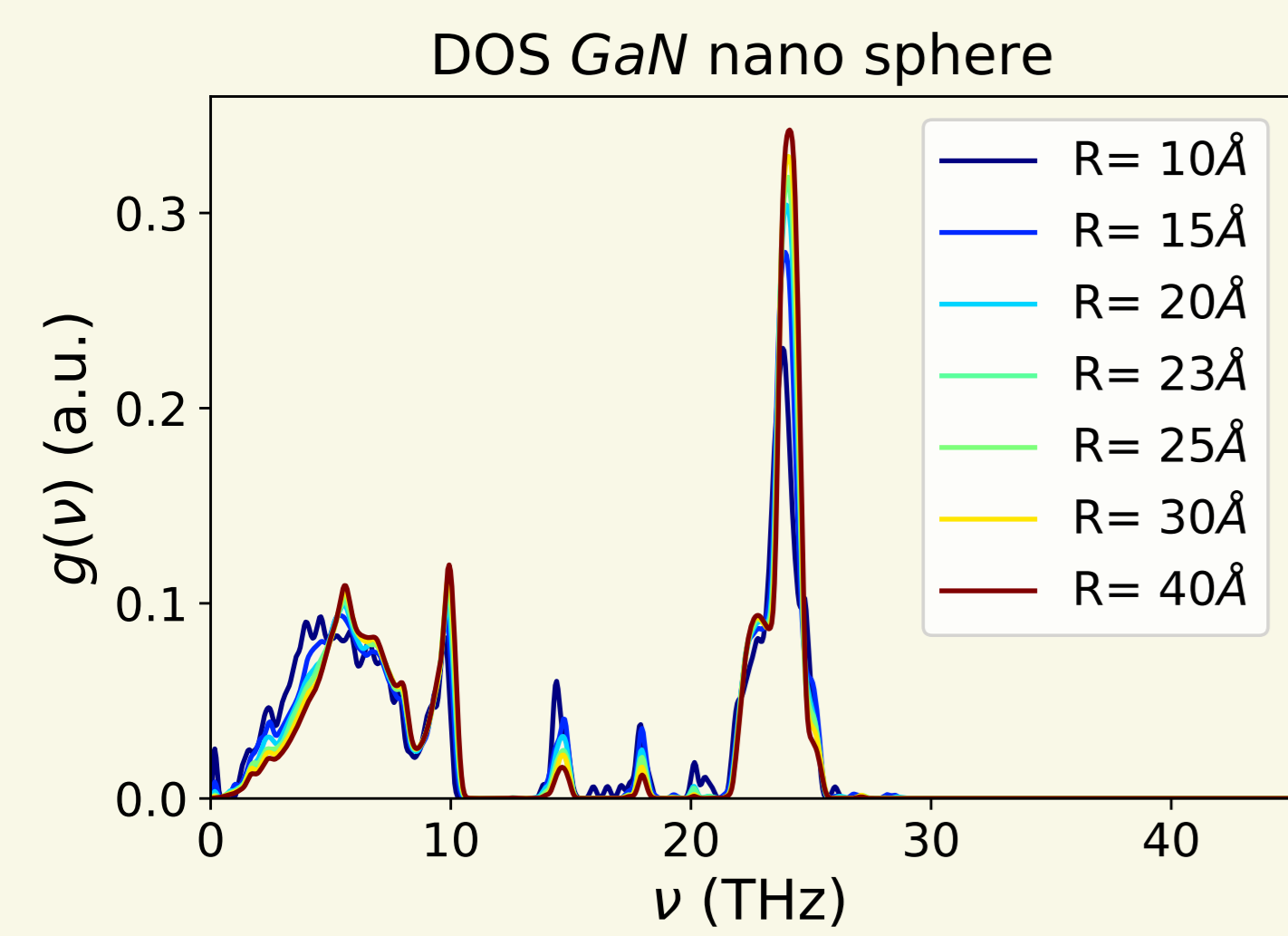
With the increasing demand of efficiency in electronic devices, a good thermal management starts to be crucial. In this regard nanocomposite can be a good solution to tune the conductivity of materials. Here we further investigate previous results [5], that shows that the thermal conductivity can depend significantly on the relative orientation of *c* - GaN inclusion in a *a* - SiO<sub>2</sub> matrix. Which is not taken into account in the Effective Medium Approach. We try to understand how this percolation can take place through molecular dynamics simulation.



## 4 VDOS nano sphere Composites

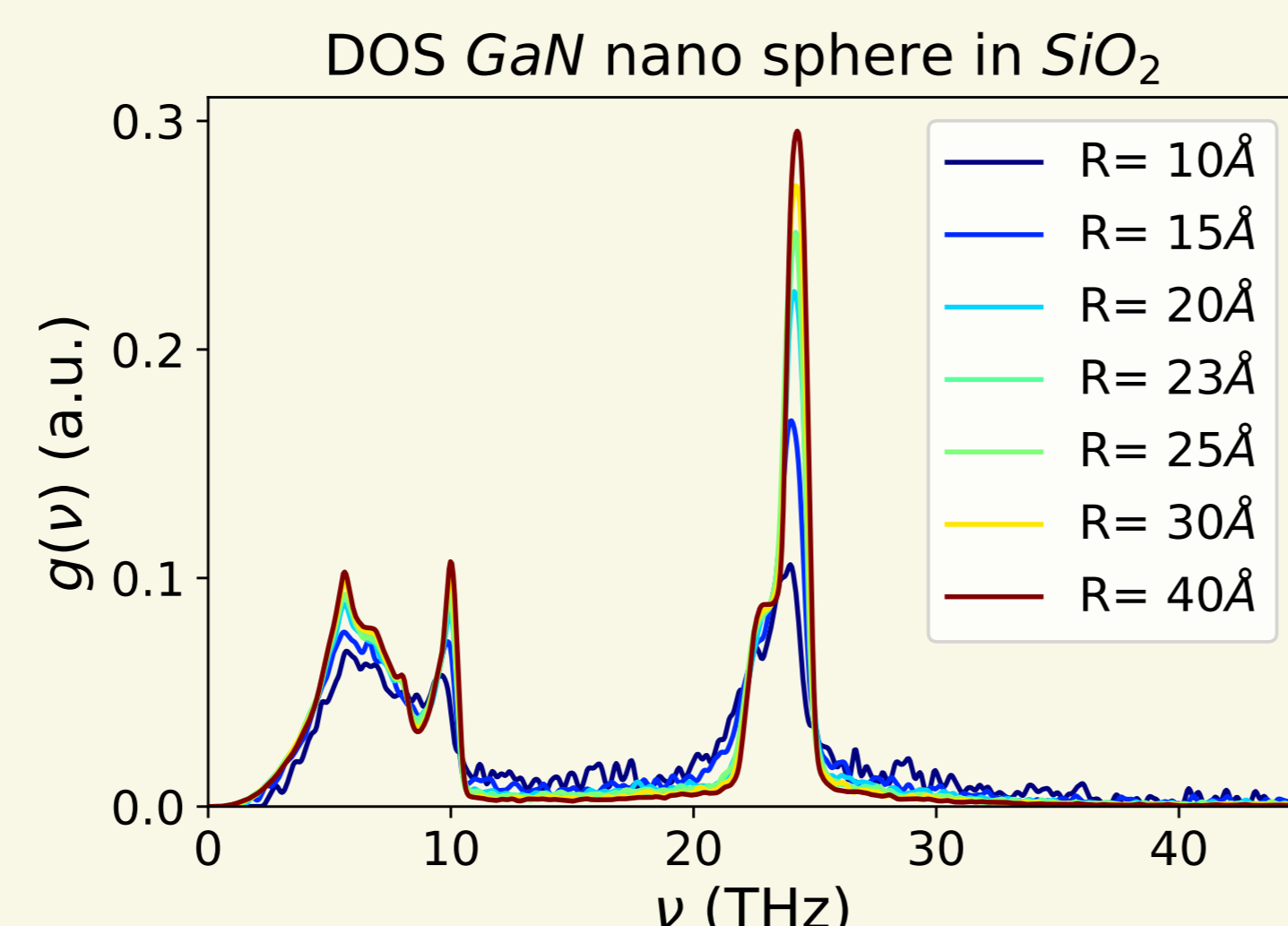
The VDOS is influenced by the size of the nano inclusion

### Inclusions Size



VDOS free GaN sphere

### Matrix Interface



VDOS GaN sphere in *a* - SiO<sub>2</sub>

### Red Shift of the acoustic peak

- Modes relative importance [4]

### In both case with the reduction of the radius

- filling of the band gap
- reduction of the sharpness of the main peaks

### Influence on the thermal conductivity

- tailoring of the EMA

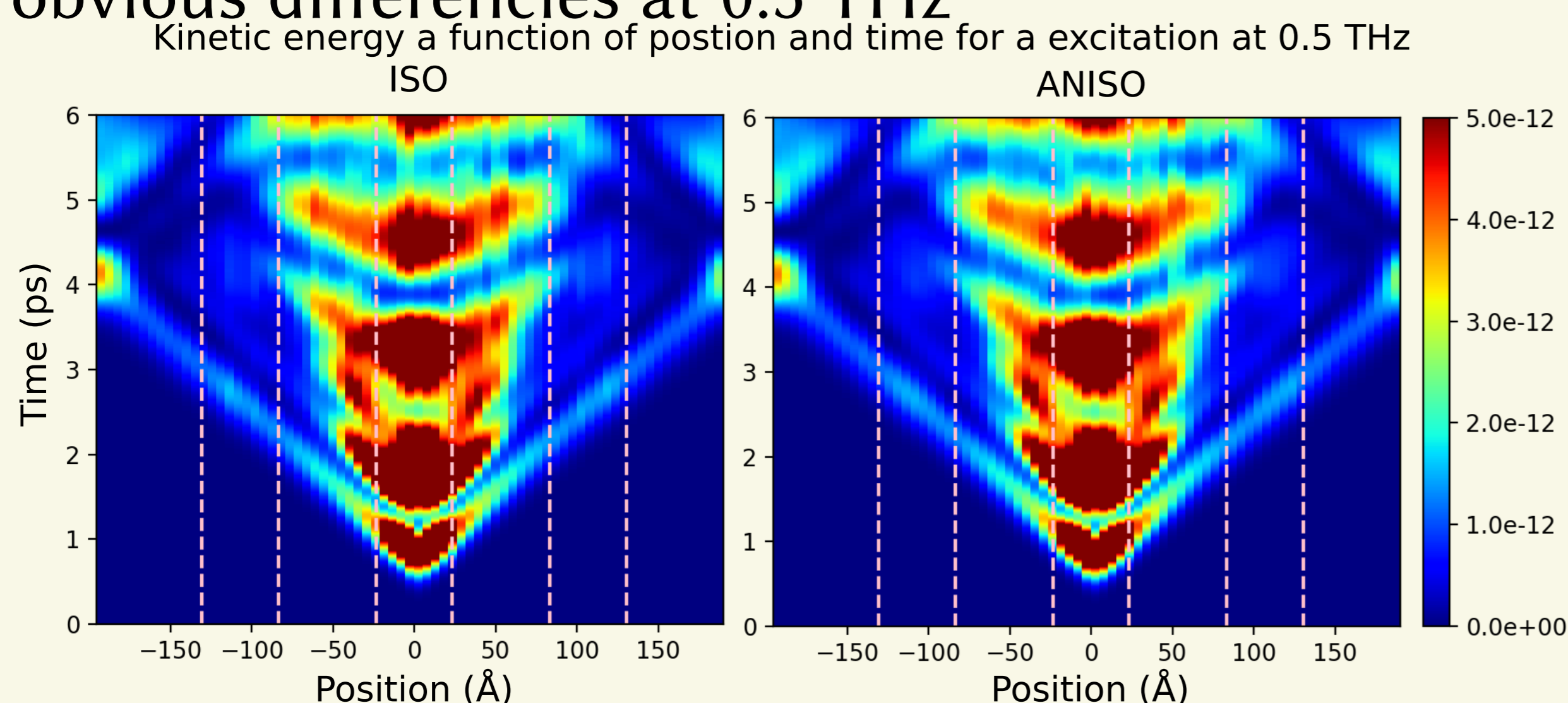
### More high frequencies modes

- little to no existing studies

## 6 Wave packet propagation

Comparison of the propagation of an excitation from the inclusion in the middle

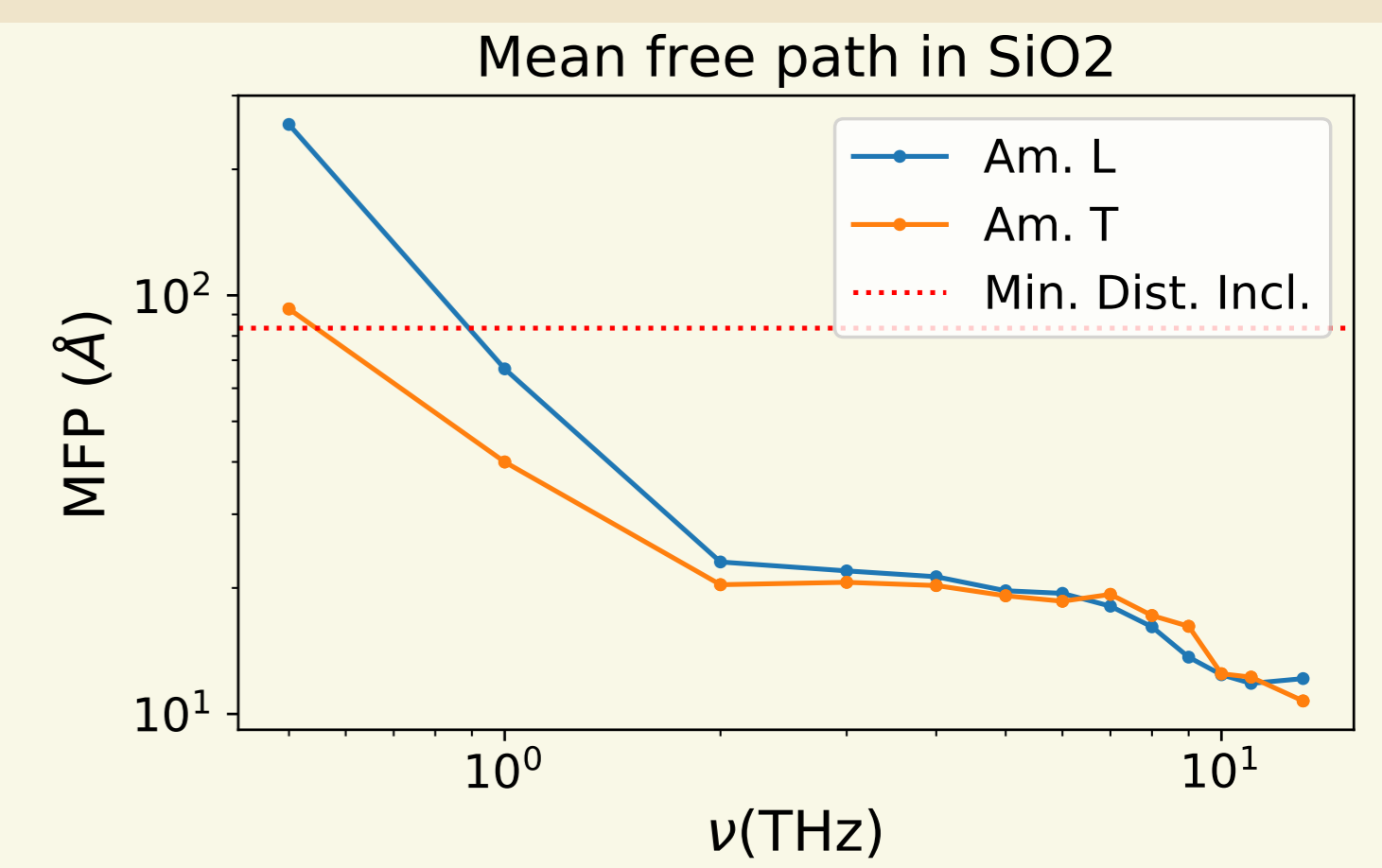
### No obvious differences at 0.5 THz



## 2 Energie transport

### Orientation dependant thermal conductivity

- Coherent wave transmission between inclusions
- Possible if Mean Free Path in SiO<sub>2</sub> ~ *l*<sub>incl</sub>
- If possible at low frequency for longitudinal waves
- ▶ Coherent with experimental results [7, 6]



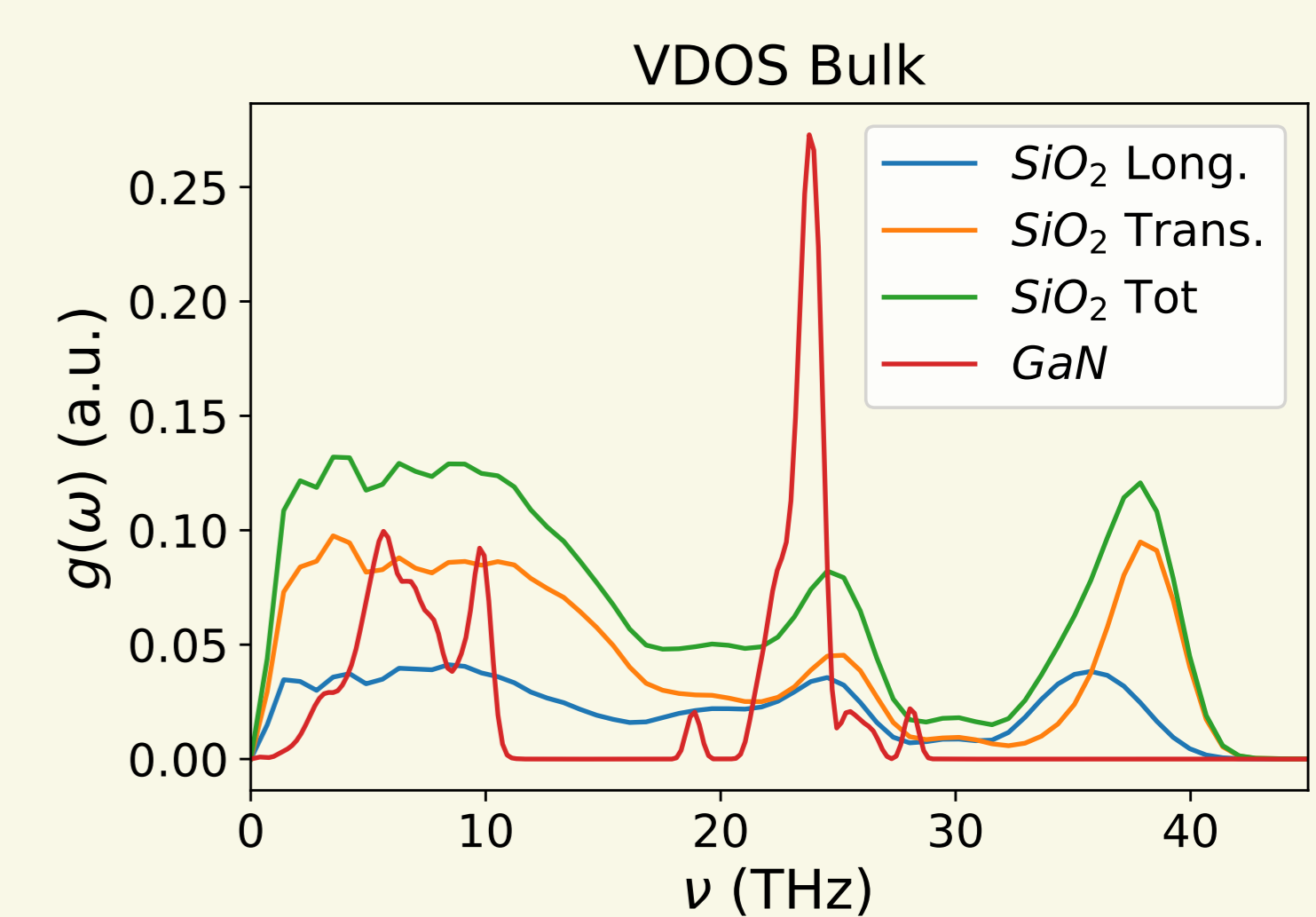
Mean Free Path in SiO<sub>2</sub> from wave packet attenuation [1]

## 3 Vibrational Density of State

To be transmitted mode of the frequency that travels should be allowed in both matrix and inclusion

### Overlap between the DOS at low frequency

- in DOS of the disjunct materials



Transverse as non compressive [2]

## 5 Dynamical Structure Factor

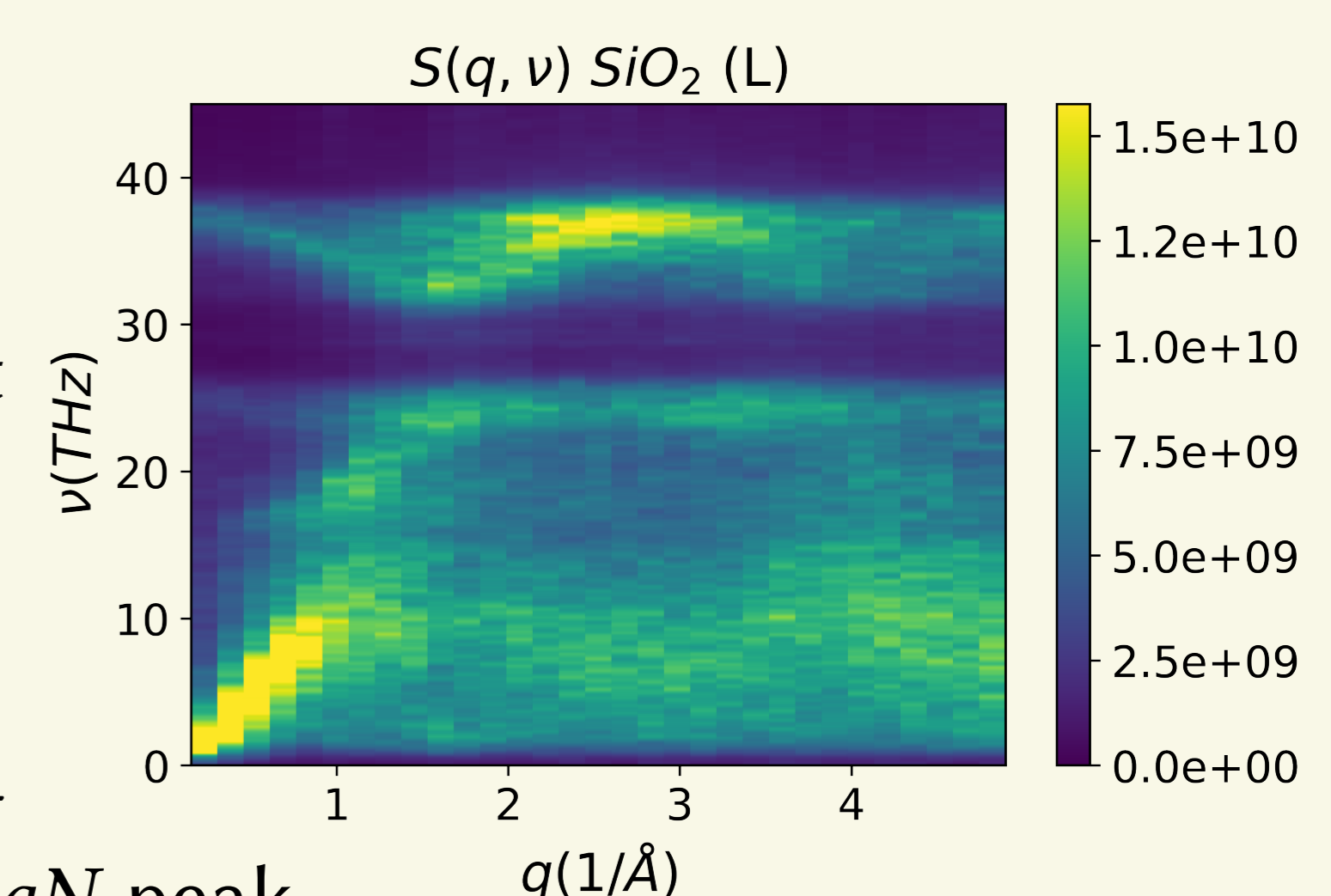
We use the mode resolved dynamical structure [3]

### for Bulk *a* - SiO<sub>2</sub>

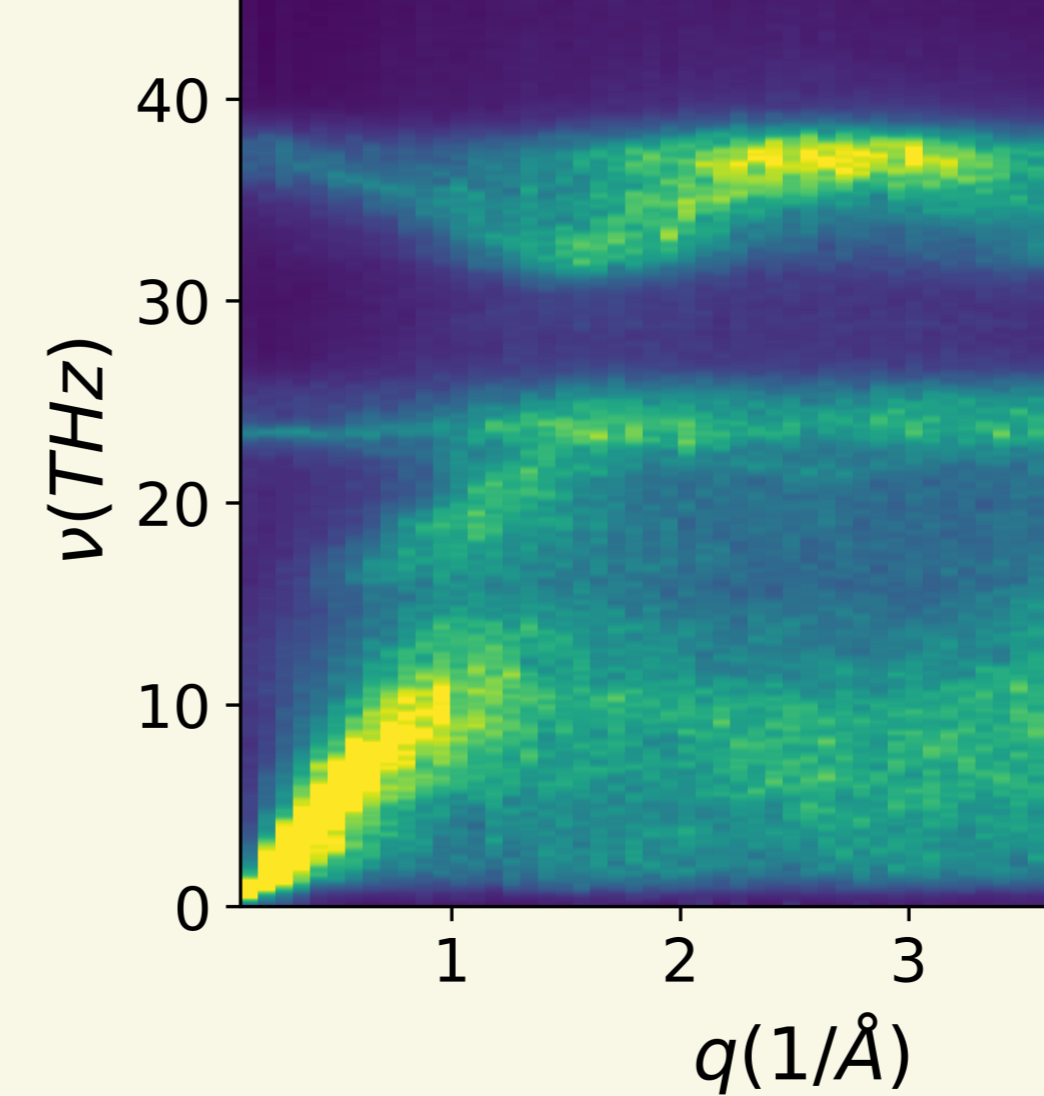
- From the slope of the first phonons
- $v_L(\nu) > v_T(\nu)$

### ISO/ANISO

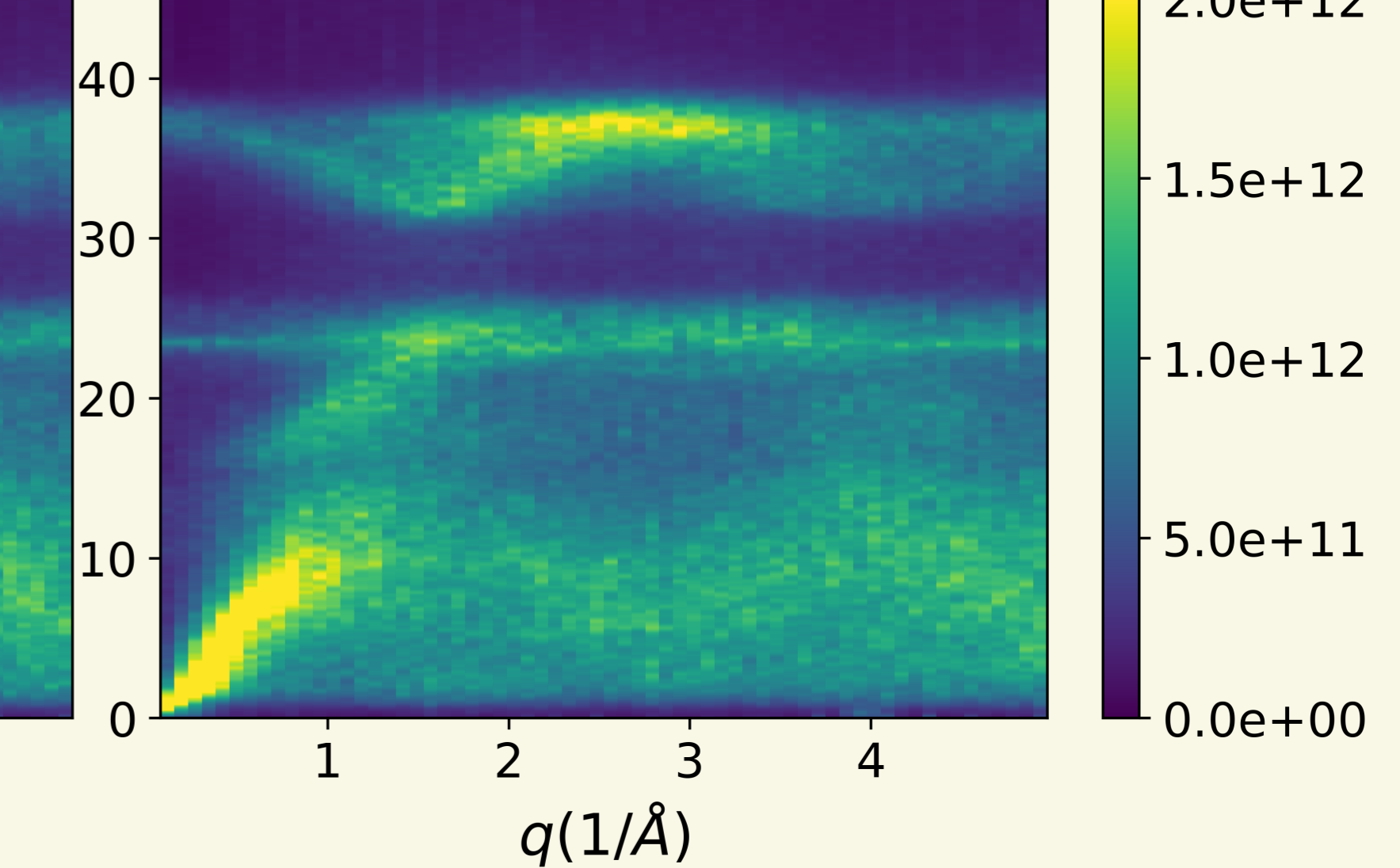
- Apparition of a new band frequency corresponding to the GaN peak
- no obvious differences



### S(q, ν) ISO (L)



### S(q, ν) ANISO (L)



## Summary and prospective

### Non trivial effect of size / interface to the VDOS

### No obvious difference on the propagative part

- no supplementary channel in  $S(q, \omega)$

### Prospective

- Computation of  $\kappa$  via another method (NEMD)
- Test of the propagation at characteristic frequencies
  - ▶ Size of the inclusions
  - ▶ Distance between inclusion

## References

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