トポロジカルデータ解析による熱伝導とナノスケール構造の相関解明

Elucidating the Correlation between Thermal Conductivity and Nanoscale Structures through Topological Data Analysis

阪大産研　南谷英美

SANKEN, Osaka Univ. Emi Minamitani

E-mail: eminamitani@sanken.osaka-u.ac.jp

Amorphous structures, which are neither completely ordered nor entirely random, exhibit physical properties significantly different from those of crystals. Understanding the correlation between structure and physical properties is crucial for their application. However, due to the complexity of amorphous structures, theoretical analysis has been extremely challenging. A typical example is thermal conductivity.

In crystals, thermal conduction is described by the relaxation of phonons through anharmonic effects. In contrast, in amorphous structures, heat is believed to be transferred through interactions between vibrational modes called diffusons, which are spatially extended and somewhat collective but lack periodicity. Considering the delocalized nature of diffusons, it is expected that the medium-range order in amorphous structures would affect thermal conduction by diffusons. However, there has been no theoretical method to quantitatively discuss which atomic connections give rise to medium-range order and how this structure determines the thermal conductivity.

Recently, we have attempted to apply persistent homology, a representative technique of topological data analysis, to this problem. We have shown that the thermal conductivity can be predicted by quantifying the atomic connections, ring structures, and voids in amorphous Si using persistent homology. Furthermore, inverse analysis allows discussion of the relationship between local structures, medium-range order, and thermal conductivity. In this presentation, we will introduce this research and discuss the potential for elucidating the correlation between nanoscale structures and thermal conductivity by combining topological data analysis with physical property simulations.

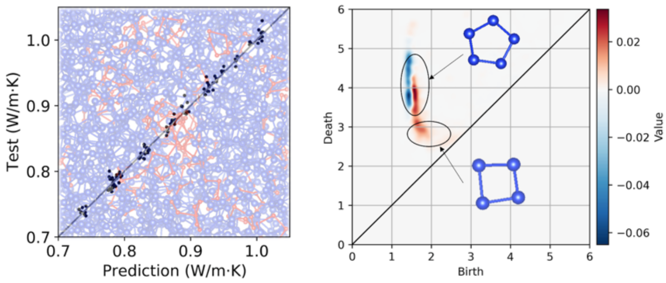

Fig 1 Prediction and inverse analysis results of thermal conductivity based on persistent homology.

References

[1] H. Edelsbrunner, J. Harer, *Computational Topology: An Introduction* (AMS, 2010).

[2] E. Minamitani et al., *J. Chem. Phys.* **156**, 244502 (2022).