熱伝導率が異なるアモルファス材料の構造的要因の トポロジカルデータ解析による解明

Structural Insights into Thermal Conductivity of Amorphous Germanium Using Topological Data Analysis

○呉　彦儒[1]，赤木 和人[2]，後藤　真宏[3]，徐 一斌[1]

○Yen-Ju Wu[1], Kazuto Akagi[2], Masahiro Goto[3], Yibin Xu[1]

1 Center for Basic Research on Materials, National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan

2 Advanced Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan

3 Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan

E-mail: Wu.YenJu@nims.go.jp

Due to their thermal properties, amorphous materials are attracting increasing attention for industrial use. Compared to crystalline materials, amorphous materials exhibit distinct thermal and lattice vibration properties because of lack of periodicity. However, analyzing atomic networks in the transmission electron microscopy (TEM) images of amorphous materials is challenging.

In this study, we applied topological data analysis (TDA) to detect a hidden order in TEM images referring to the atomic arrangements obtained by molecular dynamics simulations of amorphous germanium (a-Ge) and characterized the structural factors influencing the thermal conductivity of a-Ge based on principal component analysis (PCA). Our findings indicate that larger atomic rings, formed at higher deposition temperatures, significantly enhance thermal conductivity by facilitating heat transfer.

By utilizing data science, this study quantitatively distinguishes and characterizes previously difficult-to-identify structural factors in amorphous materials. This method introduces a new approach for incorporating metastable phases into the development of thermal insulators and thermoelectric materials. Our results suggest that manipulating atomic networks through controlled deposition processes can optimize the thermal performance of amorphous materials, opening new avenues for material innovation.

Reference:

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