Team takes data science approach to identifying thermal conductivity-related structural factors in amorphous materials

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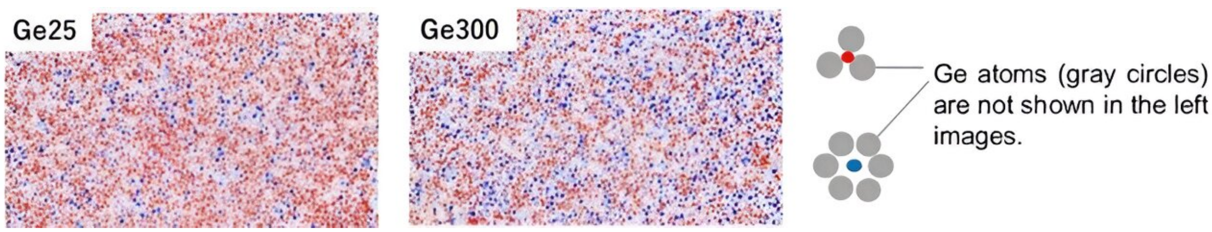

Distribution of atomic rings extracted from TEM images: Smaller (red dots) atomic rings are dominant in Ge25 while Ge300 contains a higher proportion of larger (blue dots) atomic rings. Credit: *International Journal of Heat and Mass Transfer* (2023). DOI: 10.1016/j.ijheatmasstransfer.2023.125012

A Tohoku University research team has discovered that different thermal conductivities exhibited by an amorphous material with the same composition are attributable to the sizes of atomic rings in its atomic structure. This is one of the first studies demonstrating that the structural features of amorphous materials can be correlated with their physical properties.

The paper is published in the *International Journal of Heat and Mass Transfer*.

It is already feasible to synthesize amorphous materials with the same compositions but different thermal conductivities. However, the structural factors responsible for differences in thermal conductivity had yet to be identified due to a lack of appropriate analytical methods.

It had been impossible to identify structural differences between amorphous germanium (Ge) materials with different thermal conductivities based only on high-resolution transmission electron microscope (TEM) observation. The research team analyzed amorphous Ge material TEM images using data science techniques—topological data analysis and principal component analysis—and identified structural differences between the materials.

The team found that the atomic structures of thin film specimens deposited at lower temperatures tended to be dominated by smaller atomic rings (Ge25) while specimens deposited at higher temperatures contained higher proportions of larger atomic rings (Ge300).

Larger atomic rings had been shown theoretically to be associated with higher thermal conductivity. This study found that Ge300 had higher thermal conductivity than Ge25—results consistent with the theoretical evidence.

The data science techniques developed in this research project can be used to identify metastable phases in materials—a task impossible to achieve using conventional structural analysis techniques. These techniques are therefore expected to be useful in developing metastable phase-integrated thermal control materials. They may also be useful in identifying structural features associated with the mechanical, electrical and other properties of amorphous materials in addition to their thermal properties.

This research was carried out by a research team consisting of Yibin Xu

(Leader, Data-driven Inorganic Materials Group, Center for Basic Research on Materials, NIMS) and Kazuto Akagi (Associate Professor, Advanced Institute for Materials Research, Tohoku University). This work was conducted as part of a JST CREST Exploring Unknown Materials project (research supervisor: Professor Hiroshi Kitagawa).

More information: Yen-Ju Wu et al, Topological data analysis of TEM-based structural features affecting the thermal conductivity of amorphous Ge, *International Journal of Heat and Mass Transfer* (2023). DOI: 10.1016/j.ijheatmasstransfer.2023.125012

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