# Predicting grain boundary thermal conductivities based on their atomic arrangement

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## Abstract

Most of functional and structural materials are used as polycrystalline materials. Grain boundaries (GBs) formed between the grains have different atomic structures than the grain inside. Thus, they exhibit various properties and consequently have a significant effect on macroscopic properties such as mechanical, electrical and thermal properties. By clarifying the correlations between GB structures and properties, novel material designs based on the GB microscopic structures will be possible. In this study, we have obtained thermal conductivities of 92 MgO GBs using atomic-level calculations. With these data, we constructed a model that accurately predict GB thermal conductivities from their atomic arrangement using machine learning techniques. In other words, the correlation between GB structure and thermal conductivity was quantitatively clarified for MgO for the first time.

## Background & Results

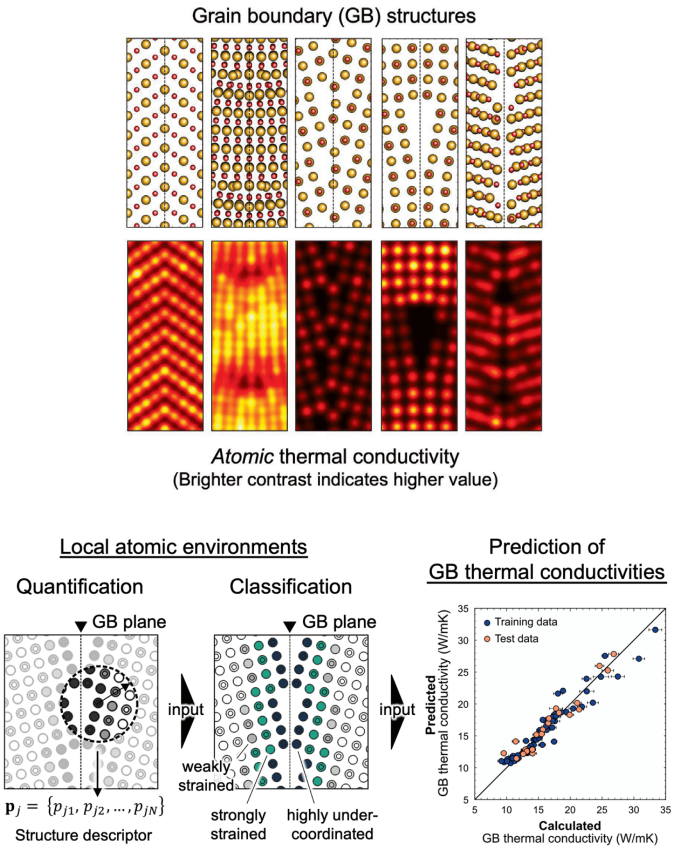
Thermal conductivity is crucial for many technological applications such as thermoelectrics. GBs are well known to reduce thermal conductivity. However, it remains unclear for many years what kind of GB atomic arrangement effectively reduces thermal conductivity. This is due to the difficulty of systematic evaluation of GB structures and their properties, and the lack of methods to quantitatively investigate structure-property relationships for GBs.

In this study, we have obtained 92 MgO GBs and their thermal conductivities using molecular dynamics method. This method can simulate the vibrational state of atoms and thus heat transport via lattice vibration. First, MgO GB structures were determined by simulated annealing method; amorphized MgO was sandwiched between crystal grains, then a high temperature was induced to promote spontaneous rearrangement of atoms, resulting in a stable GB structure. Thermal conductivities of these GBs were calculated by perturbed molecular dynamics. The visualization of *atomic* thermal conductivities revealed that local disorder of atomic arrangement significantly suppresses thermal conduction.

Then, local atomic environments (LAEs) that constitute GB structures were converted into a vector using a structure descriptor. This vector is unique to the LAE of an atom, so it can be considered as a fingerprint of LAE. Using these vectors of GB atoms, LAEs near GBs were classified into several groups by hierarchical clustering (e.g., highly under-coordinated, strongly strained). A prediction model for thermal conductivity was constructed by linear multiple regression using the number density of LAEs near the GBs. It was found that GB thermal conductivities can be accurately predicted by classifying LAEs into only six groups, and small distortions of LAEs can sufficiently reduce the thermal conductivity.

## Significance of the research and Future perspective

The constructed model should accelerate the material design for thermally functional materials. In addition, by clarifying the structure dependence of macroscopic properties other than thermal conductivity, it will be possible to achieve simultaneous control of multiple properties by GB distribution, leading to the development of new materials with multiple functions.




**Patent**

**Treatise**

Fujii, Susumu; Yoshiya, Masato et al. Quantitative prediction of grain boundary thermal conductivities from local atomic environments. Nature Communications. 2020; 11(1): 1854. doi: 10.1038/s41467-020-15619-9

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