Theoretical Studies on Novel Physical Properties Arising from Many-Body Interaction

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Education
2005 B.S. Osaka University
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Professional Employment
2010 Postdoctoral Fellow, Osaka University
2011 Special Postdoctral Researcher, RIKEN
2013 Assistant Professor, The University of Tokyo
2015 Lecturer, The University of Tokyo
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Awards
2008 L'Oréal–UNESCO Japan National Fellowships for Women in Science
2011 Best Poster Award in ISSS-6 Internal Symposium on Surface Science
2017 Young Scientist Award of the Physical Society of Japan
2019 The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology
The Young Scientists' Prize
2020 The 1st Award for Early Career Women Scientists of the Japan Society of Vacuum and Surface Science
2021 The 2nd Fumiko Yonezawa Memorial Prize of the Physical Society of Japan

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Keywords Quantum Many-Body Interaction, Density Functional Theory, Quantum Field Theory

Quantum many-body interaction is a source of novel physical properties in condensed matters. In our group, we develop theoretical methods by combining quantum field theory and density functional theory, and carry out collaborative research with experimental groups. As specific targets, we focus on magnetism in nanostructure and energy dissipation.

For magnetism in nanostructure, we are interested in the Kondo effect and spin–orbit interaction. The Kondo effect arises from the interaction between the localized spin and conduction electrons, which forms a characteristic many-body state so-called the Kondo singlet state. The spin–orbit interaction originating from the relativistic effect constrains the magnetic moment direction to a specific direction. We investigate the possibility of novel physical phenomena induced by these interactions in the nanostructure and molecules on surfaces.

For energy dissipation, we focus on the effect of electron–phonon interaction. The electron–phonon interaction is one of the most fundamental interactions in the condensed matter physics, and the quantitative evaluation in realistic materials is highly demanding. We adopt the ab-initio calculation to analyze the signal of electron–phonon coupling in surface spectroscopy and thermal properties in various kind of solids.

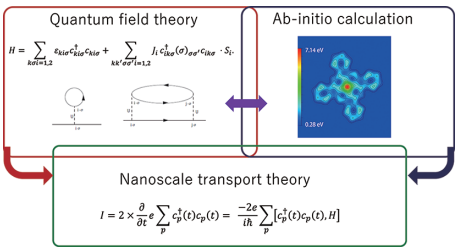

Figure 1. Schematic image of the theoretical method developed in our group.

Selected Publications

- E. Minamitani, N. Tsukahara, D. Matsunaka, Y. Kim, N. Takagi and M. Kawai, "Symmetry-Driven Novel Kondo Effect in a Molecule," *Phys. Rev. Lett.* **109**, 086602 (2012).
- E. Minamitani, R. Arafune, N. Tsukahara, Y. Ohda, S. Watanabe, M. Kawai, H. Ueba and N. Takagi, "Surface Phonon Excitation on Clean Metal Surfaces in Scanning Tunneling Microscopy," *Phys. Rev. B* **93**, 085411 (2016).
- R. Hiraoka, E. Minamitani, R. Arafune, N. Tsukahara, S. Watanabe, M. Kawai and N. Takagi, "Single-Molecule Quantum Dot as a Kondo Simulator," *Nat. Commun.* **8**, 16012 (2017).
- E. Minamitani, M. Ogura and S. Watanabe, "Simulating Lattice Thermal Conductivity in Semiconducting Materials Using High-Dimensional Neural Network Potential," *Appl. Phys. Express* **12**, 095001 (2019).
- E. Minamitani, "Ab Initio Analysis for the Initial Process of Joule Heating in Semiconductors," *Phys. Rev. B* **104**, 085202 (2021).
- E. Minamitani, T. Shiga, M. Kashiwagi and I. Obayashi "Topological Descriptor of Thermal Conductivity in Amorphous Si," *J. Chem. Phys.* **156**, 244502 (2022).

1. Topology and Machine Learning Reveal a Hidden Relationship between Thermal Conductivity and Amorphous Structure

The structure of amorphous materials is characterized by the absence of long-range order (LRO) and the presence of some medium-range order (MRO) beyond the short-range order (SRO). Revealing the quantitative correlation between the structural and physical properties of amorphous materials remains a challenging task. Thermal conductivity is a fundamental physical property that shows unique behavior in amorphous materials owing to the strong interaction between lattice vibrations and disorders. The lack of LRO reduces the lattice thermal conductivity by several orders than that of a crystal with the same stoichiometry. The heat carriers, vibrational modes, in amorphous materials are generally classified into propagating and non-propagating modes. The former is exhibited in the low-frequency range and has characteristics similar to those of phonons in the crystal. In contrast, the latter carries heat in a diffusive manner rather than propagating energy as phonons do in the crystal. It is expected that the MRO affects the propagation and diffusion of these vibrational modes, and thus the thermal conductivity.

Previous studies indicated that determination of the atomic structure corresponding to the MRO and extraction of the correlation between the MRO and the lattice thermal conductivity is essential to precisely control the thermal properties of amorphous Si. However, these tasks remain challenging because determining the essential features of MRO from the traditional structural analysis is difficult, such as the pair distribution function and bond-orientation order analysis.

Recently, persistent homology, an emerging technique in the field of topological data analysis, has been employed to describe the atomic structures corresponding to MRO in SiO_2 glass, metallic glass, and amorphous ice. The advantage of persistent homology is that multiscale topological information can be extracted from complicated structures. For the analysis of persistent homology, we considered a growing sequence of network structures for given data points with different scale lengths defined by the filtration procedure. A schematic of the filtration procedure is shown in Figure 2. As can be seen, we considered spheres centered at the respective data points. Subsequently, the radius of each sphere gradually increases. The sequence of increases in radius is often referred to as "time." At some radius, the spheres start to intersect with each other, and we set an edge between the centers of the spheres. When the edges form a closed ring, this corresponds to a topological feature called a "cycle." As the radius further increases, the ring gets fully covered by circles. This is interpreted as the cycle converting into another class of topological features called a "boundary." The topology of the data is represented by the pairs of birth and death times at which the cycle appears and is converted into a boundary. The two-dimensional visualization of birth and death time pairs is called a persistence diagram (PD).

In this study, using persistent homology, we constructed reliable descriptors for lattice thermal conductivity, reflecting the topological features of the MRO in amorphous Si.

A structural model of amorphous Si was generated via the melt–quench method using classical molecular dynamics (MD), where the system temperature was increased above the melting temperature and then gradually cooled to room temperature. The difference in structural characteristics was introduced by changing the cooling rate in the MD simulation from 10^{14} to 10^{11} K/s. We selected 570 snapshots from the equilibrated MD simulation after the melt–quench procedure, and the thermal conductivity mediated by non-propagating modes and the PD were evaluated for each structure.

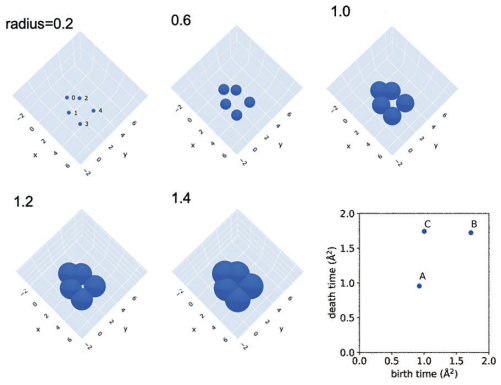

Figure 2. Schematic of the filtration procedure used to obtain a PD from data points.

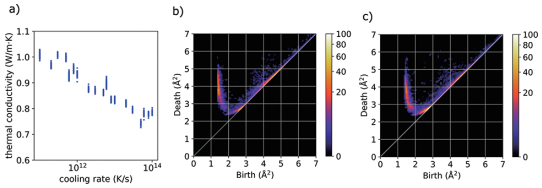

Figure 3. a) and b) Persistent diagrams for amorphous structure generate by the cooling rate of 10^{14} and 10^{11} K/s, respectively.

As shown in Figure 3, both thermal conductivity and PD depend on the cooling rates. Therefore, we constructed a descriptor of the topological features using the persistent image of the PD. We demonstrated that supervised training for the dataset of these descriptors and lattice thermal conductivities could achieve accurate predictions. In addition, from the inverse analysis by volume-optimal cycle, we determined the typical ring features correlated with the thermal conductivity and MRO.[1)] Our study demonstrates that the physical properties of amorphous Si can be predicted based on topological features. In addition, our results illustrate the hidden relationship between MRO and the physical properties of amorphous Si. This study could open an avenue for controlling material characteristics through the topology of nanostructures.

2. Other Ongoing Projects:

- Mechanical Properties in Amorphous Solids

Reference

1) E. Minamitani, T. Shiga, M. Kashiwagi and I. Obayashi, *J. Chem. Phys.* **156**, 244502 (2022).