Symposium (Oral) | Symposium：Vibronics: Energy transport science of vibrations in solid

Fri. Sep 20, 2024 9:30 AM - 11:50 AM JST | Fri. Sep 20, 2024 12:30 AM - 2:50 AM UTC A23 (TOKI MESSE 2F)

[20a-A23-1~5] Vibronics: Energy transport science of vibrations in solid

Junichiro Shiomi(Univ. of Tokyo), Kazuhiro Yanagi(Tokyo Metropolitan Univ.)

Symposium Sponsor

Science Edge

English Presentation
9:30 AM - 9:35 AM JST | 12:30 AM - 12:35 AM UTC
[20a-A23-1]
Opening
〇Masahiro Nomura[1] (1.Univ. of Tokyo)

English Presentation
9:35 AM - 10:05 AM JST | 12:35 AM - 1:05 AM UTC
[20a-A23-2]
Easy Measurement of Phonon Dispersion at SPring-8
〇Alfred Q. R. BARON[1,2], Daisuke ISHIKAWA[1,2], Hiroshi FUKUI[2,1], Taishun MANJO[2,1] (1.Materials Dynamics Laboratory, RIKEN SPring-8 Center, 2.Precision Spectroscopy Division, SPring-8/JASRI)

English Presentation
10:05 AM - 10:35 AM JST | 1:05 AM - 1:35 AM UTC
[20a-A23-3]
Phonon transport of group IV semiconductor alloys
〇Ryo Yokogawa[1,2], Atsushi Ogura[1,2] (1.Meiji Univ., 2.MREL)

English Presentation
10:50 AM - 11:20 AM JST | 1:50 AM - 2:20 AM UTC
[20a-A23-4]
Elucidating the Correlation between Thermal Conductivity and Nanoscale Structures through Topological Data Analysis
〇Emi Minamitani[1] (1.SANKEN, Osaka Univ.)

English Presentation
11:20 AM - 11:50 AM JST | 2:20 AM - 2:50 AM UTC
[20a-A23-5]
Vibration transport at topological edges of mechanical metamaterials
〇Motonobu Tomoda[1] (1.Hokkaido Univ.)

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Junichiro Shiomi(Univ. of Tokyo), Kazuhiro Yanagi(Tokyo Metropolitan Univ.)

English Presentation

9:30 AM - 9:35 AM JST | 12:30 AM - 12:35 AM UTC

[20a-A23-1] Opening

〇Masahiro Nomura[1] (1.Univ. of Tokyo)
Keywords：Phonon、Heat transfer、Energy transfer

An overview of the energy transport science of solid-state vibrations, named vibronics, is given, as well as the purpose of this symposium.

Easy Measurement of Phonon Dispersion at SPring-8

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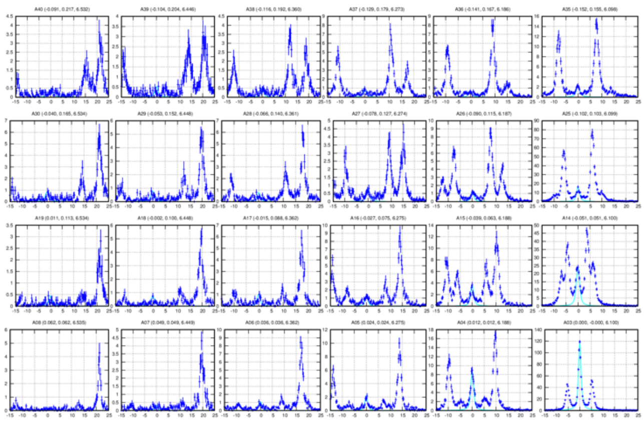
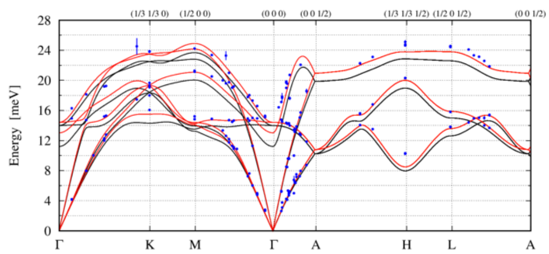
Alfred Q.R. BARON, Daisuke ISHIKAWA, Hiroshi FUKUI, Taishun MANJO

SPring-8, in Hyogo prefecture, has the world's most advanced facilities for measuring phonons using x-rays. The spectrometers at the SPring-8 beamlines, BL35XU [1] and BL43LXU [2], provide world-leading flux in small beam sizes (from 0.005 to 0.1 mm) that can be used to investigate atomic dynamics on meV energy scales over ~nm to Å correlation lengths via inelastic x-ray scattering (IXS) (see [3] for a general introduction). These measurements are used to investigate many classes of materials, focusing on issues relevant to thermal transport, ferroelectricity, superconductivity, formation of charge density waves, phase transformations, localized phonon modes, interactions of phonons with magnons, *etc.* The instruments are also effective for investigating liquids, phonons in thin films, and elastic properties of materials in extreme (high-pressure and high temperature) conditions, even those approaching those of the Earth's inner core – measurements that can be difficult or impossible by other methods.

Perhaps most notably the samples for IXS can be small: a comfortable size sample is ~ 0.5 mm scale, but the method also has been used on ~ 0.005 mm samples, or even 0.0001 mm films. This makes it easy to investigate samples that are not available in the large (cubic-centimeter scale) needed by inelastic neutron scattering, the main competing technique. The figure below gives an example of measured dispersion from a relatively simple hexagonal sample [4]. The plot at left shows a set of 24 spectra that were measured in a single 1-hour scan, while that at right show the dispersion measured in about half a day of data collection.





IXS measurements of a simple hexagonal material. At left is a set of 24 spectra measured in a single 1-hour scan (the horizontal axis is energy transfer in meV) while the plot at right shows the dispersion compared to a couple different models. After [4].

The present talk will describe the main principle of operation of the meV-IXS spectrometers at SPring-8, discuss the variety of samples that may be investigated, and the range of available sample environments.

SPring-8 is a user facility. We are happy to consider collaboration with new groups, and/or on new materials, or in new setups or geometries. Please do contact us if you may be interested. We can be reached most easily by e-mail at baron@spring8.or.jp, disikawa@spring8.or.jp, fukuih@spring8.or.jp, manjo.taishun@spring8.or.jp.
Additional information can also be found on the web pages:

https://beamline.harima.riken.jp/bl_info/bl43lxu_info.html
https://beamline.harima.riken.jp/bl43lxu/
http://www.spring8.or.jp/wkg/BL35XU/instrument/lang-en/INS-0000001397/instrument_summary_view

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Phonon transport of group IV semiconductor alloys

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【Introduction】 Group IV semiconductor alloys have attractive characteristics such as high carrier mobility and low thermal conductivity. As example of device application, silicon-germanium (SiGe) is one of the promising candidates for 3D transistors and thermoelectric devices. For thermoelectric devices, it is gradually becoming more important to reveal the phonon scattering mechanism of the alloy material and control the thermal transport as miniaturization proceeds to the nanometer scale. However, the phonon properties of the group IV semiconductor alloys have not been investigated in a sufficiently rigorous manner yet. In this paper, we introduce the information on the phonon properties of group IV semiconductors alloys such as bulk SiGe and germanium-tin (GeSn) thin films by using inelastic x-ray scattering (IXS) with synchrotron radiation and Raman spectroscopy.

【Phonon energy measurement techniques】 IXS with synchrotron radiation is a powerful technique to evaluate phonon energy and dispersion relation nondestructively. The IXS measurements were performed on the BL35XU and BL43LXU beamlines at the SPring-8 synchrotron facility. The incident x-ray energies were set to 17.795 and 21.750 keV, which corresponds to Si (9 9 9) and (11 11 11) reflections, respectively [1]. Although it can only give information on optical phonon modes at the Brillouin zone center (Γ point), Raman spectroscopy is also useful with high energy and spatial resolution compared to IXS. We also used Raman spectrometer with a focal length of 2,000 mm [2] (high-wavenumber resolution) to discuss optical phonon transport through Raman spectra of group IV semiconductor alloys.

【Main results】 We obtained clear phonon dispersion curves of bulk SiGe by IXS measurements [3]. Moreover, we also observed phonon spectra of GeSn thin film by utilizing grazing incidence IXS technique [4]. Interestingly, anomalous modes distinct from both optical and acoustic modes of bulk SiGe [5] and GeSn thin films [4] in phonon dispersion curves were observed at low-energy side. We found that the anomalous mode of bulk SiGe had no momentum and Ge fraction dependences. These behaviors were consistent with the molecular dynamics (MD) calculations. We consider that the origin of the anomalous mode is local vibrational mode (LVM) originated from the Ge (Sn) clusters surrounded by Si (Ge) atoms through a combination of IXS measurements and MD simulations [6,7]. From the above, it can be confirmed that group IV semiconductor alloy crystals exhibit unique phonon transport properties compared to pure Si and Ge from IXS results. On the other hand, Raman spectra of SiGe [8] and GeSn alloys are often used to characterize fine structures, LVMs, and strain states. We will introduce the Raman spectroscopy analysis of SiGe [9] and GeSn incorporating IXS measurements.

【Acknowledgements】 The IXS measurements were performed at SPring-8 with the approval of the JASRI (Proposal Nos. 2016A1496, 2017B1630, 2019A1678, 2019B1750, 2020A0662, 2020A1463, 2021A1363, 2021B1203, 2022A1470, and 2023B2088). Part of this work was supported by the CREST under Project. No. JPMJCR19Q5 of the Japan Science and Technology Corporation (JST). This work was supported by JSPS KAKENHI Grant Nos. 21K14201 and 24K17313, Japan.

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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

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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.

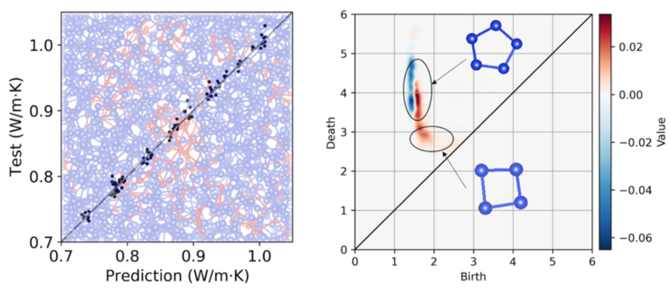

Fig 1 Prediction and inverse analysis results of thermal conductivity based on persistent homology.

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Vibration transport at topological edges of mechanical metamaterials

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The topological phases that originated from the discovery of the quantum Hall effect have recently garnered attention for their applications in classical wave phenomena. In the quantum Hall effect, it is well-known that electrons are transported along the boundaries of a sample due to the bulk's topological properties. However, it has been found that topologically protected transmission can be realized not only with electrons but also with photons [1] and phonons [2]. In the case of phonons, topological waveguides exhibit inherent robustness against bends and defects, preventing backscattering. This promises the realization of more efficient waveguides and non-reciprocal acoustic devices. To realize a phononic analog of quantum Hall (QH) systems, it is necessary to break time-reversal symmetry. Since most phononic systems do not interact with magnetic fields, theories have been proposed to introduce Coriolis forces through rotational motion [3]. On the other hand, quntam valley Hall (QVH) systems, can be realized by breaking the spatial inversion symmetry of the unit cell.

We are developing mechanical metamaterials that extend a wave machine into two dimensions to achieve vibration propagation through topological edge modes and to experiment with further control methods. To realize a QH system, we created a honeycomb lattice wave machine that maintains its equilibrium position despite rotation due to centrifugal force. To realize a QVH system, we created a suspended honeycomb lattice wave machine [4]. The vibrations of these wave machines were quantitatively measured using a motion capture system and compared with a theoretical and simulation results.

These achievements can not only provide insights into highly advanced wave propagation based on topological phononics but also contribute to a new science called "vibronics," which comprehensively considers vibrational phenomena within solids.

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