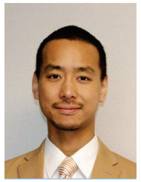
【Grant-in-Aid for Scientific Research (S)】

Meta-phononics of disordered solid system including mass transport



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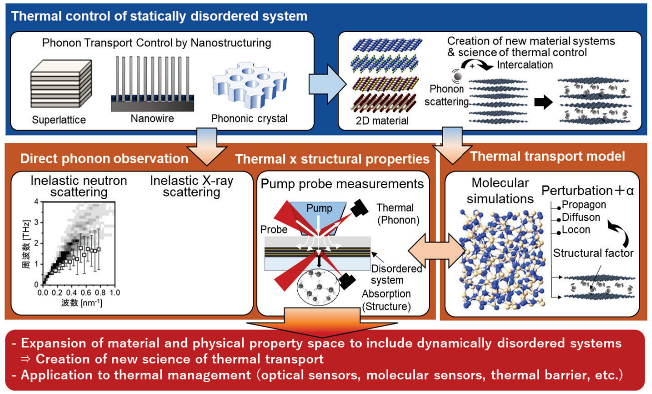
Project Information	Project Number : 22H04950 Keywords : Dynamic disorders, phonon and mass transport, nanostructures	Project Period (FY) : 2022-2026

Purpose and Background of the Research

●Outline of the Research

Recent progress in the science of phonon transport has been remarkable, and the controllability of thermal conduction in crystalline materials has been dramatically improved by nanostructuring. For further innovation, it is necessary to expand the material search space to disordered systems. To achieve the ultimate goal, we aim to significantly expand the controllability of thermal conduction by creating static and dynamic disordered nanostructures. For static systems, we will fabricate superlattices, nanowires, and phononic crystals made of amorphous materials. On the other hand, as a dynamic system, "super disordered materials," in which some of the constituent elements move around like superionic conductors, will be fabricated. We will directly measure phonon states and relaxation by inelastic scattering experiments and develop a new method to simultaneously measure phonon and mass transports to evaluate their correlation. Furthermore, by analyzing these results, we will construct a new theory of heat transport in the super-disordered systems. Ultimately, we will develop solid-state materials with ultimately small thermal conductivity, which will lead to improved sensitivity and energy conservation in optical and molecular sensors.



- Expansion of material and physical property space to include dynamically disordered systems
  ⇒ Creation of new science of thermal transport
- Application to thermal management (optical sensors, molecular sensors, thermal barrier, etc.)

Figure 1. Overall flow of research

● **Background and Objectives** Thermal conduction in non-metallic solids is carried by phonons. In recent years, "phonon engineering," in which the thermal conductivity of solids is understood from phonon picture and controlled by nanostructures, has been rapidly developed. As a result, crystalline materials with thermal conductivity higher than that of diamond and smaller than that of homogeneous amorphous materials have been found, and thermal conductivity is no longer a physical property determined by the material but can be controlled over a wide range by devising the nanostructure, contributing to improved performance in heat dissipation, insulation, thermoelectric conversion, etc.

Now that phonon engineering in crystalline systems has gradually matured, what is next? We believe it is phonon engineering of disordered systems. Heat transport by phonons can be described as the propagation of well-defined eigen modes in periodic systems such as crystals, but not in amorphous materials where atoms are arranged irregularly. Although theories have been proposed to describe this, our recent work has shown that nanostructuring of amorphous materials can yield thermal conductivities smaller than their theoretical limits, indicating the possibility that thermal conductivity can be controlled by disordered systems beyond conventional understanding.

In this study, we consider "dynamically disordered systems" in addition to such static disordered nanostructures. This is a system in which some groups of elements that make up the solid can move dynamically. By introducing ions and water into the interior of layered materials such as graphite, we create materials in which phonon transport and mass transport coexist and interact strongly and find a new controllability of heat transport. Furthermore, with new methods to measure and simulated phonon transport and dynamic structure simultaneously, we aim construct a generalized theoretical model of heat transport.

Expected Research Achievements

In this project, (1) as static systems, superlattices, nanowires, and phononic crystals made of amorphous materials are fabricated to show the controllability of heat transport by nanostructures, and (2) as for dynamic systems, "super-disordered solid system“, in which some of the constituent elements move around inside two-dimensional layered materials, are fabricated to find new controllability of heat transport. Furthermore, we (3) directly measure phonon states and relaxation by inelastic scattering experiments and develop a new method to simultaneously measure thermal transport and dynamical structure and evaluate their correlation, and (4) analyze them to clarify mode-wise thermal transport and construct a theory of heat transport in super-disordered solids.

There exits a theory to understand heat transport in static disordered structures such as amorphous by separating phonons that propagate as in crystals and those that diffusive in random directions reflecting disorder, but it does not reproduce heat transport in amorphous nanostructures. Therefore, we update a theoretical model that describes the effects of nanostructures and their interfaces. Furthermore, there is currently no fundamental theory for dynamically disordered solid systems. Therefore, we build a theoretical model by capturing its characteristics through state-of-the-art measurements and molecular simulations. Based on the theory obtained, we design and demonstrate an optimized disordered nanostructure that ultimately reduces thermal conductivity.

In the field of thermal science of solids, there has been progress in understanding and controlling materials with complex structures, from crystals to amorphous materials, and even ionic conductors in which ions diffuse inside the solid. On the other hand, in fluid dynamics, the miniaturization of channels has been progressing, and recently, angstrom channels with two-dimensional heterostructures have been realized and found to give rise to unique confinement properties. Since the flow in angstrom channels is on the same scale as that of phonons, we believe that a synergistic effect can be achieved by placing the channels in a solid. In other words, this research will create a "new fusion area“, where thermal science of solids, which has developed from crystalline systems to disordered systems, and fluid mechanics of liquids, which has deveoped by flow channel miniaturization, meet.

Homepage Address, etc.	http://www.phonon.t.u-tokyo.ac.jp/?lang=en