Report of MERIT Long-Term Dispatch

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Overview

I stayed and studied at the group of Dr. Natalio Mingo, CEA (Commissariat à l'énergie atomique et aux énergies alternatives) Grenoble, Isère, France. The report of this stay including the conducted research and my life is described below.

Background

Dr. Natalio Mingo's group is leading the field of theory and calculation of thermal properties for energy materials such as thermoelectrics and developing ShengBTE and its successor almaBTE packages, which solve the space- and time-dependent Boltzmann transport equation of phonons, using only ab-initio calculated quantities as inputs. I had not met each other, but we had contact regarding a certain material that out group had synthesized and they had calculated. This experience brought me to contact Dr. Mingo and he kindly accepted my stay.

Research

My main purpose of this stay was to learn theory and computational protocol of anharmonic vibrational properties such as lattice thermal conductivity, to unravel the origin of peculiar phonon conduction in some promising thermoelectric materials we are experimentally focusing on, and to obtain some design guidelines toward further high-performance thermoelectrics.

At the beginning, I discussed the computational feasibility and overview protocol regarding our target materials with Dr. Mingo and Dr. Ankita Katre, and decided to begin with a layered chalcogenide which is not so time-consuming, and then move on to more complex materials and defect-containing structures. Dr. Katre kindly taught me how to install the prerequisite software and how to use them. The results of calculations for each materials during the stay are described below.

Layered telluride In_2Te_5 is a novel promising thermoelectric material due to high valence band degeneracy and extremely low lattice thermal conductivity below 0.5 W / m K at high temperature. Our calculation revealed strong anisotropy of lattice thermal conductivity of this layered material: lattice thermal conductivity is 6-fold lower for van der Waals interlayer direction than for *a*-axis direction in which Te-plane is formed.

$CuTaS_3$ has quasi-one dimensional crystal structure in which CuS_4-tetrahedra and TaS_6-octahedra form infinite chains along *b*-axis and large open tunnel. Polycrystalline samples exhibit relatively low lattice thermal conductivity around 1 W / m K. Our calculations showed that $CuTaS_3$ has strongly

anisotropic phonon dispersion: the slope of optical modes along Γ-Y direction is surprisingly steep, which indicates not only acoustic modes but also optical modes have high group velocity. The lattice thermal conductivity is strongly anisotropic due to the anisotropy of phonon group velocity. In addition, comparison between open tunnel $CuTaS_3$ and some Zintl phases with tunnel structure which is intrinsically filled with alkaline or alkaline earth cation suggests that filling forth element into tunnel of $CuTaS_3$ can reduce group velocity and lattice thermal conductivity along tunnel direction.

Life during the stay

Grenoble in Auvergne-Rhône-Alpes is a beautiful city surrounded by French Alps and Rhône river. We can enjoy many hiking course and some important cultural properties such as “La Basille de Grenoble”. Many researchers visit to this city because it has MINATEC, the largest campus in Europe which is consists of some institutes, as well as synchrotron and neutron facilities. Grenoble and Tsukuba-shi have been sister city since 2013, which gives some researchers in Tsukuba opportunities to visit to Grenoble.

Working time in CEA is so-called “European style”. In Dr. Mingo’s group, everyone comes to office by 9 a.m. and they begin to leave around 5 p.m. What was most surprising to me was they basically don’t have and routine meetings with handouts or presentations. Instead, they have scrum meetings every morning around 10 a.m., in which all the members gather and give a very short (shorter than 1 minute!) speech regarding what they did yesterday and what they will do today. These meetings ended within 15 minutes including discussion. Despite these short meetings, Dr. Mingo grasped the progress of whole group and gave sufficient and adequate suggestions to us. He seems to consider so that all the members don’t waste their time and we can focus on research itself by reducing the amount of documentation and any other extra output. I was impressed by this style because lots of Japanese researchers are required to waste their time by miscellaneous duties.

Acknowledgements

I would like to express my gratitude to all the people who kindly took care of me during the stay. Especially, I appreciate Dr. Natalio Mingo for accepting my stay, giving me a lot of tender supports regarding my daily life as well as study in CEA. I also thank all the member including Dr. Ankita Katre for supporting the operation of cluster machines that I was not familiar with. Finally, I would like to say special thanks to MERIT program, my advisor Prof. Kaoru Kimura and my assistant advisor Prof. Yuichi Ikuhara for letting me have this great opportunity and supporting this dispatch.