（別紙様式５）

変革を駆動する先端物理・数学プログラム（FoPM）

国外連携機関長期研修　報告書

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Activity during stay

I worked on molecular simulation research on dislocations in quartz under the supervision of Professors Patrick Cordier and Philippe Carrez at the University of Lille. I primarily engaged in discussions on Earth sciences with Professor Cordier, while Professor Carrez provided guidance on simulation techniques. I had a desk in the same room as other doctoral students and postdocs, allowing me to conduct my research alongside them in the same space. Also, I lived in campus housing, which was located in the same building as that of regular students.

Research topics

Quartz is one of the major constituent minerals of the Earth's crust. Its plastic deformation is of particular importance considering crustal deformation processes. Furthermore, quartz exhibits unique properties of interest in materials science, such as significant weakening with the addition of small amounts of water, and transition of the active slip systems with temperature increase. One of the fundamental processes of plastic deformation is dislocation motion. Dislocations are lines of atomic-level misalignment within a crystal. Thus, atomistic simulations are an effective tool for investigating their properties. I am conducting research using atomistic simulations to investigate the structure, energy, and mobility of dislocations in quartz, with the aim of elucidating the causes of the unique characteristics of quartz's plastic deformation.

During my time in Lille, I focused my research on screw dislocations along the a-axis among the various types of dislocations. This type of dislocation is an ideal subject for the first part of research, since it is involved in deformation in the slip system active even at relatively low temperatures, and it is technically simpler to simulate than other types of dislocations.

I also received guidance on simulation techniques. I learned how to use Atomsk, a software package for preparing and analyzing atomic configurations developed by the group at the University of Lille, as well as how to design simulation setups to obtain accurate results.



Figure 1. A quartz specimen densely containing screw dislocations with the same direction. The accumulation of dislocation-induced displacement has resulted in a visible twist. Owned by Professor Cordier.

Research outcomes

First, we selected the interatomic potentials, which define interactions in atomic simulations. We calculated the generalized stacking fault energy using three types of potentials, the BKS potential traditionally used for silica systems, the ReaxFF potential specialized for chemical reactions, and the ACE potential developed using the latest machine learning techniques (Erhard et al., 2024), and compared the results. A generalized stacking fault is created by dividing a crystal along a specific plane (in this case, a plane containing a-axis dislocations) and introducing a displacement on one side of the boundary. The ability to accurately calculate its energy is considered crucial for accurately reproducing the dislocation core structure. The results showed that the BKS potential and the ACE potential yielded similar results, while the ReaxFF potential produced spurious jumps. Considering other factors such as the stability of structural optimization, it was determined that the ACE potential should be adopted.

Using this potential, we investigated the stable structures of screw dislocations along the a-axis. While the predictions from previous studies (Baeta & Ashbee, 1969, Heggie & Nylen, 1984) matched with dislocations in some of the stable positions, we found that structures in other positions did not conform to the predictions.

Furthermore, we performed simulations of dislocation motion using the Nudged Elastic Band (NEB) method. This method involves specifying the structures before and after a reaction and searching for the energetically optimal path connecting the two. In this study, we investigated dislocation motion by inputting crystals containing screw dislocations at different positions as the pre- and post-reaction structures. As a result, we were able to determine changes in the width of the dislocation during the migration process and the magnitude of the energy barrier required for migration.

Finally, we proceeded to calculate the stress required to move a dislocation (Peierls stress). There are two methods available: one that utilizes the calculation results from the NEB method, and another that derives the stress from independent simulations. The former calculates the Peierls stress by differentiating the energy with respect to the dislocation position determined from the atomic arrangement along the reaction path obtained by the NEB method. The latter method involves subjecting a system containing dislocations to shear deformation to move the dislocations, and defines the Piers stress as the stress acting on the system at the moment of movement. We found that both methods present difficulties specific to quartz. Though we were unable to obtain definitive values, we decided to continue working on this after returning to Japan.