MERIT Internship Report

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MERIT 6th
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○Period

November 25, 2019 - December 26, 2019

○Destination

Department of Fundamental Technology Research, Research Institute for Advanced Materials and Devices, KYOCERA Corporation

○Theme

Research on combinatorial optimization using quantum annealing

○Research contents

I worked on the application of combinatorial optimization using quantum annealing on the D-Wave machine to the crystal structure prediction. To reduce the problem to the Ising model that can be solved using quantum annealing, I decided to optimize the crystal structure whose atomic species are represented as {0, 1}. Specifically, I considered the problem of replacing Ag atoms with Cu atoms up to 25% in the Ag-Cu substitutional alloy. Since there is only one pattern of replacement due to the symmetry in the conventional cell, the $2\times2\times2$ supercell was taken. In order to evaluate the crystal stability, I used the EAM model potential of the Ag-Cu system. Assuming that the coefficient Qij of the Ising model is unknown, Qij is estimated using Bayesian optimization from the training set of the combination and the corresponding energy.

In the case where each atom is fixed in the symmetrical position after replacements, the

two-body model potential can be accurately represented in the Ising model. Although the coefficient Q_{ij} has 528 parameters, it could be optimized with a small number of samples less than 110. This is probably because the correct Q_{ij} has high symmetry.

The Ising model cannot accurately represent the energy after local optimization since the crystal symmetry breaks down. Because of the lack of the symmetry in the correct Q_{ij}, the fitting of the Q_{ij} with a small number of samples was failed. Therefore, assuming that the Q_{ij} does not change significantly during the local optimization, I reduced the fitting parameters by imposing the same symmetry on the Q_{ij} as the crystal. Then, it turned out that the energy can be predicted to some extent with the symmetric Q_{ij}. As long as the Q_{ij} is good to some extent, the candidate of the most stable structure can be searched efficiently.

○Impression

I think it was good that I obtained those non-trivial results in the limited period of one month and will be able to write a paper. The experience in the different environment like a company was a good opportunity to take a distance from my research at the university and to reflect on my future and research itself.

○Acknowledgement

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