MERIT Internship (Domestic)

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8th generation student of MERIT course
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Period

September 23rd, 2020 - October 30th, 2020

Place

Amagasaki Research and Development Center, Nippon Steel Corporation

Theme

Magnetism and state of impurities in fcc Fe

Research Activities

Paramagnetic fcc structure becomes thermodynamically stable in Fe at temperatures between 911 and 1392 °C, while it exhibits ferromagnetic bcc structure at room temperature. There are many papers which reported the state of impurities in bcc Fe, but few studies have been done for fcc Fe. One of the difficulties in calculation of fcc Fe is that the magnetic moment at each Fe is randomly directed, and this randomness is hard to treat in DFT calculations.

Recently, DFT calculations for impurities in fcc Fe were reported, which combined Special Quasirandom Structure (SQS) and Magnetic Sampling Method (MSM) to calculate the solution enthalpy. However, the reported method shows high computational cost. In the present study, we calculated solution energy of substitutional impurity V in fcc Fe using a $2\times2\times2$ supercell ($Fe_{31}V_1$), while the previous study used a $3\times3\times3$ supercell ($Fe_{107}V_1$). We revealed that, when we used good quality SQS of the

$2 \times 2 \times 2$ supercell, solution energy and magnetic structure of $Fe_{31}V_1$ were almost the same as those obtained with $Fe_{107}V_1$. By using this SQS, the computational cost was reduced to about 1/10 of the previous study with little deterioration in the quality of the calculation results.

Impressions

I was not very familiar with iron, so I studied it from the ground up and did research. However, I achieved more than I expected by deepening the research through frequent discussions with the researchers in Nippon Steel Corporation. I feel that I have demonstrated my expertise in physics in this internship. It will be a valuable experience for my career to work on the basic research at the company.

Acknowledgments

I would like to thank Nippon Steel Corporation for accepting us for this internship despite the difficulties of COVID-19. In particular, I would like to express my sincere thanks to Dr. Hideaki Sawada and Dr. Kazuma Ito for their help for my research. I would also like to thank Ms. Kazumi Arima from CCMS, ISSP, for helping me on the office work and coordination of this internship. I also sincerely thank my supervisor Prof. Hiroshi Okamoto and secondary supervisor Prof. Kyoko Ishizaka for their promise of this internship. Finally, I would like to thank MP-CoMS for matching me with Nippon Steel Corporation, and the MERIT program for providing me with the valuable opportunity.