

MERIT internship (domestic) report

Department of Physics

MERIT 12-th

Yuuki Kubo

1. Internship overview

Duration

2024/10/1-2024/10/31

Hosting company

Simulation Technology Development Department, Tokyo Electron Technology Solutions Ltd.

2. Implementation overview

This internship was conducted in person at the Hosaka Office of Tokyo Electron Technology Solutions Ltd. in Nirasaki City, Yamanashi Prefecture. In the internship meetings, we discussed strategies for applying my graduate research on data assimilation structural determination methods to long-standing issues at the host company. The internship lasted approximately eight hours each day. At the end of the internship period, I gave a final presentation to the Simulation Technology Development Department members and my academic supervisor. Additionally, I was allowed to observe semiconductor manufacturing equipment developed by TEL and equipment currently under development.

3. Research

3.1. Background

One of the long-standing technological development items at the host company is amorphous films. Most of the thin films deposited during semiconductor manufacturing processes have an amorphous structure, and predicting the quality of these films is a critical technology for process and equipment development. However, a fully established method for structural modeling at the atomic scale has yet to be developed. Therefore, during this internship, I investigated whether it would be possible to improve existing structural modeling methods using the data assimilation approach that I have been developing as part of my graduate research.

3.2. Method and Result

In infrared spectroscopy, atomic-scale structural information of materials can be obtained from their unique vibrational characteristics. During this internship, I explored the potential of data-assimilated structural modeling using IR spectra as experimental data. First, melt-quench simulations using *ab initio* molecular dynamics prepared multiple amorphous model structures. The IR spectra of each structure were then evaluated. Due to computational constraints, the time evolution of the dipole moment was tracked using *ab initio* molecular dynamics, and the IR spectra were obtained by performing a Fourier transform of the autocorrelation function of the dipole moment. The calculated spectra showed good agreement with the experimental data overall, although slight differences in the reproducibility of certain peaks were observed among the models. Since these models had no significant energy differences, combining these methods with data assimilation could lead to more plausible model structures.

4. Impression

During this internship, I worked on modeling amorphous structures and calculating the IR spectra of the resulting structures. While I encountered several challenges early on due to my unfamiliarity with some of the calculations, the extensive support from the Simulation Technology Development Department members enabled me to progress faster than initially expected and gain valuable insights. In addition to atomic simulations, I had the opportunity to interact with researchers working on plasma simulations, an area that I had little exposure to before. I also gained a broad understanding of semiconductor manufacturing processes, making this a highly fulfilling internship experience. Furthermore, I was given a chance to observe equipment under development and participate in discussions with individuals who offered perspectives different from those in academia. These experiences allowed me to gain firsthand experience in research and development in a corporate setting.

5. Acknowledgments

I would like to express my gratitude to the Tokyo Electron Technology Solutions Ltd. members for allowing me to undertake this internship. I am deeply thankful to Dr. Masaaki Matsukuma, Director of the Simulation Technology Development Department, who personally guided me throughout the internship, and to Ms. Yuki Hosaka from the Human Resources Department, who provided extensive support with various aspects of daily life. I also sincerely thank all the other Simulation Technology Development Department members for their generous assistance. Additionally, I am grateful to my academic supervisor, Prof. Shinji Tsuneyuki, and my co-supervisor, Prof. Shin-ichi Ohkoshi, for approving my participation in this internship. Finally, I would like to thank the MERIT Program for offering me this wonderful opportunity.