Evaluation of etching rates for reactive ion etching (RIE) and atomic-layer etching (ALE): beam experiments, atomic-scale simulation, and machine learning

Satoshi Hamaguchi[1], Kazuhiro Karahashi[1], Tomoko Ito[1], Kazumasa Ikuse[1], Shunya Tanaka[1], Yudai Kotani[1], Hojun Kang[1], Nicolas A. Mauchamp[1], Erin Joy Capdos Tinacba[1], Hiori Kino[2], Nathaniel Saura[3], Sadruddin Benkadda[3]

[1]*Graduate School of Engineering, Osaka University, Osaka, Japan*
[2]*NIMS, Tsukuba, Ibaraki, Japan*
[3]*CNRS PIIM Laboratory UMR 7345, Aix-Marseille Université,Marseille, France*

Abstract: Etching rates of various materials under specific plasma processing conditions are some of the most fundamental data for advanced manufacturing processes of semiconductor devices. Discussion is presented on how such data can be obtained systematically from well-controlled beam experiments, atomic-scale simulations such as molecular dynamics simulations and quantum-mechanical simulations, and machine learning techniques.

1. Introduction

Efficient development of manufacturing processes for advanced semiconductor devices requires fundamental data of materials and processes. For example, the prediction of process parameters, such as etching rates for unconventional materials in unexplored processes, may be achieved qualitatively with good knowledge of similar materials and processes[1]. However, for a more quantitative and reliable prediction, high-performance computation of physics-based models of the system and a large amount of fundamental data on materials and processes supporting such simulations are needed. The goal of this study is to establish a systematic method to collect fundamental and reliable data on etching properties based on well-controlled experiments and atomic-scale numerical simulations, such as molecular dynamics (MD) simulations and density-functional-theory (DFT) simulation, and machine learning (ML) techniques.

2. Discussion

Mono-energetic mass-selected ion beams have been used to determine the etching rates/sputtering yields of various materials by various ion species as functions of the ion incident energy[2]. Although actual reactive plasmas are far more complex, such ion beam data serve as essential building blocks for a better understanding of plasma-surface interactions. Atomic-scale simulations can also reproduce the same beam-etching processes *in silico*, giving further insights into the underlying physical and chemical mechanisms. However, the development of the interatomic potential (force-fields) for atomic-scale simulations for such simulations is not a trivial task as they depend on simplified but still complex modeling of electron orbital structures of the system. In addition to classical treatments of such models for modern etching systems[3], efficient ML-based techniques to develop such models[4] (Fig.1), together with their possible limitations, will be discussed in this study.

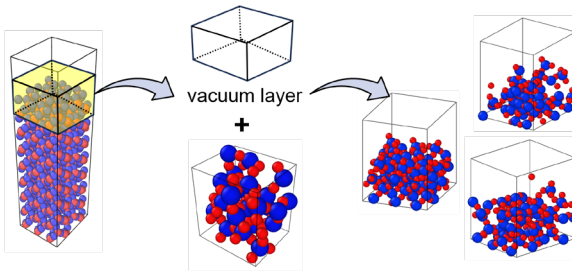

Fig. 1. Schematic diagram of active learning to obtain atomic configurations for additional ML data: (from left to right) Select a snapshot of MD simulation based on the current ML model when the surface becomes sufficiently rough, select a surface structure, repeat this process many times during the MD simulation to collect a large number of atomic structures. These collected structures are used for DFT calculations to supply more data for the ML process.

Acknowledgments

This work was partially supported by the JSPS Grant-in-Aid for Scientific Research (A) 21H04453 and the JST's ASPIRE" Grant Number JPMJAP2321.

References

[1] G.S. Oehrlein, et al., J. Vac. Sci. Tech. B, 42, 041501 (2024).
[2] K. Karahashi and S. Hamaguchi, J. Phys. D: Appl. Phys. 47, 22 224008 (2014).
[3]H. Kang, et al., Proc. International Sym. Dry Process 2024, p. 195.
[4] S. Tanaka, et al., AVS 70th International Sym. Exhib. (2024) PS1-WeA-2.