Evaluation of Nickel Self-Sputtering Yields by Molecular Dynamics Simulation

Mauchamp Nicolas, Michiro Isobe, Hamaguchi Satoshi
Center for Atomic and Molecular Technologies, Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka 562-0871, Japan
E-mail: mauchamp@ppl.eng.osaka-u.ac.jp

In the manufacturing process of magnetic random access memories (MRAMs), stacks of thin layers of magnetic materials and insulators are deposited and etched to form magnetic tunnel junction (MTJ) cells. Typically, ion milling with energetic Ar+ ions are used to produce such MTJ cells in the etching processes. However, for further miniaturisation of MTJ cells and increase of MRAM integration, less damaging and more selective etching processes for magnetic materials and insulators are needed. The ultimate goal of this study is to establish reactive ion etching (RIE) processes for MTJ cells and we approach this goal by examining etching characteristics of magnetic materials with various reactive ions theoretically, using molecular dynamics (MD) simulations and first-principle quantum mechanical (QM) simulations. In this study, we focus on nickel (Ni) as a sample magnetic material and evaluate its self-sputtering yields over a wide range of the ion incident energy and incident angle, using MD simulation. The goal of this study is to clarify how the evaluated sputtering yield depends on the inter-atomic potential model used in the MD simulation. The self-sputtering yield is the simplest example of a sputtering yield as it depends only on the interaction among the single atomic species (i.e., Ni in this study).

There have been many earlier studies on classical MD simulations of Ni. However, it has been found that most interatomic potential models that were used for such studies cannot reproduce the self-sputtering yields of Ni that agree with those obtained from ion beam experiments, especially at high ion incident energies. Since the Ni self-sputtering yield at a high ion incident energy sensitively depends on the short-range repulsive atomic interaction, we have determined the short-range interatomic functions based on experimentally observed Ni self-sputtering yields. It has been found that the newly obtained interatomic potential model for Ni, which is based on the embedded atom model (EAM), can reproduce experimentally obtained Ni self-sputtering yields over a wide range of the ion incident energy with high accuracy. Using the newly created interatomic potential model, we have also determined the dependence of the Ni self-sputtering yield on the ion incident angle.