The early stage of deposition process at surface and interface for magnetic multilayer systems: Molecular dynamics simulation

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Magnetic Random Access Memory (MRAM), thin film multilayers of ferromagnetic (Co or CoFe) / insulator(Al_2O_3) / ferromagnetic (Co or CoFe), is the device for reading and storing data by controling its spin dependent tunneling. Spin tunneling can only be observed in the 1-2 nm thick insulating thin film. The performance of the junction largely depends on the uniformity, orderness of the film and the atomic structure of the interface between the films[1]. Understanding the deposition behavior in the atomic scale is thus crucial to improve the performance of the MRAM devices.

In this study, the deposition behavior for magnetic multilayer systems according to various deposition conditions was investigated by molecular dynamics simulation which is known to be capable of simulating the accurate atomic nature of interface characteristics of nanometer-scale multilayer thin film. In the early stage of deposition process, in spite of the low adatom incident energy of 0.1 eV, transition metals(TM; Fe, Co, Ni)-Al intermixing occurred actively at the surfaces of Al(001) at room temperature. Interestingly, we observed the ~ 4 eV of local acceleration of TM atom at the very moment of interaction between TM and Al atoms. The local acceleration was always the same order of magnitude irrespective of the initial kinetic energy and incident atomic positions. At the interface region of TM/Al(001), an intermetallic compound was formed and found to be of B2 structure at 300 K. This result showed that the formation of thermodynamically stable phase can occur in the atomic scale even at the moderate temperature. Moreover, the Co/Al system showed different layer coverage and pair correlation function characteristics, in comparison with Fe/Al and Ni/Al systems. It was found that substrate temperature is the key parameters for determining the interface structure. The structural characteristics of Al and Ni thin film growth on Ni(111) substrate according to the incident energy of adatoms were investigated. In case of Al on Ni(111), Al adatoms were grown basically through the layer-by-layer growth mode. On the other hand, Ni thin films on Ni(111) surface at low incident energy were shown to favor island growth. The steering effect due to atomic attraction, which results in rougher surface, was significantly observed at low incident energy. The growth mode of Ni film was, however, changed to follow layer-by-layer growth mode for the incident energy of 6 eV. The different aspects of surface morphology between Al and Ni deposition on Ni(111) surface could be successfully explained by the surface diffusion and impact cascade diffusion.

Reference

[1] J. M. D. Teresa, A. Barthelemy, A. Fert, et al., Science **286**, 507 (1999)