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Atomic investigation of Ti/Al(001) interface by molecular dynamics simulation

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The morphology of interface in metallic multilayers plays critical role in determining the device characteristics for magnetic storage systems. Various schemes for improving the growth of sharp interface have been suggested to control the surface or interface energy of the growing film. Ti interlayers in Fe/Al systems, which are used for magnetic tunnel junctions, increased the stability of interface between Fe and Al thin-films by blocking Fe diffusion into Al substrate. However, it is required to study the mixing behavior of Ti atoms during the deposition process on Al substrate. In this paper, interface mixing behavior of the Ti atoms on Al(001) surface at room temperature has been investigated by using molecular dynamics simulation.

The size of Al(001) substrate was (8×8×6) a_0 with the surface perpendicular to the z-axis, where a_0 is the bulk lattice constant of Al. The periodic boundary conditions were applied in both x and y directions and the position of the bottommost two layers were fixed. The temperature of other layers was isothermally maintained at 300K. The incident energy of adatoms was set to 0.1eV. The adatom was added at a distance of 20Å from the substrate surface. The positions of the adatoms were randomly selected in the x, y-plane and the incident angles were normal to the surface. The time step was set to 1fs.

When Ti atoms were deposited on Al(001), surface-confined intermixing was observed at the interface of Ti/Al(001). This intermixing phenomenon of Ti/Al(001) system was found to be different from other well-intermixing transition metal(TM)/Al system. Only first layer of the Al substrate was penetrated by Ti adatoms whereas none of the Ti adatoms were found at the second layer of the substrate.

The origin of surface-confined mixing phenomenon of Ti/Al(001) system could be explained by the locally accelerated energy of adatom. The local acceleration of Ti adatoms on the clean Al(001) surface was calculated. For more quantitative analysis, the energy barrier during incorporation of the Ti adatoms into Al substrate was also calculated.