

Molecular dynamics simulations on the direct sputtering of Al_2O_3 insulating film in a magnetic tunneling junction

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Abstract

The molecular dynamics (MD) simulation is used to study the direct deposition of aluminum-oxide (Al_2O_3) to grow an insulating thin film on cobalt substrate in a magnetic tunneling junction (MTJ). The direct deposition of Al_2O_3 may produce a very thin film with very smooth surface and form an averagely oxidized insulator. A high magnetoresistance ratio is desired in an MTJ device, so that smooth surface and good structural integrity for the insulating thin film is anticipated. The MD simulation is an effective way in determining optimal processing parameters that can be used to fabricate high-quality MTJ devices. The Buckingham and many-body tight-binding potentials are applied in the MD simulations for different interactions between particles. The effects of the cluster size and the incident energy on the thin film's surface morphology and Al_2O_3 purity are investigated. Some optimal parameters that could be used as the reference for practical processing purposes are derived.

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1. Introduction

Although the tunneling phenomenon between ferromagnetic (FM) films was discovered by Julliere [1] nearly three decades ago, the researches of the magnetoresistance (MR) effect on the magnetic tunneling junctions (MTJs) were not flourished until late 1990s (e.g. see Refs. [2–4] and

references therein). An MTJ basically consists of two layers of FM material separated by an insulating thin oxide film that is acting as a tunnel barrier, much like a sandwiched structure [2]. The spin electrons “tunnel” through the insulator, forming the current flowing perpendicularly to the layers. The resistance of an MTJ is smallest when two FM layers are parallel and largest when antiparallel [5]. This phenomenon, also referred as tunneling magnetic resistance (TMR) [6], corresponds to the binary states of 0 and 1, which are the basis for data storage. Owing to this characteristic, the MTJ is a promising technology for

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the magnetic random access memory (MRAM), which could possibly replace current static and dynamic random access memory (SRAM and DRAM) as the mainstream RAM applications [7], because of the MRAM technology's non-volatility, higher memory array density than that for DRAM, and faster data access speed than that in SRAM [4].

The typical material used for the tunnel barrier is Al-oxide (AlO_x) [6,8–10]. Ferrous metals, such as Fe, Co, or Ni, are generally used for the FM films, although other alloys, such as CoFe and permalloy, have been used as well [2,3]. The tunnel resistance depends not only on the surface roughness of the interface between FM and insulating layers, but also the micro-structural characteristics of the thin Al-oxide film. As Ando et al. [11] indicated, the corresponding tunnel resistance was very small for the junction with the rough interface. The magnetic properties of those layers are also related to the structural characteristics of the interface [12]. Since a high MR ratio is desired in a tunneling magnetoresistive device, it implies that smooth surface and good structural integrity are anticipated to exist on a thin Al-oxide film that is acting as the insulating layer. From the manufacturing point of view, therefore, how to achieve such qualities during fabrication processes becomes a key engineering objective.

The magnetron sputtering is widely used to fabricate MTJs on glass substrates or Si wafers (e.g. see Refs. [3,6,13]). While most tunneling barriers are processed by the technique that the Al film is first deposited followed by oxidation, it is important that the Al layer, but not the FM layer underneath, is oxidized entirely in the process. Zhu et al. [14] have investigated the oxidation depth of Al-oxide films in MTJs using Fourier transform infrared spectroscopy. They measured the plasma oxidation depth in a wedged Al thin film and estimated it to be 1.3 nm. They also found the oxide/aluminum interface abrupt and indicated that the thickness of the oxide layer increases slowly with exposure to oxygen. Thus a tunnel barrier may not be oxidized fully and uniformly beyond 1.3 nm. The technology of depositing Al followed by oxidation, however, is typically able to fabricate the Al_2O_3 layer in the range of 1–5 nm of

thickness. This technique can be further categorized into two kinds, depending upon the method of oxidation. One is the natural oxidation in which the deposited Al layer is oxidized in air at room temperature for 24–48 h [15,16], the other is plasma oxidation where the tunneling barrier is formed in oxygen plasma for several seconds to minutes [3,8]. A thickness of 1–5 nm of the Al_2O_3 layer can be formed by both methods. The insulating layer can be also generated by directly depositing Al_2O_3 film using Al_2O_3 ceramic target. This technique has been applied on the fabrications of double tunnel junctions for MRAM devices [13,17], tunnel giant magnetoresistance [18], and organic thin film transistors [19], although less observed for conventional FM/insulating/FM MTJs. Depending on the final applications, this method may yield a very thin Al_2O_3 film, e.g. 0.75 nm as obtained by Tanoue and Yamasaki [13], and a very smooth surface such as the results from Ha et al. [19].

Given the facts that the oxidation depth, surface smoothness, and micro-structural integrity of the insulating film are correlated and will significantly affect the MR ratio, which in turn determines the overall performance of an MTJ device, we believe the direct deposition of Al_2O_3 can yield fully and uniformly oxidized Al films with a desired thickness, as many MTJs have the thickness of the tunnel barrier greater than 1 nm. Therefore, in this study we use molecular dynamics (MD) simulations to examine the micro-structural characteristics of the insulator/FM interface formed by Al_2O_3 direct deposition.

The MD simulation is an effective way to study micro-scale molecular interactions. In this research the MD method is used to simulate the thin Al_2O_3 film growth in the ionized cluster beam deposition (ICBD) process. The ICBD process is one of the methods used by semiconductor and microelectronics industries to grow thin solid films. Generally the ICBD process starts by evaporating materials in a specially designed crucible. The molecular clusters may be formed through adiabatic expansion or by mixing with some reactive gases. These clusters then are bombarded at the ionization electrode by electron beams from an electron gun. The ionized clusters are accelerated

toward the substrate by an electric field. Thin films are formed upon the impact of the ionized clusters and the substrate [20–22]. The ICBF process can produce thin films with high packing density, good adhesion, and low surface roughness [23].

We use the MD simulation to investigate part of the ICBF process in which Al_2O_3 target is sputtered, causing Al_2O_3 clusters deposited onto Co ferromagnetic substrate and thus forming the thin oxide film. We assume an ideal case of simulation in which the Al_2O_3 target and the Co substrate both have 100% purity and in a system with a constant temperature of 300 K. The variations of the surface roughness and the structural purity of the thin oxide film will be examined through the change of the incident energy and the size of the Al_2O_3 clusters, hence determining some of the optimal processing parameters.

2. Physical model

Fig. 1 shows the MD simulation model where the Al_2O_3 clusters are deposited onto a Co substrate. The substrate is formed by six layers of Co atoms in the hexagonal close-packed crystal structure, with the dimensions of $29a \times 25b \times 12.5c \text{ \AA}$ where a , b , and c represents the lattice distance for Co in X , Y , and Z direction and

corresponds to $\sqrt{6}/2$, $\sqrt{2}$, and $\sqrt{3}/3$, respectively. Without loss of generality, the dimensions are set to be equivalent to $3.55 \times 3.54 \times 0.72 \text{ nm}$, which is nearly a square in the X – Y plane. Periodic boundary conditions are specified along the boundary of this square. Those Co layers are further designated into three categories for different functions in simulation. The first layer at bottom is a fixed layer that supports all other particles in the system. The second and third layers are thermal control layers that maintain the system's steady temperature, which is set at 300 K. The fourth through sixth layers are free motion layers that simulate the interactions and motions of particles after the impacts of incident clusters. The temperature of the free motion layers is calculated according to the heat transfer from thermal control layers.

An Al_2O_3 molecule is generated by perfectly aligning Al and O atoms in the (100) direction. Fig. 2 depicts the molecular structure of Al_2O_3 , from which a cluster can be formed. The cluster size can be changed in different simulations depending on the number of the Al_2O_3 molecules in a cluster. Clusters are set to be vertically striking into the Co layers, after both of which reach an equilibrium state of energy, i.e. 300 K. After the impact but before the energy is in equilibrium, the next impact of cluster on substrate should be withheld. Otherwise the energy of the second

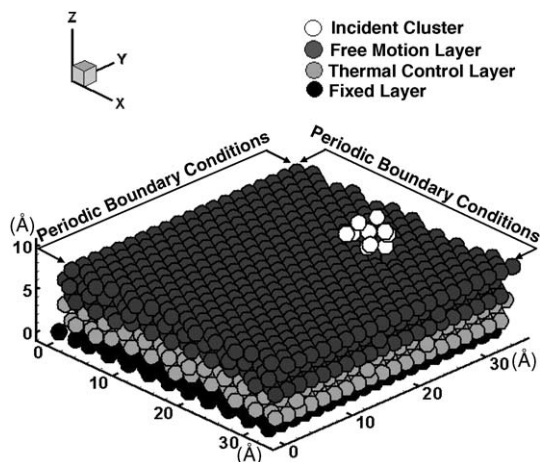


Fig. 1. Schematic drawing for the simulation model.

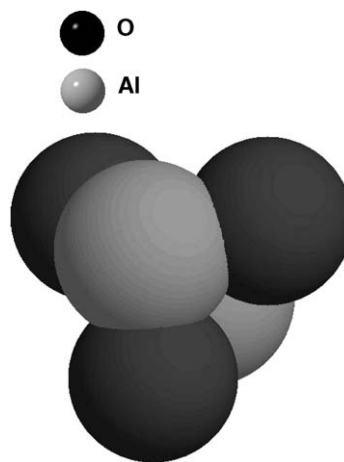


Fig. 2. Molecular structure of Al_2O_3 .

impact will be added to the first one, causing the errors magnified. Therefore, the characteristic incident frequency of 0.1 atom/ps is adopted in the simulations in order to prevent such errors from happening.

3. Molecular dynamics simulation

Molecules of Al_2O_3 are used to form the clusters in our MD simulations. The incident direction is assumed to be perpendicular to the plane of the Co substrate. The location where an incident cluster is initially placed is defined by a random distribution function [24]. The velocity of an incident cluster is calculated by the following equation:

$$V = \sqrt{2E/M}, \quad (1)$$

where E is the prescribed incident energy and M is the atomic mass of the cluster.

The Buckingham potential and many-body tight-binding potential are used in our MD simulations for different interactions between particles. The Buckingham potential $S(r_{ij})$, which represents the short-range interactions between ion pairs i and j , assumes the form [25]

$$S(r_{ij}) = A_{ij} \exp(-r_{ij}/\rho_{ij}) - C/r_{ij}^6, \quad (2)$$

where r_{ij} is the distance between atoms i and j ; A , C , and ρ are parameters determined by simultaneously fitting to the lattice parameters of a variety of oxides. Parameters used in the current simulations, namely for interactions between O^{2-} – O^{2-} , Co^{2+} – O^{2-} , and Al^{3+} – O^{2-} , are listed in Table 1.

The many-body tight-binding potential is summed by the band energy, which is resulted from the large d -band density of state, and the Born-Mayer ion–ion repulsions, hence incorporat-

ing the total cohesive energy of a system as [26,27]

$$E_i = - \left\{ \sum_j \xi^2 \exp \left[-2q \left(\frac{r_{ij}}{r_0} - 1 \right) \right] \right\}^{1/2} + \sum_j B \exp \left[-p \left(\frac{r_{ij}}{r_0} - 1 \right) \right]. \quad (3)$$

In Eq. (3) ξ denotes an effective hopping integral, and r_0 is the first-neighbors distance. B , q , and p are parameters determined by experimental data and related to the cohesive energy, the relative interatomic distance, and the compressibility of the bulk metal, respectively. The values for these parameters employed in our simulations, namely Al–Al [26], Co–Co [28], and Al–Co, are listed in Table 2. Note that the cross parameters for Al–Co are approximated by using an averaging algorithm evaluating data from those of pure elements.

As the surface roughness is usually measured from a given baseline, it is defined as the root mean square of the surface heights for clusters on the exposed layers. The surface roughness, R , can be calculated from the following equation:

$$R = \sqrt{\sum_{j=0}^n \frac{(z_j - \bar{z})^2}{n}}, \quad (4)$$

where n is the total number of the exposed clusters which are either stationary or migrating in layer j at a particular time step, z_j is the height for exposed clusters, and $\bar{z}$ is the mean height of the film surface. Note that $j = 0$ corresponding to the top surface layer. For simplicity and without loss of generality, z is a dimensionless coordinate defined by the Z coordinate—in the unit of Å—divided by unity, i.e. Z/r_1 , where $r_1 = 1$ Å.

Table 1
Parameters of Eq. (2) for short-range interatomic potential [25]

Interaction	A (eV)	ρ (Å ^{−1})	C (eV Å ^{−6})
O^{2-} – O^{2-}	9547.96	0.2912	32.0
Co^{2+} – O^{2-}	778.02	0.3301	0.0
Al^{3+} – O^{2-}	1725.20	0.28971	0.0

Table 2
Parameters for many-body tight-binding potential

Interaction	B (eV)	ξ (eV)	p	q	r_0 (Å)
Al–Al	0.1221	1.316	8.612	2.516	4.050
Co–Co	0.0950	1.488	11.604	2.286	2.502
Al–Co	0.1077	1.399	10.108	2.401	3.276

4. Results and discussions

4.1. Effects of incident energy and cluster size on surface morphology

Fig. 3 shows the distributions of the Al_2O_3 thin film surface roughness against the incident energy for various cluster sizes. There is a similar pattern observed in all three curves: the surface roughness decreases to a minimum as the incident energy increases at relatively lower levels, then a transition zone follows before the incident energy passing beyond a value referred to as the critical cluster incident energy [29] where the surface roughness starts to be irrelevant to the cluster size. Fig. 3 indicates such value to be approximately 80 eV/cluster. It also implies the incident energies at which the minimum surface roughness occurs are 45, 55, and 65 eV/cluster for $1\text{Al}_2\text{O}_3$, $2\text{Al}_2\text{O}_3$, and $4\text{Al}_2\text{O}_3$ clusters, respectively.

An incident cluster may be split into AlO_x sub-clusters or Al and O atoms upon the impact with substrate, and those kinds of particles may be also sputtered off the deposited film, depending on the magnitude of the incident energy. The scattered particles and bombardments of incident clusters will generate surface defects and, therefore, in-

crease the surface roughness. The migrating atoms or particles scattered from clusters and film surface, in contrast, tend to fill up those defects and hence reducing the surface roughness. The curves in Fig. 3 are the results of the interaction between these two factors.

The migrating ability of the atoms in Al_2O_3 clusters is enhanced when the incident energy increases [30]. In the low levels of incident energy where surface roughness decreases as the incident energy increases, the migrating ability of atoms is more influential than the incident energy itself on the deposited film's surface morphology. The incident energy, smaller than the binding energy between the particles in a cluster, is too low to break up the cluster while it is bombarded onto the substrate, as illustrated in Fig. 4. The deposited clusters are piled up on the substrate and no Al or O atoms can further migrate, hence forming the hole-like defects which in turn result in a rough surface.

As the incident energy keeps increasing, the minimum surface roughness can be reached when the effects of the incident energy and the particle migrating ability are in balance. Fig. 5 illustrates such condition where some of the surface atoms are scattered while others, including those in clusters, move to fill up defects. When the incident energy is larger than that having the minimum

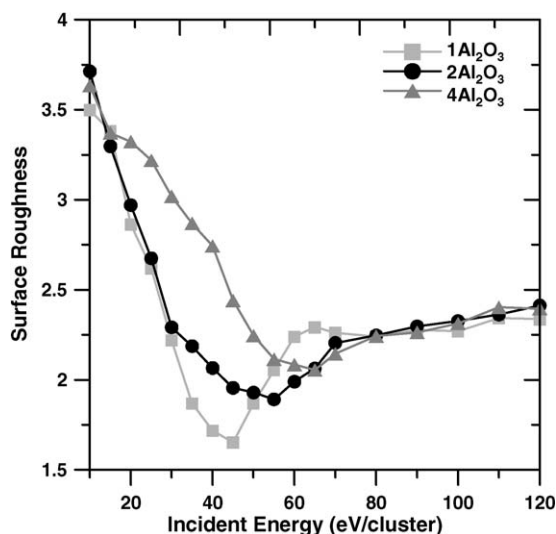


Fig. 3. Surface roughness vs. incident energy for Al_2O_3 clusters in three sizes.

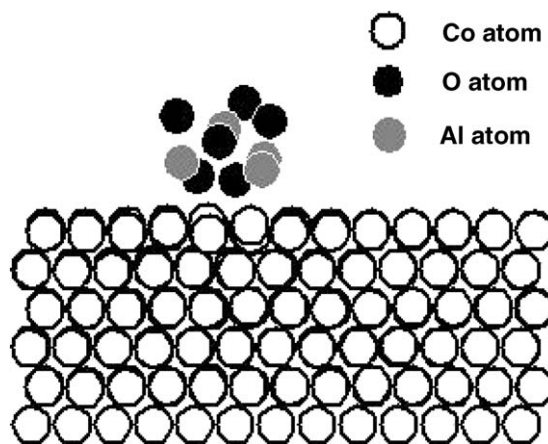


Fig. 4. Schematic side view of the substrate and a depositing cluster at low incident energy levels. Note that the atoms forming the cluster are still bound together.

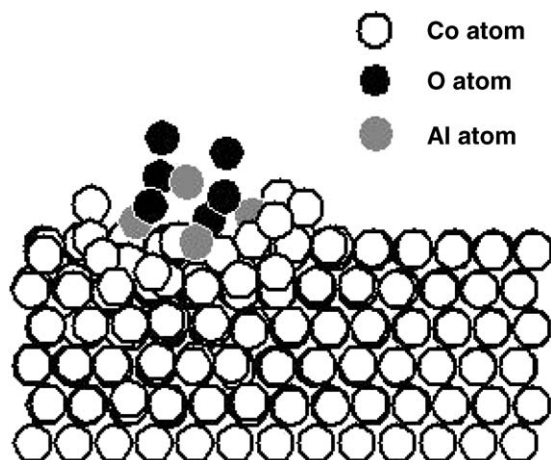


Fig. 5. Schematic side view of the substrate and a deposited cluster when a minimum surface roughness is obtained. Note that part of the cluster has been embedded into substrate.

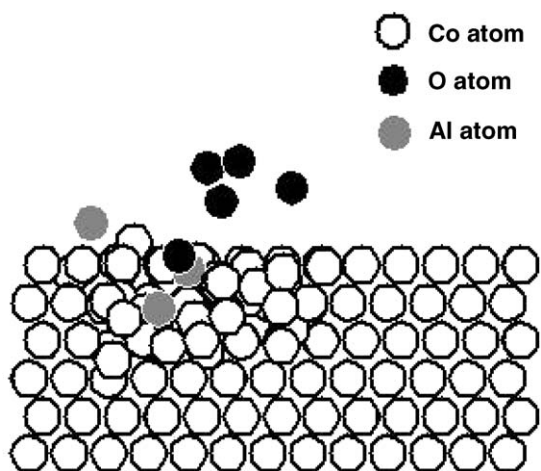


Fig. 6. Schematic side view of the substrate and a deposited cluster at high incident energy levels. Note that some of the cluster atoms are scattered.

surface roughness, the bombardments of the incident clusters are powerful enough to scatter deposited Al and O atoms from film surface (see Fig. 6). At this level of incident energy, the effect of particle migration is overcome. Thus the surface roughness increases as the incident energy increases at a relatively high level.

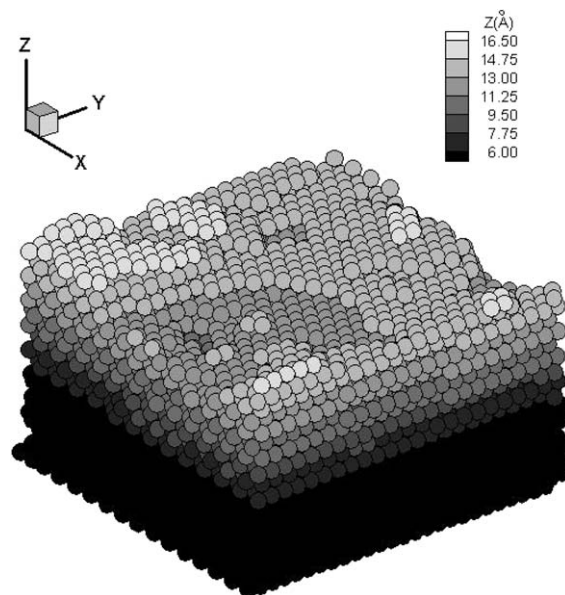


Fig. 7. Surface morphology of thin film deposited by $1\text{Al}_2\text{O}_3$ clusters with incident energy of 45 eV/cluster.

As mentioned earlier, higher incident energy will enhance the migrating ability of particles. Consequently smaller clusters require less energy to achieve the same level of the migrating ability. In addition, smaller clusters are able to break up into smaller AlO_x sub-clusters, which in turn will fill up smaller holes on the film surface, resulting in lower overall surface roughness. Fig. 7 shows the surface morphology of the thin film deposited by clusters composed of only one single Al_2O_3 molecule, at the incident energy of 45 eV/cluster that is associated with the minimum surface roughness for such clusters. In comparison to Fig. 8, which shows the best surface morphology for the $2\text{Al}_2\text{O}_3$ clusters at the incident energy of 55 eV/cluster, Fig. 7 has demonstrated an even better surface morphology. When the incident energy is higher than the critical cluster incident energy, the incident clusters, regardless of sizes, most likely will be disintegrated into AlO_x sub-clusters or Al and O atoms upon impact with substrate. Those scattered particles may migrate to fill hole-like defects on the film surface, offsetting the effect that larger clusters attribute to rougher surfaces.

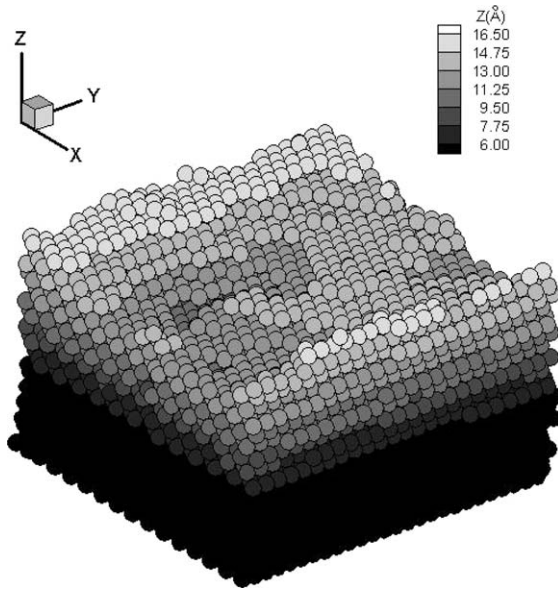


Fig. 8. Surface morphology of thin film deposited by $2\text{Al}_2\text{O}_3$ clusters with incident energy of 55 eV/cluster.

4.2. Effects of cluster size and incident energy on thin film purity

To investigate the extent of the deposited film purity, we use the Al-oxide percentage, $\text{Al}_2\text{O}_3\%$, to represent the ratio of the number of deposited Al_2O_3 molecules to the number of all incident Al_2O_3 molecules. Mathematically the Al-oxide percentage can be expressed as

$$\text{Al}_2\text{O}_3\% = \frac{D_{\text{Al}_2\text{O}_3}}{T_{\text{Al}_2\text{O}_3}} \times 100\%, \quad (5)$$

where $D_{\text{Al}_2\text{O}_3}$ is the number of molecules with complete Al_2O_3 structure (as seen in Fig. 2) in the deposited thin film, and $T_{\text{Al}_2\text{O}_3}$ is the total number of all incident Al_2O_3 molecules. The value of 100% implies the molecular structure of the thin film is formed by pure Al_2O_3 without any other AlO_x sub-clusters or single Al and O atoms.

Fig. 9 shows the Al-oxide percentage distributions for different incident cluster sizes at various incident energies. In general, the Al-oxide percentage value of a multi-molecular cluster is lower than that of a single-molecular cluster at a given incident energy. For the $1\text{Al}_2\text{O}_3$ clusters, the

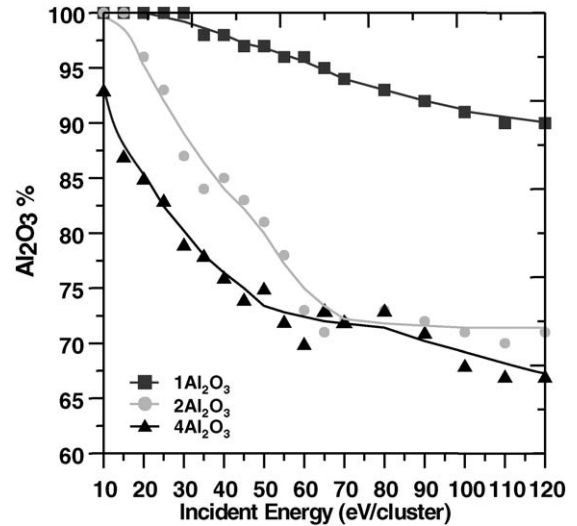


Fig. 9. $\text{Al}_2\text{O}_3\%$ vs. incident energy for different Al_2O_3 cluster sizes.

$\text{Al}_2\text{O}_3\%$ value, starting at 100% for low incident energies, remains high across various incident energies and is still about 90% at the high incident energy of 120 eV/cluster. On the other hand, the $\text{Al}_2\text{O}_3\%$ value for multi-molecular clusters reduces notably as the incident energy increases and it is only about 70% at high incident energies. The mechanisms behind those phenomena are described as follows.

For a multi-molecular cluster, there exists intracuster interactions [31] that makes the free energies of the molecules in an incident cluster larger than those of the molecules in the film surface. Fig. 10 are snapshots showing such motions for a $1\text{Al}_2\text{O}_3$ cluster and a $2\text{Al}_2\text{O}_3$ cluster, both under 30 eV/cluster of incident energy, from the initial stage of deposition, 10 ps, to the instant just after impact, 14 ps. Apparently the $2\text{Al}_2\text{O}_3$ cluster demonstrates more effectively spreading of atoms over the substrate surface upon impact. The kinematics of such observation is that most break-away atoms in the $1\text{Al}_2\text{O}_3$ clusters may be easily regrouped and form Al_2O_3 structures again, while the secondary bonding in the $2\text{Al}_2\text{O}_3$ clusters is more inclined to break and results in more dispersed sub-clusters. As a result, the AlO_x sub-clusters or Al and O atoms of the incident cluster

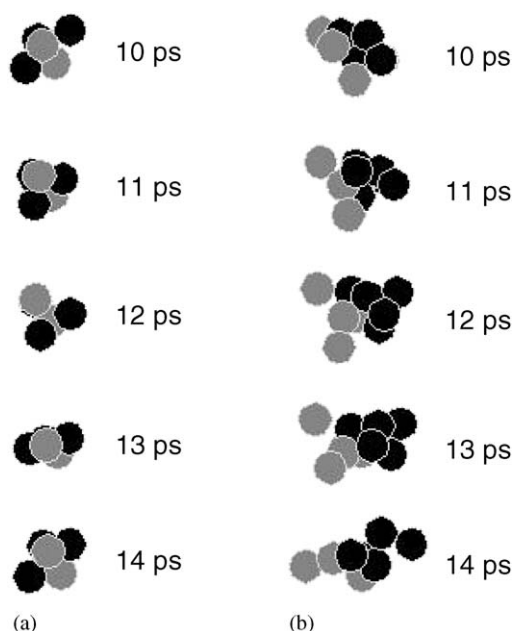


Fig. 10. Snapshots showing shape changes for a cluster, under 30 eV/cluster of incident energy, from an initial stage to the moment after impact: (a) $1\text{Al}_2\text{O}_3$; (b) $2\text{Al}_2\text{O}_3$.

tend to be scattered off the film surface when the impact of the incident cluster and the substrate occurs. A larger cluster, e.g. the $4\text{Al}_2\text{O}_3$ compared to the $2\text{Al}_2\text{O}_3$, produces more scattered particles because of its relatively large size. In addition to the particles scattered from an incident cluster, the AlO_x sub-clusters or Al and O atoms in the deposited film may be also sputtered out of the film surface. Those particles will substantially reduce the $\text{Al}_2\text{O}_3\%$ value. A larger size of cluster has a larger cross sectional area which, upon the impact, may result in more sputtered particles from the deposited film. All of those factors explain the fact that the $\text{Al}_2\text{O}_3\%$ value reduces when the cluster size becomes bigger. For the same cluster size, larger incident energy simply contributes more disintegrated and sputtered particles. Thus the $\text{Al}_2\text{O}_3\%$ value decreases in general as the incident energy increases.

For the $1\text{Al}_2\text{O}_3$ clusters, however, the effect of the internal relative motions between molecules is not as significant as in a multi-molecular cluster because there is only one single-molecular clusters

(see Fig. 10). Obviously the free energy of a single-molecular cluster is smaller than that of a multi-molecular cluster. Consequently the destruction of the single-molecular cluster's structure and the deposited film surface due to sputtering is relatively minor. The dominant factor on the thin film purity for single-molecular clusters is left to incident energy. Low levels of incident energy are not large enough to disintegrate the single-molecular clusters upon impact, hence keeping the thin film's purity while the full Al_2O_3 molecules are deposited. As the incident energy increases, incident clusters may break up into AlO_x sub-clusters or Al and O atoms when the clusters strike onto the film surface. Generally the higher the incident energy is, the more AlO_x sub-clusters or Al and O atoms may be scattered. This attributes the decline of the $\text{Al}_2\text{O}_3\%$ value for increased incident energy. Some particles may also be scattered out of the film surface upon the impact of the clusters and the film surface. Since the cross sectional area of a $1\text{Al}_2\text{O}_3$ cluster is relatively small, scattered particles are less than those from a multi-molecular cluster. Thus the $\text{Al}_2\text{O}_3\%$ value of the $1\text{Al}_2\text{O}_3$ clusters is overall higher than that of the $2\text{Al}_2\text{O}_3$ or $4\text{Al}_2\text{O}_3$ clusters.

5. Conclusions

The molecular dynamics method is employed to simulate the direct deposition of Al_2O_3 as the insulating thin film in a magnetic tunneling junction that could be used in the promising MRAM applications. The effects of the incident energy and the cluster size on the deposited thin film's surface roughness are studied. At low incident energies, the surface roughness decreases as the incident energy increases mostly because the migrating ability of the incident particles increases. At higher incident energies, however, incident clusters and film atoms may be scattered upon impact of the clusters and film surface, causing surface defects and therefore increasing surface roughness. The interaction of both factors make the surface roughness increase when the incident energy increases at relatively high levels. Thus the minimum surface roughness is obtained under the

condition that the influences of the incident energy and the particle migrating ability are in balance. Our MD simulations imply that the incident energies at which the minimum surface roughness occur are 45, 55, and 65 eV/cluster for $1\text{Al}_2\text{O}_3$, $2\text{Al}_2\text{O}_3$, and $4\text{Al}_2\text{O}_3$ clusters, respectively. Smaller minimum surface roughness is found on smaller incident clusters. The influences of cluster size and incident energy on Al_2O_3 purity of the thin film are examined as well. We found in general that smaller incident clusters may yield higher percentage of the Al_2O_3 purity in a deposited thin film. In particular the incident clusters with single Al_2O_3 molecule has a much better Al-oxide percentage value over all incident energies than that for multi-molecular clusters. The value of $\text{Al}_2\text{O}_3\%$ decreases as the incident energy increases, basically due to debonding of the molecules within a cluster or of the atoms within a molecule.

An MTJ with good performance is expected to have a high MR ratio, which requires superior surface morphology and aluminum-oxide purity within the insulating film surface. Given the results of our MD simulations, we conclude that the incident energy of roughly 45 eV/cluster in the ICBF process for single- Al_2O_3 clusters may yield best qualities for such thin films. Overall, the MD simulation is considered as an effective way to study the thin film deposition and determine the optimal processing parameters. The control of sputtering only $1\text{Al}_2\text{O}_3$ clusters from Al_2O_3 target, however, poses an engineering challenge and may need further study.

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References

- [1] M. Julliere, Phys. Lett. A 54 (1975) 225.

- [2] J.S. Moodera, L.R. Kinder, T.M. Wong, R. Meservey, Phys. Rev. Lett. 74 (1995) 3273.
- [3] W.J. Gallagher, S.S.P. Parkin, Y. Lu, X.P. Bian, A. Marley, K.P. Roche, R.A. Altman, S.A. Rishton, C. Jahnes, T.M. Shaw, G. Xiao, J. Appl. Phys. 81 (1997) 3741.
- [4] S.S.P. Parkin, K.P. Roche, M.G. Samant, P.M. Rice, R.B. Beyers, R.E. Scheuerlein, E.J. O'Sullivan, S.L. Brown, J. Bucchigano, D.W. Abraham, Y. Lu, M. Rooks, P.L. Trouilloud, R.A. Wanner, W.J. Gallagher, J. Appl. Phys. 85 (1999) 5828.
- [5] J.C. Slonczewski, Phys. Rev. B 39 (1989) 6995.
- [6] Y. Ando, J. Murai, T. Miyazaki, J. Magn. Magn. Mater. 199 (1999) 161.
- [7] R.L. Comstock, J. Mater. Sci. – Mater. Electron. 13 (2002) 509.
- [8] S. Tehrani, B. Engel, J.M. Slaughter, E. Chen, M. DeHerrera, M. Durlam, P. Naji, R. Whig, J. Janesky, J. Calder, IEEE Trans. Magn. 36 (2000) 2752.
- [9] H. Kyung, C.S. Yoon, C.K. Kim, Mater. Sci. Eng. B–Solid State Mater. Adv. Technol. 90 (2002) 55.
- [10] M. Urech, V. Korenivski, D.B. Haviland, J. Magn. Magn. Mater. 249 (2002) 513.
- [11] Y. Ando, M. Yokota, N. Tezuka, T. Miyazaki, J. Magn. Magn. Mater. 199 (1999) 155.
- [12] J.R. Fermin, A. Azevedo, B. Li, F.M. de Aguiar, S.M. Rezende, J. Appl. Phys. 85 (1999) 4943.
- [13] S. Tanoue, A. Yamasaki, J. Appl. Phys. 88 (2000) 4764.
- [14] W. Zhu, C.J. Hirschmugl, A.D. Laine, B. Sinkovic, S.S.P. Parkin, Appl. Phys. Lett. 78 (2001) 3103.
- [15] T. Miyazaki, S. Kumagai, T. Yaoi, J. Appl. Phys. 81 (1997) 3753.
- [16] N. Tezuka, M. Oogane, T. Miyazaki, J. Magn. Magn. Mater. 199 (1999) 149.
- [17] K. Inomata, Y. Saito, K. Nakajima, M. Sagoi, J. Appl. Phys. 87 (2000) 6064.
- [18] K. Takanashi, S. Mitani, J. Chiba, H. Fujimori, J. Appl. Phys. 87 (2000) 6331.
- [19] W.H. Ha, M.H. Choo, S. Im, J. Non-Cryst. Solids 303 (2002) 78.
- [20] K. Kakishita, S. Kondo, T. Suda, Nucl. Instrum. Methods Phys. Res. Sect. B–Beam Interact. Mater. Atoms 121 (1997) 175.
- [21] J.Q. Xie, Y. Zheng, J.Y. Feng, Nucl. Instrum. Methods Phys. Res. Sect. B–Beam Interact. Mater. Atoms 122 (1997) 239.
- [22] E.Z. Kurmaev, K. Endo, T. Ida, T. Otsuka, S.Y. Kim, G.S. Chang, A. Moewes, N.Y. Kim, C.N. Whang, D.L. Ederer, Org. Electron. 3 (2002) 15.
- [23] S.J. Cho, D.K. Park, T.W. Kwon, D.S. Yoo, I.G. Kim, Thin Solid Films 417 (2002) 175.
- [24] J.M. Haile, Molecular Dynamics Simulation: Elementary Methods, Wiley, New York, 1992.
- [25] R.W. Grimes, S.P. Chen, J. Phys. Chem. Solids 61 (2000) 1263.

- [26] F. Cleri, V. Rosato, *Phys. Rev. B* 78 (1993) 22.
- [27] M.-H. Su, C.-C. Hwang, J.-G. Chang, S.-H. Wang, *J. Appl. Phys.* 93 (2003) 4566.
- [28] N. Levanov, V.S. Stepanyuk, W. Hergert, O.S. Trushin, K. Kokko, *Surf. Sci.* 400 (1998) 54.
- [29] C.-C. Hwang, J.-G. Chang, G.-J. Huang, S.-H. Huang, *J. Appl. Phys.* 92 (2002) 5904.
- [30] C.-I. Weng, C.-C. Hwang, C.-L. Chang, J.-G. Chang, S.-P. Ju, *Phys. Rev. B* 65 (2002) 195420.
- [31] Y. Hu, S.B. Sinnott, *Surf. Sci.* 526 (2003) 230.