Effect of oxide barrier height in spin dependent tunneling in MTJ of FeO-MgO multilayer structure

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Abstract. We study the spin dependent tunneling current properties through oxide multilayers in a magnetic tunnel junction (MTJ). For this purpose, nonequilibrium Green's function approach along-with the density-functional theory have been applied. We employed three structural models of FeO-MgO-FeO multi-layer with three different width of FeO and MgO layer. An atomistic model is considered to describe the effect of oxide multilayers of different heights. Spin dependent study for tunneling reveals that the parallel spin shows higher tunneling current whereas anti-parallel spin conducts very less. Further, the lowest tunneling current is obtained for the case where the FeO and MgO each has 3 atomic layers of height whereas the tunneling current is highest in 4 atomic layers of FeO/1 atomic layers of MgO/4 atomic layers of MgO multilayer structure. Importantly, when the MgO or FeO layers are increased or decreased from this level, the tunneling current decreases significantly. The study reveals that the layer height in the tunneling domain can be important factor for tuning and adjusting tunneling current in the nanoscale regime of oxide layer thickness.

Keywords: Tunneling, MTJ, barrier height, spin dependent current.

1. Introduction

Magnetic tunnel junction (MTJ) with MgO and Al_2O_3 barrier is one of the very active areas of research because of their high tunnel magnetoresistance (TMR) alongside their applications related to magnetic random access memories (MRAM) [1]. Theoretically, it has been shown that Fe/MgO/Fe layers in MTJ can exhibit TMR up to 1000% whereas many groups have experimentally fabricated Fe/MgO/Fe multilayer MTJ, which shows a TMR of maximum ~200% at room temperature [2,3]. The same experimental TMR value for MgO barrier is increased up to 604% when the ferromagnetic electrodes were replaced by CoFeB. The deviation in the result of theoretical and experimental value is attributed to the interfacial properties of the barrier and electrode. It also has been reported that the spin dependent tunneling depends highly on the different properties of the interface [4]. Therefore, the study of interfacial properties in MTJs is important for the improvement in tunneling properties. Thus far, the first principal calculation for Fe/MgO interface has been performed by many research groups [5]. It has also been showed that the growth of FeO layer at the barrier electrode interface gives rise the structural coherency, which leads to high TMR values [6]. Theoretical investigations of interfaces in Fe/MgO/Fe based MTJs also revealed that the interface roughness can play an important role in TMR [7]. Experimentally, the morphologies, diffusion, and reactions at the interfaces of multilayers are now investigated using spectroscopic techniques using third generation synchrotron radiation sources, which highlights that increase in structural order due to annealing gives rise to lower TMR value [8,9]. MgO can be grown on Fe (001) using molecular beam epitaxy (MBE), pulsed laser deposition (PLD), RF-sputtering etc. However, at the time of growth it is predicted and investigated that there is a possibility of growth of thin FeO layer at the interfaces, which affects the spin dependent tunneling current and changes the TMR value significantly. In this direction, the present study focuses to a theoretical discussion on the height of FeO and MgO layer over spin dependent tunneling properties and the effects of different layer heights on tunneling current.

2. Theoretical Formulation and Results

In this paper, investigation has been carried out with oxide multilayer effect of FeO-MgO with different thickness in which the overall barrier height is taken to be constant.

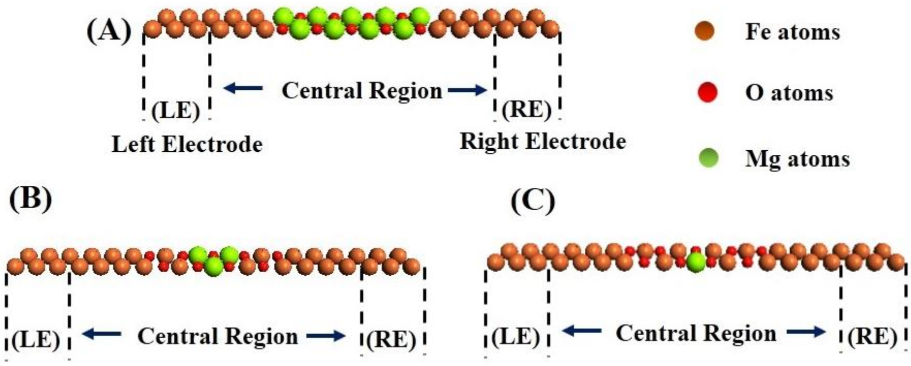

Figure 1: Schematic diagram of the atomistic device where (a) consists of 9 atomic layers of MgO, (b) consists of 3 atomic layers of FeO/ 3 atomic layers of MgO/ 3 atomic layers of MgO and (c) consists of 4 atomic layers of FeO/ 1 atomic layers of MgO/ 4 atomic layers of MgO.

The device configurations used for the simulation are shown in Figure 1. We employed three structural models of FeO-MgO-FeO multi-layer with three different width of FeO and MgO layer as described in the later. The device configuration is simple where oxide layers are put in between two Fe electrodes in order to measure the spin dependent tunneling current through the oxide multilayer. The oxide region taken here is 9 atomic layers thick and both the electrodes are 3 atomic layers thick. The lattice constant of Iron used for the simulation is 2.866 Ǻ. Total 42 numbers of atoms are there in the device. Such small number of atoms is taken because the simulation time increases drastically once the number of atoms in the device is larger. The left and right electrodes are of 3 atomic layers each. The simulations have been performed in an iron/insulator/iron system. Three sets of simulation has been carried out by using different combination of oxides like (a) nine atomic layer MgO, (b) three atomic layer FeO/ three atomic layer MgO/ three atomic layer FeO, (c) four atomic layer FeO/ one atomic layer MgO/ four atomic

layer FeO. In all the simulations, the oxide multilayer height has taken the same as nine atomic layers. Total numbers of atom used in all the simulations are 42 out of that 6 atoms are used for both the electrodes. The calculation is performed to calculate the I-V characteristics after constructing the device. The calculator used here is “ATK-DFT (Device)” with 300 K electron temperature. SGGA (Spin dependent General Gradient Approximation) has been implemented as exchange correlation. The numbers of Monkhorst-Pack grid points are taken as 1, 1, and 100 which is used to resolve the Brillouin Zone along A, B and C directions respectively. The voltage bias between left and right electrode is applied from 0.25 Volt to 1 Volt. The final I-V characteristics for -1 to 1 bias voltage are obtained after symmetrizing each of the plots.
Here we study the spin dependent tunneling current properties through oxide multilayers in a magnetic tunnel junction (MTJ) as described earlier. For that purpose nonequilibrium Green’s function approach along-with the density-functional theory have been applied. Three different structural models of FeO-MgO-FeO multi-layer with different width of FeO and MgO layer are employed.

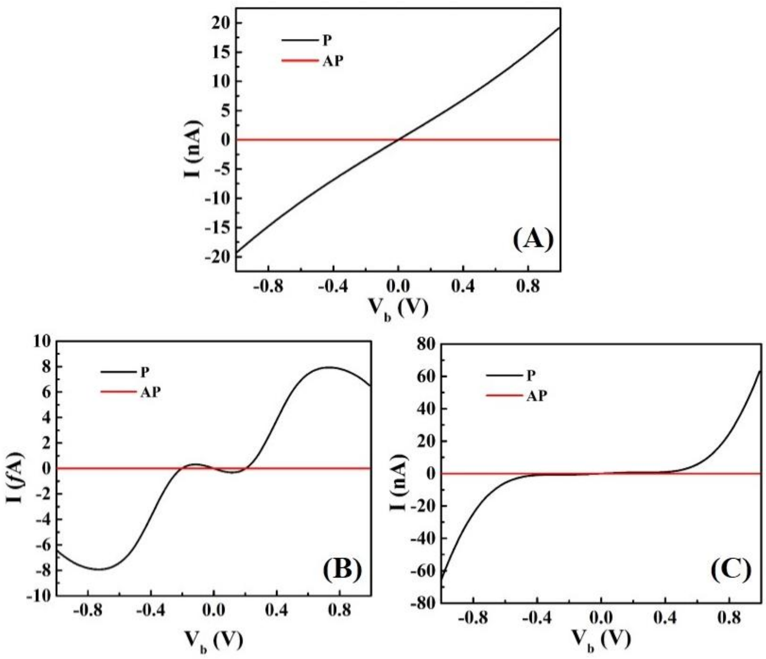

Figure 2: The spin dependent tunneling current in parallel (P) and anti-parallel (AP) situation for (A) 9 atomic layer MgO barrier (B) 3 atomic layers of FeO/ 3 atomic layers of MgO/ 3 atomic layers of MgO (C) 4 atomic layers of FeO/ 1 atomic layers of MgO/ 4 atomic layers of MgO. The current in case of 3 atomic layers of FeO/ 3 atomic layers of MgO/ 3 atomic layers of MgO is in femtoampere (*f*A) but in other two cases the current is in nanoampere (nA).

Figure 2 shows the tunneling current through the oxide multilayer in 3 different combinations of FeO and MgO layer and in each case the current in anti-parallel condition is negligible compared to parallel condition. The electrons in the case of anti-parallel magnetization scatter more that leads to a less current through the device. Moreover the tunneling current changes at different three combinations as shown in Figure 2.

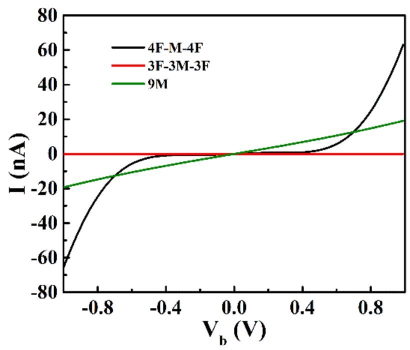

Figure 3: Tunneling current through (a) 9 atomic layer MgO barrier (9M), (b) 3 atomic layers of FeO/ 3 atomic layers of MgO/ 3 atomic layers of MgO barrier (3F-3M-3F), (c) 4 atomic layers of FeO/ 1 atomic layers of MgO/ 4 atomic layers of MgO (4F-M-4F) barrier in parallel magnetization condition.

The current through the MTJ in all 3 mentioned configurations in parallel condition are described in Figure 3 and it is clear that the tunneling current is highest in case of structure (c). However, the tunneling current shows almost linear characteristics in case of structure (a). So the growth of FeO layer may create an obstacle in tunneling and thus the growth of FeO is an important issue in fabricating Fe/MgO/Fe MTJ. Moreover, the structure (c) shows an interesting characteristics where the current start rising after a certain bias voltage. This characteristics is very similar to a diode characteristics where the mentioned critical bias voltage can be correlated with the threshold voltage.

3. Conclusions

In summary, this study of tunneling current through a multi-layer oxide barrier reveals the effect of height of oxide layer in MTJs to improve the tunneling current through it. Moreover electron spin shows a significant effect in electron transport not only in single layer but in the multi-layer structure as well. In each case of the present study suggests that the tunneling current is higher in case of parallel magnetization condition. The highest value of tunneling current is achieved in the third case of the study with 4 atomic layers of FeO/ 1 atomic layers of MgO/ 4 atomic layers of MgO (4F-M-4F) barrier.

Acknowledgments

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