

## Compositional Change of MgO Barrier and Interface in CoFeB/MgO/CoFeB Tunnel Junction after Annealing

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Recent experiments have demonstrated high TMR ratios in MTJs with the MgO barrier [1, 2]. The CoFeB/MgO/CoFeB junctions showed better properties than the CoFe/MgO/CoFe junctions because the MgO layer had a good crystalline structure with (001) texture and smooth and sharp interface between CoFeB/MgO [3]. The amorphous CoFeB with 20 at%B starts the crystallization at 340°C [4] and this crystallization of the CoFeB helps obtaining the high TMR ratio. In this work, the compositional changes in the MgO barrier and at the interface of CoFeB/MgO/CoFeB after the CoFeB crystallization were studied in annealed MTJs. XPS depth profiles were utilized. TEM analyses showed that the MgO barrier had (100) texture on CoFeB in the junctions. B in the bottom CoFeB layer diffused into the MgO barrier and B-oxide was formed at the interface of CoFeB/MgO/CoFeB after the CoFeB crystallization.

**Key words :** magnetic tunnel junction, MgO barrier, CoFeB electrode, interface analysis

### 1. Introduction

Recent experiments have demonstrated over 100% TMR ratio in the MTJs with Fe/MgO/Fe and CoFe/MgO/CoFe [1, 2]. Later the CoFeB/MgO/CoFeB junctions showed better properties than the CoFe/MgO/CoFe junctions because the MgO layer had a good crystalline structure with (001) texture and smooth and sharp interface between CoFeB/MgO [3]. The amorphous CoFeB electrode with 20 at%B starts crystallization at 340°C [4] and this crystallization of CoFeB may help to obtain the high TMR ratio.

In this article, compositional changes of MgO barrier and interface were studied in CoFeB/MgO/CoFeB structure after the CoFeB crystallization by annealing treatment. We have focused on B distribution in the junction before and after the annealing treatment. XPS depth profiles were utilized. TEM analyses showed that the MgO barrier had (100) texture on CoFeB in the junctions and CoFeB was crystallized in the annealed junctions.

### 2. Experiments

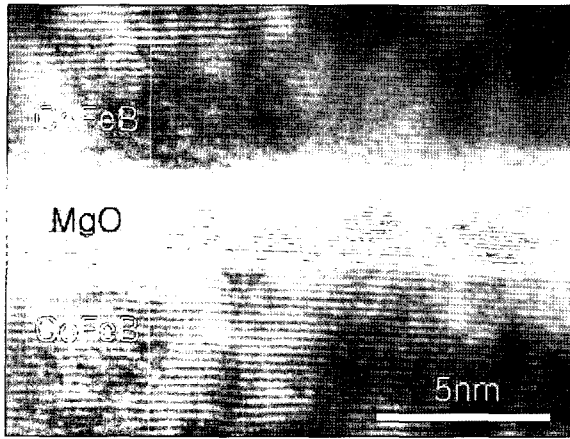
Magnetic tunnel junctions were prepared in a DC magnetron sputtering system at a base pressure of  $3 \times 10^{-8}$  Torr. The MgO barrier was deposited in rf-power system at room temperature. The samples were annealed at 340 °C in a vacuum of  $3 \times 10^{-6}$  Torr. To study the structural characteristics of the MgO layer and the CoFeB electrode, high resolution TEM was used. To investigate the compositional change at the interface of bottom CoFeB electrode/MgO barrier before and after the annealing treatment, SiO<sub>2</sub> (sub)/IrMn (5 nm)/CoFeB (4 nm)/MgO (3 nm)/Ta (5 nm) samples were measured by XPS. For the interface of MgO barrier/top CoFeB electrode, the specimens of SiO<sub>2</sub> (sub)/CoFeB (2 nm)/MgO (5 nm)/CoFeB (3 nm)/Ta (5 nm) were used.

### 3. Results and Discussions

The high resolution TEM images of CoFeB/MgO/CoFeB are shown in Fig. 1 at the annealed state. The MgO barrier had (100) texture on CoFeB in the junctions.

To investigate the effect of the heat treatment on the compositional change at the interface between the bottom

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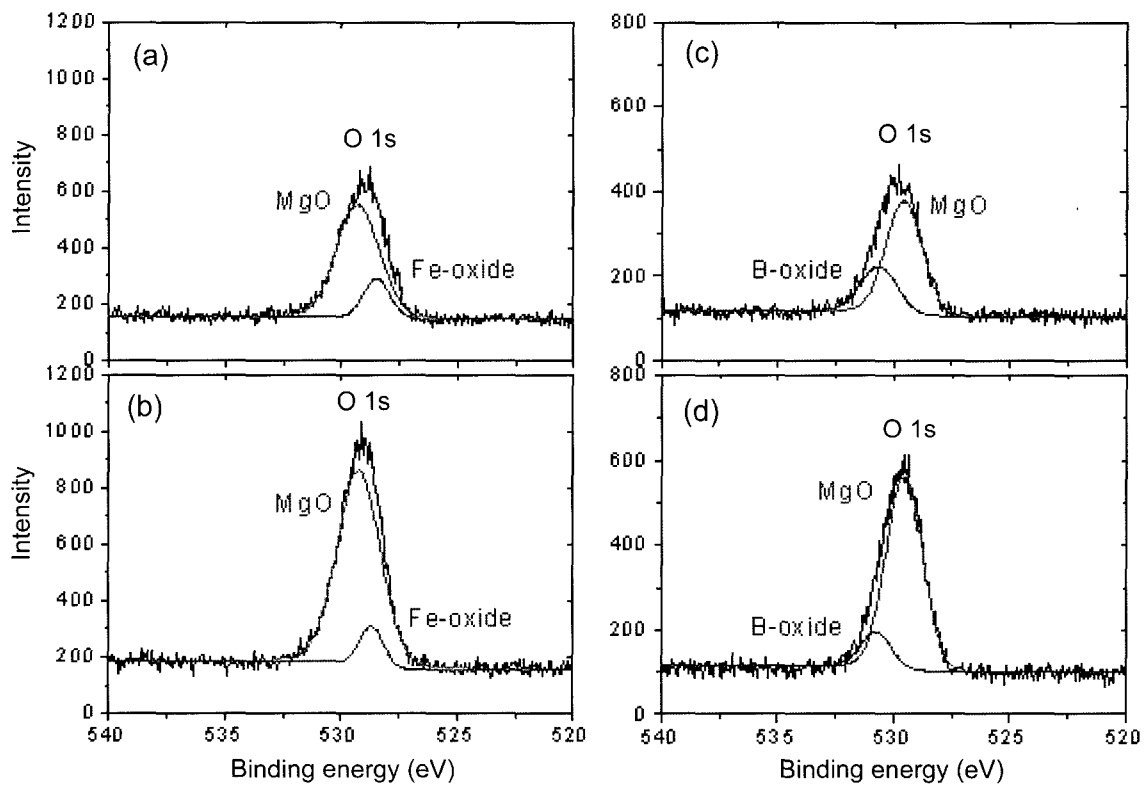


**Fig. 1.** HRTEM image of CoFeB/MgO/CoFeB at annealed state.

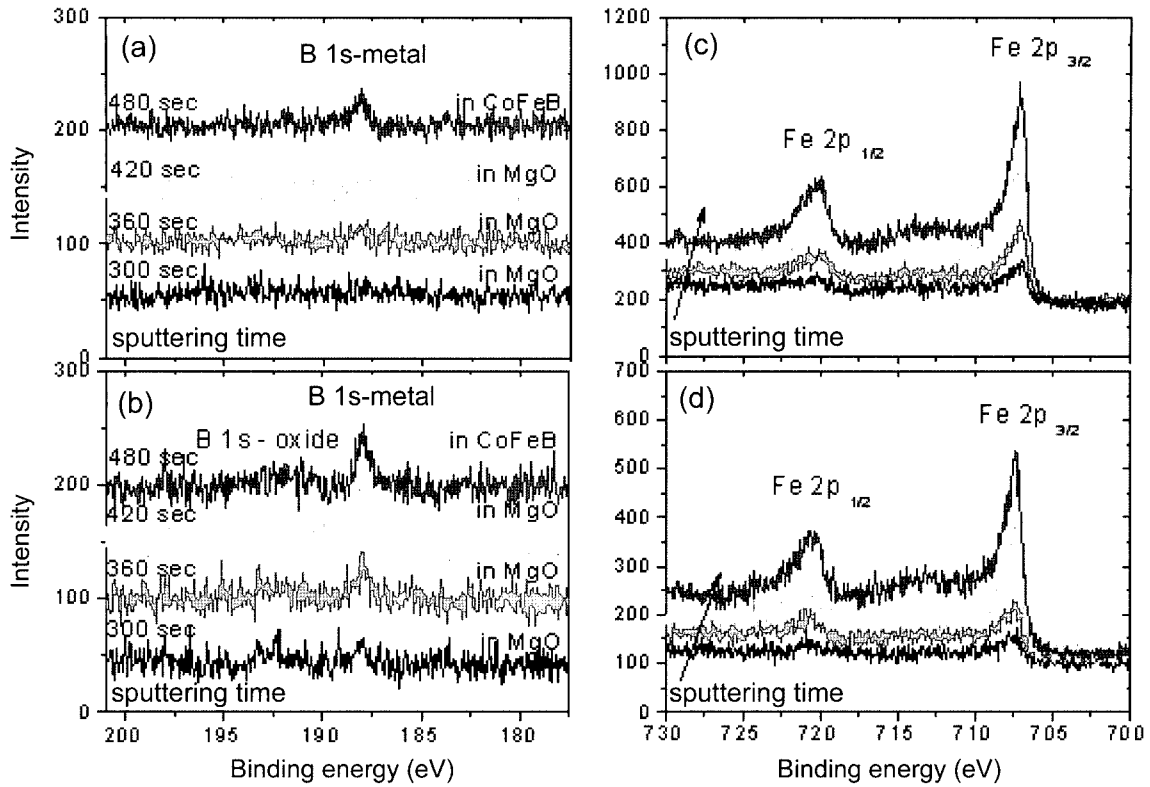
CoFeB electrode and the MgO barrier before and after annealing, IrMn/CoFeB/MgO/Ta samples were measured by XPS. Fig. 2 shows the XPS depth profiles of O 1s peaks in the MgO barrier at the as-deposited state and the annealed state. At the as-deposited state, Fe-oxide peak existed at the interfaces between the bottom CoFeB and MgO, shown in Fig. 2 a) and b). This Fe-oxide formation was predicted by the previous simulations [5, 6]. In Fig. 2

c) and d), the O 1s peaks were deconglomerated by MgO and B-oxide peaks at the interface between the bottom CoFeB and MgO after annealing, without the Fe-oxide peaks. However, the B-oxide peaks were not observed in the O 1s profiles at the as-deposited state. These results indicate that B in the bottom CoFeB layer diffused into the MgO barrier and B-oxide was formed at the interface of the bottom CoFeB/MgO during the crystallization of the bottom CoFeB layer. This was confirmed by B 1s and Fe 2p peak profiles as shown in Fig. 3. This indicates B from CoFeB pinned layer has freely diffused out to the MgO barrier side at the as-deposited state. This B was oxidized into the B-oxide (close to  $B_2O_3$ ) by gathering the excess oxygen during the annealing treatment, which existed near the interface between the bottom CoFeB layer and the MgO barrier. The heat of formation of  $B_2O_3$  is 1278 kJ/kg-mole and this is higher than that of  $Fe_3O_4$  (1014 kJ/kg-mole) and CoO (253 kJ/kg-mole). The Fe-oxide was reduced by forming B-oxide. This will increase the spin polarization of the bottom electrode.

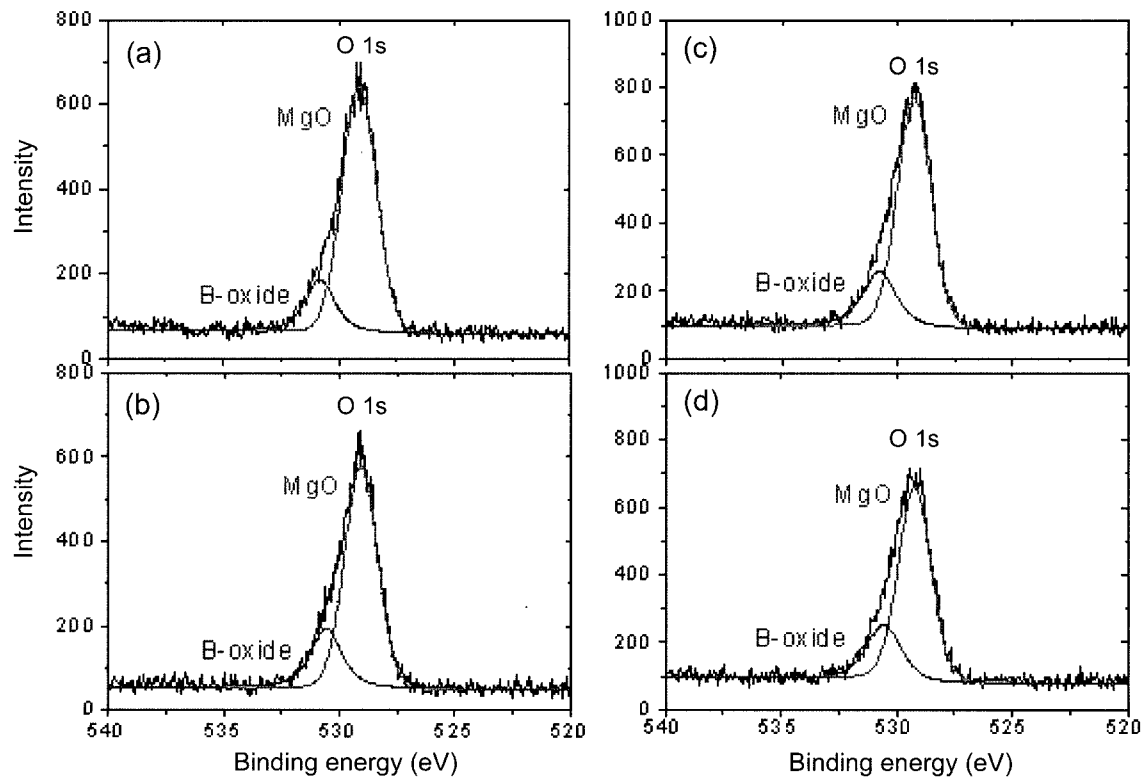
In order to study the compositional change at the interface between the MgO barrier and the top CoFeB electrode before and after the annealing treatment, CoFeB/MgO/CoFeB/Ta was analyzed by XPS. Fig. 4 shows the



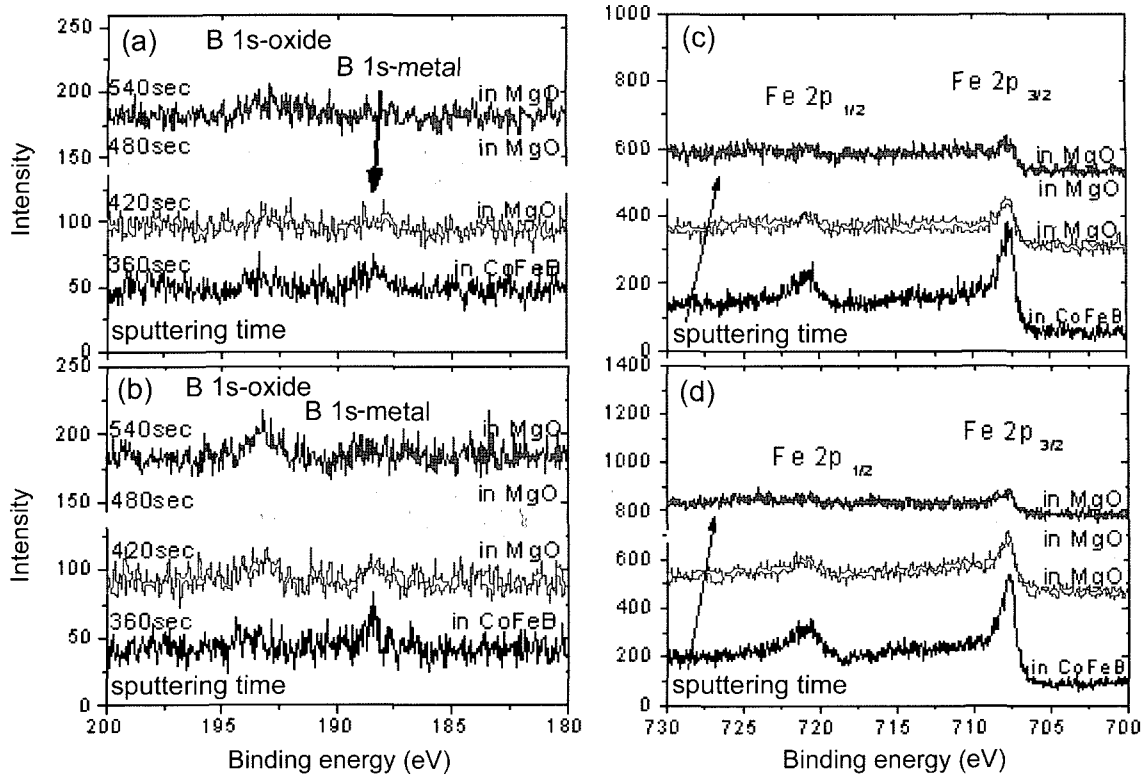
**Fig. 2.** O 1s XPS depth profile of IrMn/CoFeB/MgO/Ta in MgO barrier at sputtering time a) 420 sec (interface of bottom CoFeB/MgO) and b) 360 sec at the as-deposited state and c) 420 sec (interface of bottom CoFeB/MgO) and d) 360 sec at the annealed state.



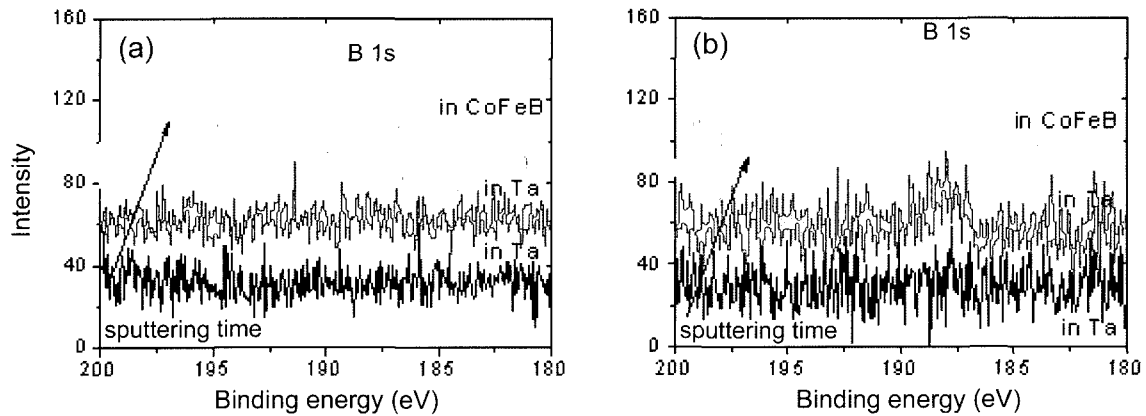
**Fig. 3.** B 1s XPS depth profile of IrMn/CoFeB/MgO/Ta at the interface of CoFeB/MgO and in MgO barrier at a) the as-deposited state and b) the annealed state, Fe 2p XPS depth profile of IrMn/CoFeB/MgO/Ta at the interface of CoFeB/MgO and in MgO barrier at c) the as-deposited state and d) the annealed state.



**Fig. 4.** O 1s XPS depth profile of CoFeB/MgO/CoFeB/Ta in MgO barrier at sputtering time a) 480 sec and b) 420 sec (interface of MgO/top CoFeB) at the as-deposited state and c) 480 sec and d) 420 sec (interface of MgO/top CoFeB) at the annealed state.



**Fig. 5.** B 1s XPS depth profile of CoFeB/MgO/CoFeB/Ta at the interface of MgO/CoFeB and in MgO barrier at a) the as-deposited state and b) the annealed state, Fe 2p XPS depth profile of IrMn/CoFeB/MgO/Ta at the interface of MgO/CoFeB and in MgO barrier at c) the as-deposited state and d) the annealed state.



**Fig. 6.** B 1s XPS depth profile of CoFeB/MgO/CoFeB/Ta at the interface of CoFeB/Ta at a) the as-deposited state and b) the annealed state.

O 1s peaks in MgO barrier at the as-deposited state and annealed state. For both cases, the B-oxide peaks existed near the MgO/CoFeB interface and the Fe-oxide peaks were not observed. These results are confirmed by the B 1s and Fe 2p peaks profiles, shown in Fig. 5. B also diffused into the Ta capping layer after annealing, shown in Fig. 6. The Fe-oxide peaks did not appear in MgO barrier at the as-deposited and annealed states in Fig. 5 c)

and d). Therefore, it is concluded that the increase of the TMR ratio upon the annealing must be mainly associated with the increase of polarization of the bottom electrode due to the formation of the chemically clean interface and the reduction of Fe-oxide at the interface. Other reason may be the increase of polarization by crystallization of the amorphous electrodes and the formation of physically sharp interface.

#### 4. Conclusions

We have studied the compositional change of MgO barrier in CoFeB/MgO/CoFeB junctions by XPS depth profile. The Fe-oxide was formed at the interface of the bottom electrode and the MgO barrier at the as-deposited state. However, the Fe-oxide peak did not exist in the MgO barrier CoFeB electrodes crystallization. Because B has no solubility in CoFe, B has diffused into MgO barrier side and formed B-oxide collecting excess oxygen and sometimes reducing the Fe-oxide. At the interface between MgO and top electrode, no Fe-oxide was formed and only B-oxide existed in the as-deposited state. Upon annealing there were no appreciable changes besides marginal increase of B-oxide. The increase of polarization at the bottom electrode sides is the reason for the higher TMR ratio in CoFeB/MgO/CoFeB junctions due to cleaner interface and/or the reduction of Fe-oxide at the interface. Another reason may be the crystallization of the CoFeB electrodes and formation of physically sharp interface.

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