

# Simulation of Tunnel Magneto Resistance

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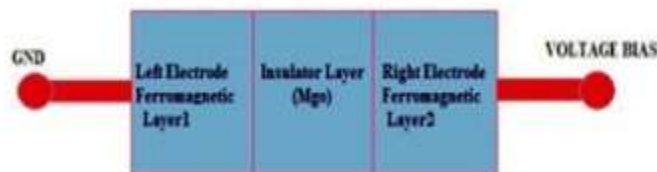
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**Abstract**— In the past two decades electronics has been reaching to its limit of miniaturization and a time will come when further miniaturization will not be possible. Spintronics is the key for opening this deadlock. The science of manipulating the spin of electron with or without the charge to get the desired result is known as Spintronics. Magnetic Tunnel junction is a vital element in Spintronics consists of two ferromagnetic electrodes separated by an insulator layer. Scarcely few works, however, have been carried out thus far in modelling and simulation of Magnetic tunnel junction. Acknowledging the fact that the simulation of tri-layer magnetic tunnel junction will provide a valuable insight for further integration of Spintronics in practical devices, a study of magnetic tunnel junction is presented. In this paper we present result of first principle simulation of TMR of Co/MgO/Co magnetic tunnel junction and various constraints affecting it using Atomix toolkit and NEMO5 Program package. The method in program package is based on carrying out density functional theory (DFT) within the Keldysh Non-equilibrium Green's function

**Keywords**— Spintronics, Tunnel Magneto resistance, Magnetic Tunnel junction, Co/MgO/Co, Non Equilibrium Green function (NEGF), DFT, LSDA

## 1. INTRODUCTION

The persistent efforts in device miniaturization by mankind in past few decades lead us to nanometre era of electronic devices where the quantum phenomena of spin and charge took prominent role in device physics. In recent years Magnetic Tunnel Junction is the centre of attraction for various researchers due to interesting physics behind it and its application in area like magnetic sensors and data storage technology. Magnetic Tunnel junction consist of an insulator layer (Mgo, Beo) sandwiched between two thin Ferromagnetic electrode (Fe, Ni or Co) in such a way that the magnetization of two ferromagnetic electrode can be switched between parallel and antiparallel state under the influence of external magnetic field.



Figur1: Magnetic tunnel junction

The following effect was discovered by M. Julliere in year 1975 by taking Fe/Ge-O/Co-junction in consideration at 4.2 K [1]. For practical device applications it is of utmost importance to make sure that insulating layer is very thin so depending upon the relative orientation of magnetization of the two ferromagnetic layers, electrons from one ferromagnetic layer can tunnel through to reach the other metal layer when a bias voltage is applied across the MTJ. This phenomenon is called spin dependent tunnelling (SDT). However TMR decrease precipitously for barrier thickness below 2 nm [2]

In earlier stages of its development magnetic Tunnel junction is usually based on Amorphous  $Al_2O_3$  [2,3] but with the theoretical prediction of WH Butler in year 2001 the course

Changes to that of MgO as it shows large Tunnelling Magneto resistance in a Fe/MgO/Fe Magnetic Tunnel Junction [4,5]. Extensive studies have started over MgO based Magnetic tunnel junction up to now however

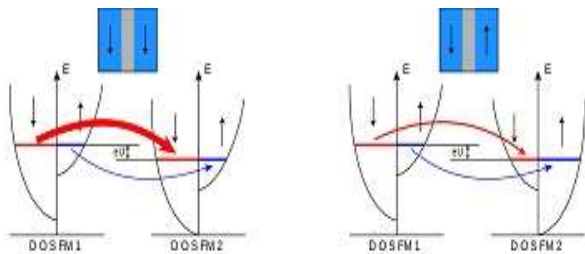
Complete understanding of tunnelling is still not attained due to complexity of metal/insulator surface. The major aspect of Magnetic tunnel junction that makes it such a promising candidate for future Spintronic devices like magnetic sensors is Tunnel magneto resistance. Magnetic Tunnel junction is made in such a way that the magnetization of two ferromagnetic electrodes can be switched

between parallel and antiparallel state under the influence of external magnetic field. This switching property caused an abrupt change in electrical conductance of Magnetic tunnel junction [6]. The Tunnel magneto resistance ratio defined the sensitivity of device more the ratio more sensitive the device is. In practical way Tunnel magneto resistance ratio can be defined in terms of conductance and Tunnelling current.

Equation 1(a) and (b)

$$\delta = \frac{G_P - G_{AP}}{G_{AP}}, \delta = \frac{I_{PS} - I_{APS}}{I_{APS}} e$$

Here  $G_P$  is conductance in parallel state,  $G_{AP}$  is conductance in antiparallel state and similar term goes to tunnelling current. With the theoretical predictions and several experiments TMR ratio is increased to several hundred percent in recent time [7,8].



**Figure2:**Tunnel Magneto Resistance in parallel and antiparallel

The simulation and modelling using first principal calculations help us in discovering various new materials for Magnetic tunnel junction application's [9, 10]. Here in this paper we have studied about Mgo based magnetic Tunnel Junction with Fe as pinned and free layer.

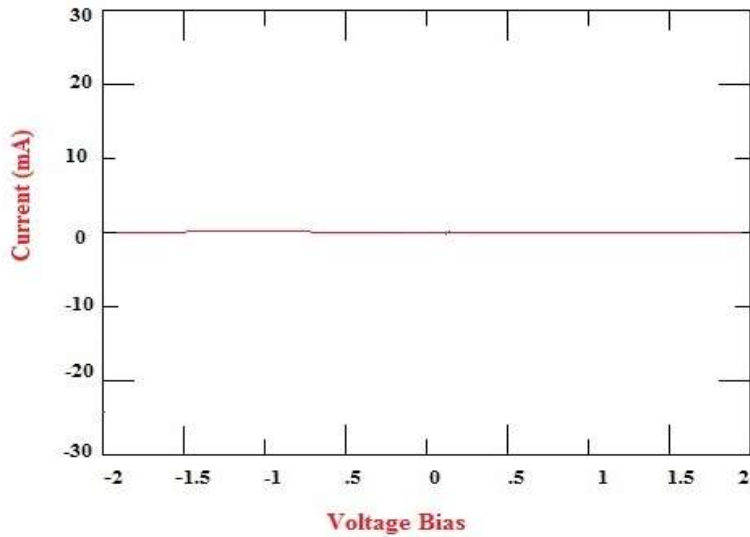
### SIMULATION SET UP

In this paper we have built Co/Mgo/Co magnetic tunnel junction on Nemo5 and then simulated it for I-V curve and Transmission spectrum in both parallel and antiparallel configurations. The left electrode has no voltage where as we applied a bias voltage on right electrode. In magnetic tunnel junction the I-V curves are result of spin polarized electron transportation. The exchange correlation used is LSDA. The insulator layer we have taken into consideration is up to 7 layers. Here we have used NEMO5 as calculator and cross checked the result with ATK11.08. The mesh cut off and temperature are 90 Hartree and 373 Kelvin. Here work is done on spin-density functional theory and non-equilibrium Green's functions to estimate the structure and low-bias current/voltage characteristics of magnetic tunnel junctions (MTJs) consisting of five to seven MgO barriers sandwiched between Co electrode in both the parallel and anti-parallel magnetization configurations. The tunnelling magneto resistance in the above two described magnetic tunnel junction with increasing bias voltage ranging from (0 to .4v). The decrease in tunnel magneto resistance with bias voltage is in accordance with the experimental values. Here we only work on deducing the effects of voltage bias on Tunnel Magneto Resistance there are other aspects also which also affect the Tunnel magneto resistance and that are thickness of Barrier layers and temperature which I will include in our next work. .

### Simulation Results

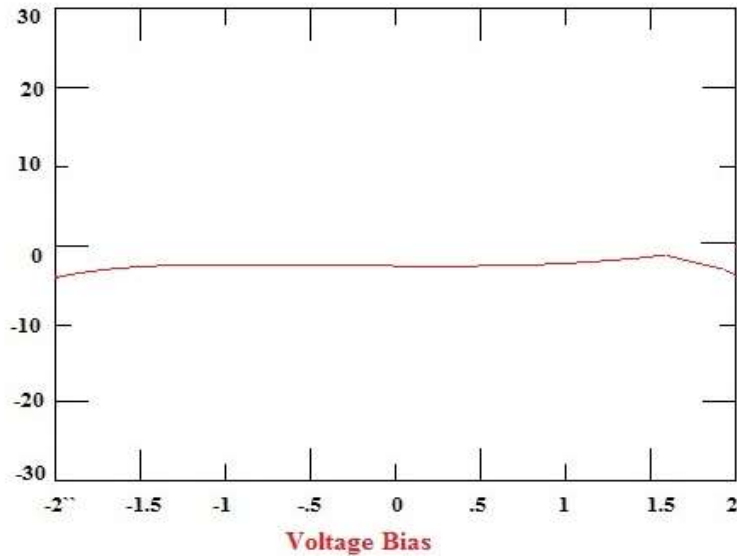
Figure 3(a) (b) I/V curve in parallel and anti - parallel configuration from the following figures we can depict that Tunnel current in parallel state and antiparallel are almost independent of bias voltage.

**I/V Curve Parallel configuration of Co/MgO/Co  
Magnetic Tunnel Junction**



**Figure 3(a)**

**I/V curve Antiparallel Configuration**



**Figure 3 (b)**

From the I/V curve we have obtained the value of TMR of the Co/MgO/Co magnetic tunnel junction at various bias voltages. From figure 3 and 4 we got the value of Tunnel Magneto Resistance at various bias voltages and what effect does bias voltage cause on the Tunnel magneto resistance of Co/MgO/Co magnetic Tunnel junction at various bias voltages. A graph has been plotted from the data, and it has been seen that the Magnetic Tunnel Junction here exhibits a TMR (ratio) of about 87%-94% when the voltage is varied between -1 to 1 volt. This is quite near to that of 100%.

copper is also one of the promising materials to be used in Magnetic tunnel junction. This is shown below in Diagram:

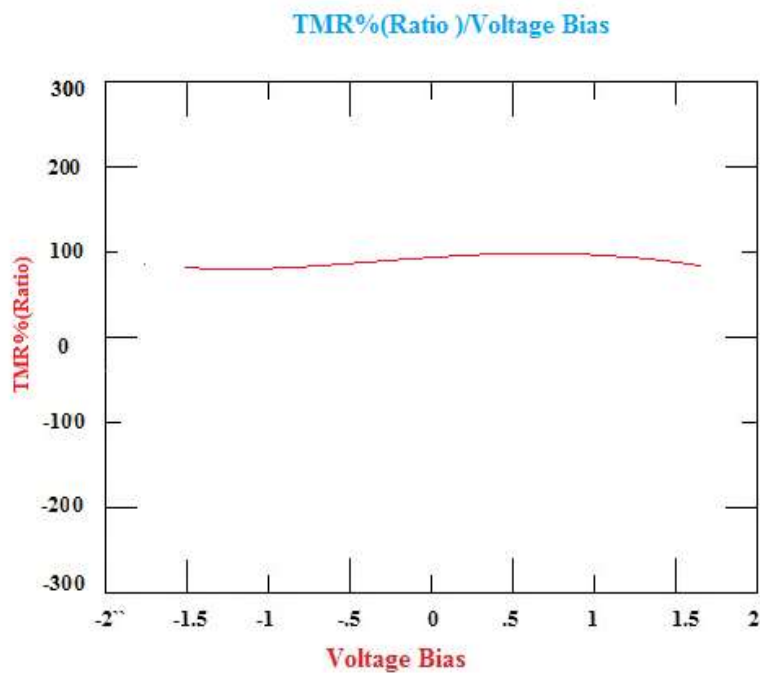


Figure 4

The electrical aspects arising from external conditions applied like bias voltage and its effects on internal condition (e.g. Tunneling Magneto Resistance) are shown precisely in the figure below. The simulation results are not exact in line with that of experimented values reported the variation in results are due to various impurities and resonant channels that are present there at the fabrication process

### Conclusion

Although several modeling approaches has been used till today to study electrical properties of Magnetic tunnel junction but none can accurately predict the electrical properties of Magnetic Tunnel Junction. In this paper we have used SGGA band structure calculation for Co/Mgo/Co

Magnetic Tunnel Junction to obtain I/V curve for parallel and anti-parallel states .From the I/V curve we have calculated The Tunnel Magneto resistance at various bias voltages(-1.5 - 1.5). The parallel and anti-parallel states are also simulated against varying insulator thickness from 4 to7 layers.A gradual increase is seen in resistance when varied through four to seven layers. In this we have used NEFG-DFT formalism to examine the case of Co/Mgo/Co magnetic tunnel junction and it is seen that tunnelling properties of magnetic tunnel junction is strongly influenced by voltage bias and insulator thickness of the layer.

### Future work

The above described work can further improved by adding various conditions like thermal and stress distribution effect on the simulated magnetic tunnel junction also the study of noise sources of MT J and the defects in the barrier can be studied for further development of Magnetic tunnel junction..

**REFERENCES:**

- [1]M. Julliere, "Tunneling between ferromagnetic films," Phys. Lett. A, vol. 54, no. 3, pp. 225–226, Sep. 1975
- [2]W. H. Butler, X. G. Zhang, T. C Schulthess and J. M MacLaren, Phys. Rev. B. 63, 054416 (2001).
- [3]W. Thomson, "On the Electro-Dynamic Qualities of Metals: Effects of Magnetization on the Electric Conductivity of Nickel and of Iron", Proceedings of the Royal Society of London, 8, pp. 546–550 (1856–1857).
- [4]N. F. Mott, "The electrical conductivity of transition metals," Proc.Roy.Soc.A153,699 (1936).
- [5]M. Julliere, "Tunneling between ferromagnetic films," Phys. Lett. A, vol. 54, no. 3, pp. 225–226, Sep. 1975
- [6]S. Maekawa and U. Gafvert, "Electron-tunneling between ferromagnetic films," IEEE Trans.Magn., vol.MAG-18, no. 2, pp. 707–708, Mar. 1982.
- [7]K. Deb, S. Agrawal, A. Pratab, T. Meyarivan, "A Fast Elitist Non-dominated Sorting Genetic Algorithms for Multiobjective Optimization: NSGA II," KanGAL report 200001, Indian Institute of Technology, Kanpur, India, 2000. (technical report style)
- [8]M. N. Baibich, J. M. Broto, A. Fert et al., Giant magnetoresistance of (001) Fe/(001) Cr magnetic superlattices, Phys. Rev.Lett. 61, 2472–2475 (1988).
- [9] W. H. Butler, X. G. Zhang, T. C Schulthess and J. M MacLaren, Phys. Rev. B. 63, 054416 (2001).
- [10] First Principles modeling of electron transport KStokbro(J.phy.:Condens. Matter(2008) 064216(7pp)
- [11]First principles modeling of TMR Fe/MgO/Fe trilayers arXiv:cond-mat/0605017
- [12]Simulation of Tunneling Magneto resistance of Fe/Mgo/Fe Magnetic Tunnel Junction by K Shiiki  
[http://iopscience.iop.org/1742-6596/303/1/012101/pdf/1742-6596\\_303\\_1\\_012101.pdf](http://iopscience.iop.org/1742-6596/303/1/012101/pdf/1742-6596_303_1_012101.pdf)