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Full Length Article

# First principle study on TMR effect in A-MgO-A (A = Fe, Co and Ni) magnetic tunnel junction

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## 1. Introduction

Magnetic tunnel junction (MTJ) provides high magneto-resistance comparing to giant magnetoresistance (GMR) devices. The function of the device is based on both tunneling and magneto-resistance effect. These MTJ are also called tunnel magneto-resistive devices (TMR). Typically TMR device consists of a non-magnetic insulator layer sandwiched by ferromagnetic layer. The resistance of TMR devices based on the magnetic orientation of the ferromagnetic materials [1–4]. Understanding of spin-dependent transport plays a vital role in predicting the performance of this device. The electrode materials highly influence the magneto-resistance changes in these devices. At present, number of investigation have been carried out on iron electrode due to its enhanced ferromagnetic behavior [5–8]. Cobalt, nickel and gadolinium elements are also exhibiting ferromagnetic nature. Out of these iron, cobalt and nickel are abundantly available in nature and shows ferromagnetic property at room temperature.

Zhang et al. analyzed tunnel magneto resistance effect in Co/MgO/Co and FeCo/ MgO/ FeCo. They found that Co/ MgO/ Co and FeCo/ MgO/ FeCo systems exhibits more tunnel magneto-resistance than Fe/MgO/Fe [9]. Santos et al. investigated the tunnel magneto resistance in C60 molecule attached in between ferromagnetic electrode [10]. Shi et al. explored the origin of magneto-resistance in organic materials. He observed more than 60 percentage magnetoresistance in this device [11]. We have previously reported the effect of electrode on 11-acene molecular junction as a spin-valve [12]. These theoretical investigation represent that iron is the best electrode for 11-acene spin valve devices. Thin film type TMR devices have been analyzed by various researchers with different combination of ferromagnetic materials [13–17]. They reported that the combination of iron based TMR devices show better TMR effect. Experimental investigation represented that two dimensional materials h-BN also exhibits tunnel magneto-resistance effect [18]. Recent analysis shows that epitaxially grown ferromagnetic materials are widely used in TMR devices, because of its high spin filtering effects [19–26]. Also it is feasible and cost effective process to make TMR devices. Theoretical investigation of this type of epitaxially grown material for TMR devices have been carried by Butler et al. [27].

The purpose of this study is to manifest the role played by the electrode material in TMR devices. To build the TMR device, an insulating layer MgO was sandwiched between the ferromagnetic electrodes. We have used cobalt, iron and nickel as ferromagnetic electrode to understand the spin-dependent transport mechanism through the MgO tunnel barrier. We separated these devices into three regions namely electrode region, electrode extension region and a scattering region as shown in Fig. 1 for spin transport calculations. We investigated total density of states, projected density of states and transmission coefficient of these devices to understand the spin transport properties.

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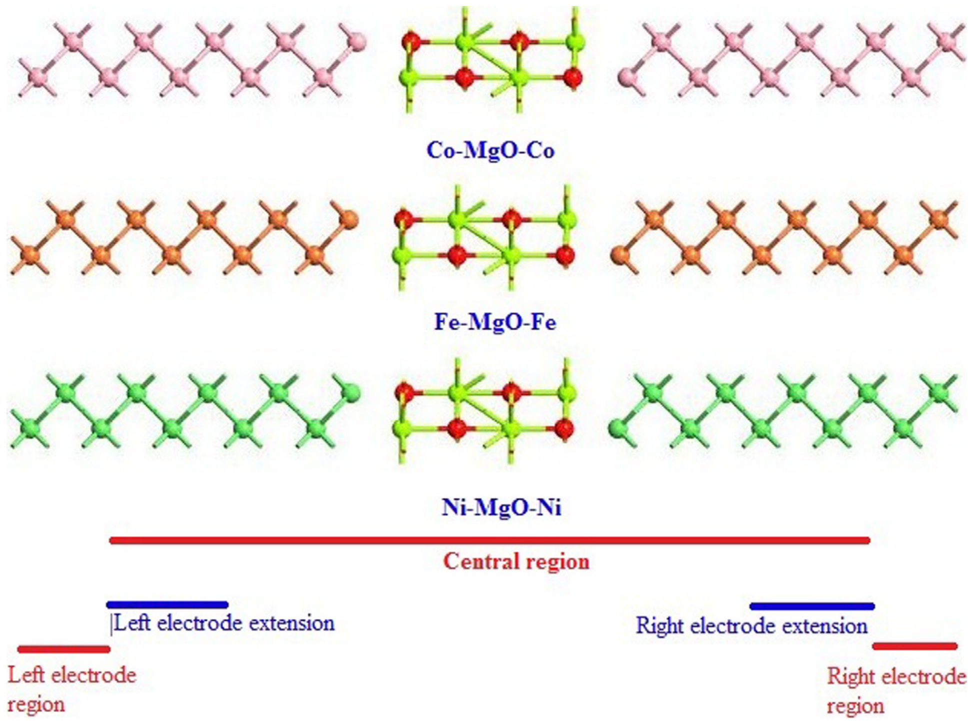


**Fig. 1.** Schematic representation of Co-MgO-Co, Fe-MgO-Fe and Ni-MgO-Ni devices.

## 2. Computational details

For Fe/MgO/Fe, Co/MgO/Co and Ni/MgO/Ni devices the spin polarized transport properties are computed by implementing full spin polarized Density Functional Theory (DFT) with Non-Equilibrium Green's Function (NEGF) [28–30] using Atomistic ToolKit package (ATK) [31–34]. The charge and spin property of electron determines the TMR function. So we have done spin polarized calculation of these devices, in which the spin and charge properties of electrons included. Different basis set are used for insulating layer and electrode material, because the accuracy of the transport property highly depends upon interfaces or junctions. We have used double zeta polarised basis set for Mg and O atoms and single zeta polarised basis set for electrode material. Convergent results are achieved by using 2 × 2 × 100 k points sampling along x, y and z directions, where z represents electron transport direction. Spin component of electron was taken into account by using spin dependent SGGA for analyzing the spin-dependent electron transport of these structures. This SGGA treats the electron density semi-locally to achieve better accuracy. To include exchange co-relation effect, we have used Perdew, Burke and Ernzerhof (PBE) function for all these calculation. In parallel configuration (PC) the spin of left and right electrode magnetic (spin) orientation kept same and in anti-parallel configuration (APC) it kept in opposite direction.

Density of states, projected density of states and transmission co-efficient of these devices was calculated in both parallel and anti-parallel spin configuration. The Local Density of states was calculated using the spectral density matrix as mentioned below.

$$\rho(E) = \rho^L(E) + \rho^R(E) \quad (1)$$

Where $\rho^L(E)$ and $\rho^R(E)$ are left and right electrode spectral density. By integrating the local density of states over all space, we obtained device density of states.

The transmission co-efficientof these systems was calculated as

$$T(E, V_b) = Tr(G_1 G G_2 G^+) \quad (2)$$

Where broadening matrices $G_{1,2} = i(S_{1,2} - S_{1,2}^+)$ are defined as the anti-Hermitian parts of self-energies $S_{1,2}$, which arises from the coupling of the central scattering region to the electrode. The conductance was calculated using the transmission coefficient.

The Tunnel magnetoresistance was calculated by the parallel and anti-parallel conductance of each device (both optimistic and pessimistic method) at zero bias. In optimistic method the difference between parallel and anti-parallel conductance will be divided by anti-parallel conductance. In the case of pessimistic method the difference between parallel and anti-parallel conductance will be divided by the sum of parallel and anti-parallel conductance.

## 3. Results and discussion

The total density of states, projected density of states of d, p and s orbital and transmission coefficient was calculated within the range of −5 eV to 5 eV for all devices in both parallel and anti-parallel configuration to explain the spin dependent electron transport property across the metal-insulator-metal interfaces.

### 3.1. Total density of states (TDOS)

To analyze the available electronic states for spin-dependent transport, total density of states of the whole device was calculated. In a parallel configuration, all the three structures show almost zero density of states for spin-up electrons at Fermi level and LUMO region. From Fig. 2, it is clearly seen that the electron transport occurs only by spin-down electrons in parallel configuration. For all these structure, by changing the magnetic alignment into anti-parallel configuration, it is observed that increase in density of spin up electronic states as well as a decrease in spin down electronic states in LUMO region (near to Fermi-level). Whereas in HOMO region (near to Fermi-level) the spin up electronic states get reduced and increase in spin-down electronic states was observed. Particularly in Fe-MgO-Fe device shows a sharp peak of spin up density of state at -1.1 eV in parallel alignment and for anti-parallel alignment, a sharp peak is observed in spin-down density of state

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