Magnetic tunnel junctions with impurities

F. Kanjouri\(^1,2\), N. Ryzhanova\(^1,3\), B. Dieny\(^3\), N. Strelkov\(^1,3\), A. Vedyayev\(^1,3\)

\(^1\)Department of Physics, Moscow Lomonosov University, Moscow 119899, Russia
\(^2\)Department of Physics, Yazd University, Yazd, Iran
\(^3\)SPINTEC, Unité de Recherche Associée 2512 CEA/CNRS, CEA/Grenoble, Département de Recherche Fondamentale sur la Matière Condensée, 38054 Grenoble Cedex, France

Abstract: The influence on the I-V characteristics and tunnel magnetoresistance (TMR), of impurities embedded into the insulating barrier (I) separating the two ferromagnetic electrodes (F) of a magnetic tunnel junction, was theoretically investigated. When the energy of the electron’s bound state at the impurity site is close to the Fermi energy, it is shown that the current and TMR are strongly enhanced in the vicinity of the impurity. If the position of the impurity inside the barrier is asymmetric, e.g. closer to one of the interfaces F/I, the I-V characteristic exhibits a quasidiode behavior. The case of a single impurity and of a random distribution of impurities within a plane were both studied.

Magnetic tunnel junctions (MTJ), consist of two metallic ferromagnetic electrodes separated by an insulating barrier. They typically exhibit tunnel magnetoresistance (TMR) of the order of 50% associated with a change in the relative orientation of the magnetization in the two ferromagnetic electrodes. They attract a lot of attention\(^1,2,3\) especially due to their applications in several spin-electronic devices especially in non-volatile MRAM (Magnetic Random Access Memory). In a pioneer paper\(^4\), a theory of TMR for ideal MTJ (without defect) was developed. Later on, it has been shown\(^5,6\) that the presence of different types of defects within the barrier can dramatically affect the I-V characteristics and TMR amplitude. In these papers, the current, averaged over the cross-section of the system, was calculated. However, it is also interesting to investigate the local current density and TMR in the vicinity of the impurity. From an experimental point of view, this is achievable by using conductive Atomic Force Microscopy approach as realized for instance in the following reference\(^7\) where the authors mapped out the spatial variations of the I(V)
characteristics through a tunnel barrier. From a theoretical point of view, a theory of local impurity assisted tunnelling in MTJ was recently developed [8]. Tight binding model and Kubo formalism were used to calculate the spin-dependent tunnel current through the MTJ. In this earlier paper, the I-V characteristics were not investigated in detail. Furthermore, the dependence of spin-dependent current on the position of cross section plane relative to the position of impurity was not calculated.

In the present paper, we report on a theoretical study of the spatial distribution of spin-dependent current across the plane of a magnetic tunnel junction. The local I-V characteristics as well as the local TMR amplitude are calculated for a single impurity and for a random planar distribution of impurities inside the barrier. In this theory, We adopted the free electron model with exchange splitting for the ferromagnetic electrodes and used the nonequilibrium Keldysh technique [9] to calculate the transport properties which are nonlinear functions of the applied voltage.

The MTJ is described as a three layers system, consisting of two thick ferromagnetic electrodes $\mathbb{F}$ separated by an insulating layer, $\mathbb{I}$. Inside the barrier, a single nonmagnetic impurity with attracting potential is located at a given distance from the $\mathbb{F}/\mathbb{I}$ interface. The two cases of parallel and antiparallel orientations of the $\mathbb{F}$-layers magnetization were investigated.

The $\mathbb{F}$-electrodes are connected to the reservoirs with chemical potentials $\mu_1$ and $\mu_2$ so that $\mu_2 - \mu_1 = eV$, where $V$ is the applied voltage.

To calculate the current through the system, the Keldysh Green function $G^{-+}$ and advanced and retarded Green functions $G^{A}$ and $G^{R}$ must be calculated. By solving the Dyson equation, we found that

$$G^{-+}(\mathbf{r}, \mathbf{r}') = G^{-+}_0(\mathbf{r}, \mathbf{r}') + \frac{G^{R}_0(\mathbf{r}, \mathbf{r}_0)WG^{-+}_0(\mathbf{r}_0, \mathbf{r}')}{1 - WG^{R}_0(\mathbf{r}_0, \mathbf{r}_0)} + \frac{G^{-+}_0(\mathbf{r}, \mathbf{r}_0)WG^{A}_0(\mathbf{r}_0, \mathbf{r}')}{1 - WG^{R}_0(\mathbf{r}_0, \mathbf{r}_0)}$$

$$+ \frac{G^{R}_0(\mathbf{r}, \mathbf{r}_0)WG^{-+}_0(\mathbf{r}_0, \mathbf{r}_0)WG^{A}_0(\mathbf{r}_0, \mathbf{r}')}{(1 - WG^{R}_0(\mathbf{r}_0, \mathbf{r}_0))(1 - WG^{A}_0(\mathbf{r}_0, \mathbf{r}_0))}$$

(1)

where $G^{-+}_0(\mathbf{r}, \mathbf{r}')$, $G^{A}(\mathbf{r}, \mathbf{r}')$ and $G^{R}(\mathbf{r}, \mathbf{r}')$ are the Green’s functions for the system in the absence of the impurity and the potential of the impurity $V$ was represented as a $\delta$-function: $V(\mathbf{r}) = W a_0^2 \delta(z - z_0)\delta(\mathbf{r} - \mathbf{r}_0)$, $\mathbf{r}_0 = (\mathbf{r}_0, z_0)$ is the position of the impurity, $a_0$ is its effective radius, $W$ is its amplitude. The explicit expressions for $G^{A}, G^{R}, G^{-+}$ have the following forms:
\[ G^R(r, r') = \int d^2k \frac{(-1)^{\epsilon - \kappa \cdot \rho'}}{2 \sqrt{q(z)q(z')} \text{den}^*} \{ E(z_2, z) [q(z_2) + ik_2] + E^{-1}(z_2, z) [q(z_2) - ik_2] \} \times \{ E(z', z_1) [q(z_1) + ik_1] + E^{-1}(z', z_1) [q(z_1) - ik_1] \}, \]

\[ G^A_0(r, r') = \int d^2k \frac{(-1)^{\epsilon - \kappa \cdot \rho'}}{2 \sqrt{q(z)q(z')} \text{den}^*} \{ E(z_2, z) [q(z_2) - ik_2] + E^{-1}(z_2, z) [q(z_2) + ik_2] \} \times \{ E(z', z_1) [q(z_1) - ik_1] + E^{-1}(z', z_1) [q(z_1) + ik_1] \}, \]

\[ G^{++}_0(r, r') = \int d^2k \frac{4k_1 q(z_1) n_2 e^{-i \kappa \cdot \rho'}}{\sqrt{q(z)q(z')} \text{den}^*} \{ E(z_2, z) [q(z_2) + ik_2] + E^{-1}(z_2, z) [q(z_2) - ik_2] \} \times \{ E(z_1, z_2) [q(z_2) - ik_1] + E^{-1}(z_1, z_2) [q(z_1) + ik_1] \}, \]

\[ G^{--}_0(r, r') = \int d^2k \frac{4k_2 q(z_2) n_2 e^{-i \kappa \cdot \rho'}}{\sqrt{q(z)q(z')} \text{den}^*} \{ E(z_1, z) [q(z_1) + ik_1] + E^{-1}(z_1, z) [q(z_1) - ik_1] \} \times \{ E(z_1, z_2) [q(z_2) + ik_2] + E^{-1}(z_1, z_2) [q(z_1) + ik_1] \}, \]

where

\[ q(z) = \sqrt{\frac{2}{\epsilon_0} + \kappa^2 - \frac{2m}{\hbar^2} \frac{(z - z_1)}{(z_2 - z_1)} eV}, \]

\[ k_1 = \sqrt{\frac{2m}{\hbar^2} (\varepsilon - \Delta_1) - \kappa^2}, \]

\[ k_2 = \sqrt{\frac{2m}{\hbar^2} (\varepsilon - \Delta_2 + eV) - \kappa^2}, \]

\[ \text{den} = \{ E(z_1, z_2) [q(z_2) - ik_2] [q(z_1) - ik_1] - E^{-1}(z_1, z_2) [q(z_2) + ik_2] [q(z_1) + ik_1] \}, \]

\[ E(z_1, z_2) \equiv e^{\int_{z_1}^{z_2} q(r) dr}, \]

\( \kappa \) is the electron momentum perpendicular to the plane of structure, \( \varepsilon \) is the energy, \( z_1 \) and \( z_2 \) are the positions of the \( \mathbb{F}/\mathbb{I} \) interfaces, \( \Delta_1 \) and \( \Delta_1 \) denote the positions of the bottom of the energy band for spin up and down subbands.

\( n_L = f^0(\varepsilon) \) and \( n_R = f^0(\varepsilon + eV) \) are Fermi distribution functions in the left and right reservoirs and \( \frac{\hbar^2 q^2}{2m} \) height of potential barrier above Fermi level.

In \( \mathbb{I}, \mathbb{I}L, \mathbb{I}R, \mathbb{I}E \) and \( \mathbb{I} \rho \) and \( z \) are in the plane and perpendicular to the plane coordinates, and we consider that \( z \) and \( z_0 \) are situated within the barrier. We have to take into account that all Green functions are matrices in spin space. \( k^\uparrow_{1F}, k^\downarrow_{1F}, k^\uparrow_{2F}, k^\downarrow_{2F} \) are Fermi wave vectors.
FIG. 1: Dependence of the current for different spin channels and P and AP configuration on the distance from the impurity in the plane of the structure at $z=15$ Å. $k_F^\uparrow = 1.1$ Å$^{-1}$, $k_F^\downarrow = 0.6$ Å$^{-1}$, $q_0 = 1.0$ Å$^{-1}$

of electron with spin $\uparrow$ ($\downarrow$) in the left and right F-electrodes. The current was calculated, using the following expression:

$$j_z(\rho, z) = \frac{e\hbar}{2m} \int d\varepsilon \left( \frac{\partial G^{-+}(z, \rho; z', \rho)}{\partial z'} - \frac{\partial G^{-+}(z, \rho; z', \rho)}{\partial z} \right)_{z=z'}$$  \hspace{1cm} (5)

In Fig.1 and Fig.2 the dependencies of the currents in different channels (up and down spin) on coordinate $\rho - \rho_0$ at one interface $\|F$ (at $z_2 = 15\text{Å}$) (another interface is at $z_1 = 0$) and inside the barrier at $z = 10$ are shown. In this calculation, the impurity is assumed to be positioned at $\rho_0 = 0$ and $z_0 = 5\text{Å}$.

In the vicinity of the impurity, a hot spot of radius approximately equal to 6Å may be observed. The current density in the center of the hot spot exceeds the value of the background current by several orders of magnitude. In Fig.3 the TMR dependence on the distance from the impurity at different $z$ is shown. It is interesting that the value of TMR in the vicinity of the impurity exceeds its background value (TMR for the ideal structure is equal 0.013) by more than an order of magnitude. Furthermore, in some cases, regions of $\rho - \rho_0$ exist in which the TMR becomes negative.

Fig.4 shows the I-V characteristics for positive and negative applied voltage. These curves
FIG. 2: The same dependence at $z = 10$ Å.

FIG. 3: Dependence of TMR on the distance from the impurity in the plane of the structure at different $z$. For parameters see Fig. I.

are quite asymmetric with respect to the sign of the voltage. This asymmetry is related to the asymmetric positioning of the impurity inside of the barrier. It is particularly pronounced if the potential of the impurity is chosen so that the bound (resonance) state of electrons with spin up is located near the Fermi energy for the positive applied voltage $V = 1.2$ V, and if this bound state lies below the Fermi energy for negative voltage. This diode behavior
FIG. 4: Local I-V curve at $\rho = \rho_0$ and $z = 15$ Å for the case of single impurity.

FIG. 5: I-V curve in the case of the layer of impurities at $z_0 = 3$ Å and $x = 0.5$.

was demonstrated so far in the case of a single impurity. We next investigate the case of a finite concentration of impurities.

In this case, we consider the same magnetic tunnel barrier structure with a monolayer of impurities of finite atomic concentration $x$, situated closer to one of the F/I interfaces. To solve the problem, as a first step, we have to find the coherent potential and effective
Keldysh Green function $G_{\text{eff}}^{-+}$. By solving the Dyson equation in the Keldysh space, the following expression was obtained for $G_{\uparrow\uparrow}^{-+\text{AP}}$:

\[
G^{-+}(z, z') = G_{0}^{-+}(z, z') + \frac{G_{0}^{-+}(z, z_0) \Sigma^{A}G^{-+}_{0}(z_0, z')}{1 - G_{0}^{-+}(z_0, z_0) \Sigma^{A}} + \frac{G_{0}^{R}(z, z_0) \Sigma^{R}G_{0}^{-+}(z_0, z')}{1 - G_{0}^{R}(z_0, z_0) \Sigma^{R}} - \frac{G_{0}^{R}(z, z_0) \Sigma^{+}G^{A}_{0}(z_0, z')}{(1 - G_{0}^{A}(z_0, z_0) \Sigma^{A})(1 - G_{0}^{R}(z_0, z_0) \Sigma^{R})} + \frac{G_{0}^{R}(z, z_0) \Sigma^{R}G_{0}^{-+}(z_0, z_0) \Sigma^{A}G_{0}^{A}(z_0, z')}{(1 - G_{0}^{A}(z_0, z_0) \Sigma^{A})(1 - G_{0}^{R}(z_0, z_0) \Sigma^{R})} 
\]

where $\Sigma^{R(A)}$ are the coherent potentials (C.P.) for the retarded and advanced Green functions, which have to be found from the C.P.A equation:

\[
\bar{t} = (1 - x) \frac{(\varepsilon^{A} - \Sigma)}{1 - (\varepsilon^{A} - \Sigma)G_{\text{eff}}(z_0, \rho_0; z_0, \rho_0)} + (x) \frac{(\varepsilon^{B} - \Sigma)}{1 - (\varepsilon^{B} - \Sigma)G_{\text{eff}}(z_0, \rho_0; z_0, \rho_0)} = 0 
\]

where $\varepsilon^{A}$ and $\varepsilon^{B}$ are the onsite energies of the host ($\text{Al}_2\text{O}_3$) and the impurity ($\text{Al}$) and $\Sigma^{++} = i(n_R + n_L)(\Sigma^{R} - \Sigma^{A})$.

Now to calculate the I-V characteristic, we can use the previously found expression for $G_{\alpha\alpha}^{-+\text{P(AP)}}$ and substitute it into the expression (5).

In Fig.5, the I-V characteristic in the AP configuration is shown. An asymmetry of the curve on the sign of the applied voltage is clearly visible.

Such a structure may be prepared for instance by sputtering a thin layer of $\text{Al}$ on the bottom $\mathbb{F}$-electrode, then oxidise it in Alumina. Thenafter, a second thicker layer of $\text{Al}$ is sputtered on the already formed Alumina barrier but this second layer is subsequently underoxidized so that a thin layer of the random alloy $\text{Al}_x\text{Al}_2\text{O}_3(1-x)$ remains inside the more or less ideal insulator $\text{Al}_2\text{O}_3$ at an assymmetric location within the barrier.

The work was partly supported by the Russian fund of fundamental research (grant N 04-02-16688a). AV, NR and NS thank CEA for financial support during their stay.

[1] J. S. Moodera, L. R. Kinder, T. M. Wong, and R. Meservey, Phys. Rev. Lett. 74, 3273 (1995).
[2] S. S. P. Parkin, Spin Dependent Transport in Magnetic Nanostructures (Taylor & Francis, 2002).
[3] J. S. Moodera and G. Mathon, JMMM 200, 248 (1999).
[4] J. C. Slonczewski, Phys. Rev. B 39, 6995 (1989).
[5] E. Y. Tsymbal and D. G. Pettifor, Phys. Rev. B 58, 432 (1998).
[6] A. Vedyayev, D. Bagrets, A. Bagrets, and B. Dieny, Phys. Rev. B 63, 064429.1 (2001).
[7] V. D. Costa, Y. Herry, F. Bordon, M. Romeo, and K. Ounadjela, Euro. Phys. J. B13, 297 (2000).

[8] E. Y. Tsymbal and D. G. Pettifor, Phys. Rev. B. 64, 212401 (2001).

[9] L. V. Keldysh, JETP 20, 1018 (1965).