Appendix A

Theoretical Model of Inverse TMR

We present here details of the theoretical model that includes the effect of spins of the tunnelling electrons and can be used to calculate, to a first approximation, the effect of band structure on the observed spin polarization and TMR. This is based on the original model due to Bürgler and Tarrach [77]. Another description has also been given by MacLaren *et al* [93].

First, the wavefunction ψ of the electrons is described in a free-electron model at the two electrodes (ψ_1 and ψ_3) and inside the tunnelling barrier (ψ_2). The wavefunctions are matched and calculated in a standard fashion and the transmission probability, $T_{\sigma\tilde{\sigma}}$, of the tunnel barrier is calculated. At the end, the net current is calculated by incorporating the densities-of-states of the two electrodes.

The terms used in the discussion below can be understood from the schematic in Fig. A.1. The free-electron wavefunctions are given by

$$\psi_1 = \begin{bmatrix} A_\uparrow e^{ik_{1\uparrow}x} + B_\uparrow e^{-ik_{1\uparrow}x} \\ A_\downarrow e^{ik_{1\downarrow}x} + B_\downarrow e^{-ik_{1\downarrow}x} \end{bmatrix}$$

$$\psi_2 = \begin{bmatrix} C_\uparrow e^{k_2 x} + D_\uparrow e^{-k_2 x} \\ C_\downarrow e^{k_2 x} + D_\downarrow e^{-k_2 x} \end{bmatrix}$$

$$\widetilde{\psi_3} = \begin{bmatrix} G_\uparrow e^{ik_{3\uparrow}(x-d)} \\ G_\downarrow e^{ik_{3\downarrow}(x-d)} \end{bmatrix}$$

$$\psi_3 = R\,\widetilde{\psi_3} = \begin{bmatrix} \cos\theta/2 & \sin\theta/2 \\ -\sin\theta/2 & \cos\theta/2 \end{bmatrix} \widetilde{\psi_3}$$

Here, $\widetilde{\psi_3}$ is the wavefunction in the second electrode at the same angle as the first and ψ_3 is the final wavefunction. This is because, when the magnetization of the second electrode is rotated by an angle θ with respect to the first, a transformation R must be used to match the wavefunctions.

To solve the above equations, we start by applying the following boundary conditions

$$\begin{array}{ll} \psi_1|_{x=0} = \psi_2|_{x=0} & \dot{\psi}_1|_{x=0} = \dot{\psi}_2|_{x=0} \\ \psi_2|_{x=d} = \psi_3|_{x=d} & \dot{\psi}_2|_{x=d} = \dot{\psi}_3|_{x=d} \end{array}$$

One can then solve for the final wavefunction, ψ_3, in terms of the initial wavefunction, ψ_1. For an incident wave, $A_{\sigma=\uparrow\downarrow}$, on the side of the first electrode, the resultant wave at the other electrode, $G_{\sigma=\uparrow\downarrow}$, is given by

$$\begin{bmatrix} G_\uparrow \\ G_\downarrow \end{bmatrix} = \begin{bmatrix} \Upsilon_\uparrow A_{22} A_\uparrow - \Upsilon_\downarrow A_{12} A_\downarrow \\ -\Upsilon_\uparrow A_{21} A_\uparrow + \Upsilon_\downarrow A_{11} A_\downarrow \end{bmatrix},$$

where A_{ij} and Υ_σ are long terms depending only upon the wavevectors $k_{i\sigma}$, the barrier width d, the potentials $\phi_{i\sigma}$ and the magnetization angle θ. Knowing these, the equations can be fully solved.

Since the flux of particles, which constitutes the current carried in a wave ψ_i is defined by

$$J_i \equiv \frac{\hbar}{2mi}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right),$$

the net current carried across the junction is

$$J_1 = \frac{\hbar}{m}\begin{bmatrix} |A_\uparrow|^2 \\ |A_\downarrow|^2 \end{bmatrix} k_1 = J_3 = \frac{\hbar}{m}\begin{bmatrix} |G_\uparrow|^2 \\ |G_\downarrow|^2 \end{bmatrix} k_3$$

In other words, the tunnelling probability, $T_{\sigma\tilde{\sigma}}$, of going from an initial state, σ in electrode 1, to a final state, $\tilde{\sigma}$ in electrode 3, can be written as

$$T_{\sigma\tilde{\sigma}} = \left|\frac{G_{\tilde{\sigma}}}{A_\sigma}\right|^2 \cdot \frac{k_{3\tilde{\sigma}}}{k_{1\sigma}}$$

This expression is equivalent to those given by both Maclaren *et al* and Bürgler and Tarrach.

We now calculate the net tunnelling current. With a bias V applied, the shaded region shown in Fig. A.1 depicts the electron states that are available. For an angle θ between the electrodes, the net current should be calculated after summing over all combinations of initial and final spin states: i.e., $\sigma =\uparrow$ to $\tilde{\sigma} =\uparrow$, $\sigma =\uparrow$ to $\tilde{\sigma} =\downarrow$, etc. We then get the result

$$I(\theta) \propto \sum_{\sigma,\tilde{\sigma}} \int_{-V}^{0} \rho_1^{\sigma}(E_F^1 + E) T_{\sigma\tilde{\sigma}}(E_F^1 + E) \rho_3^{\tilde{\sigma}}(E_F^3 + V + E) dE$$

As the integral proceeds over all states between the two fermi levels, the densities of states $\rho_i^{\sigma}(E)$ of the two electrodes are taken into account. Finally, the TMR of the junction can be calculated with the formula

$$\frac{\Delta R}{R_p} = \frac{I(\theta = 0)}{I(\theta = \pi)} - 1$$

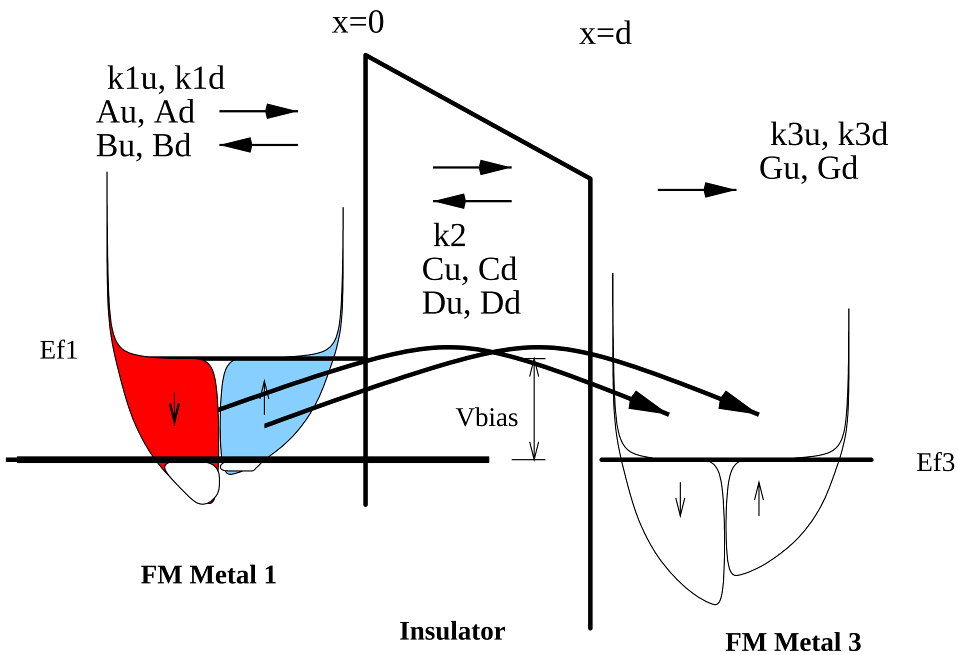

Figure A.1: Theoretical model for calculation of TMR.