Journal of Magnetism and Magnetic Materials 465 (2018) 333–338

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Research articles

Effects of temperature on the magnetic tunnel junctions with periodic grating barrier

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ARTICLE INFO

Keywords:
Magnetic tunnel junction
Tunneling magnetoresistance
Effect of temperature
Spin-polarized transport
Spintronics

ABSTRACT

We have developed a tunneling theory to describe the temperature dependence of tunneling magnetoresistance (TMR) of the magnetic tunnel junctions (MTJs) with periodic grating barrier. Through the Patterson function approach, the theory can handle easily the influence of the lattice distortion of the barrier on the tunneling process of the electrons. The lattice distortion of the barrier is sensible to the temperature and can be quite easily weakened by the thermal relaxation of the strain, and thus the tunneling process of the electrons will be significantly altered with the variation of the temperature of the system. That is just the physical mechanism for the temperature dependence of the TMR. From it, we find two main results: 1. The decrease of TMR with rising temperature is mostly carried by a change in the antiparallel resistance (R_{AP}), and the parallel resistance (R_P) changes so little that it seems roughly constant, if compared to the R_{AP}. 2. For the annealed MTJ, the R_{AP} is significantly more sensitive to the strain than the R_P, and for non-annealed MTJ, both the R_P and R_{AP} are not sensitive to the strain. They are both in agreement with the experiments of the MgO-based MTJs. Other relevant properties are also discussed.

1. Introduction

Magnetic tunnel junctions (MTJs) have received considerable attention for many years. They can be applied to the promising spintronic devices such as high-density magnetic reading head [1]. Early experimental studies were confined to the MTJs with amorphous aluminum oxide (Al-O) barriers. In 2001, Butler et al. [2] predicted theoretically that, if single-crystal MgO is used as the MTJ barrier, the tunneling magnetoresistance (TMR) can reach a extremely high value. The prediction was verified soon by Parkin et al. [3] and Yuasa et al. [4]. Since then, the MgO-based MTJs have been widely investigated over the last decade [5–14]. One of the most important and distinguished properties of MgO-based MTJs is that the parallel resistance (R_P), the antiparallel resistance (R_{AP}), and the TMR all oscillate with the barrier thickness [4,11–14], which is radically different from the case of Al-O-based MTJs where no such oscillation is found. Those oscillations have already been well interpreted by the spintronic theory developed previously by us [15]. The theory is founded on the traditional optical scattering theory [16]. Within it, the barrier is treated as a diffraction grating with intralayer periodicity. It is found that the periodic grating can bring strong coherence to the tunneling electrons, the oscillations being a natural result of this coherence. Besides the oscillations, the theory can also explain the puzzle why the TMR is still far away from infinity when the two electrodes are both half-metallic.

Experimentally, there is another important property for MgO-based MTJs, that is, the temperature dependences of the R_P, R_{AP} and TMR. It is found that, as usual, the TMR will decrease when the temperature of the system increases. However, the decrease of TMR with rising temperature is mostly carried by a change in the R_{AP}. The R_P changes so little that it seems roughly constant, if compared to the R_{AP} [3,17–25]. Theoretically, the modified version of the magnon excitation model [26] is at hand for the mechanism of the above temperature dependence. However, this model can not explain the TMR oscillation on the thickness of MgO barrier. Physically, that is because it dose not include the effect of the periodicity of the single-crystal barrier which plays a key role in the scattering process when the electrons tunnel through the barrier. Based on this reason, we would like to extend our previous theory to interpret the temperature dependences of the R_P, R_{AP} and TMR of MgO-based MTJs.

As well known, the MgO-based MTJs are fabricated through epitaxial growth. Hence there will be lattice mismatch and interfacial defects between the barrier and its neighbouring layers. Obviously,

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https://doi.org/10.1016/j.jmmm.2018.06.028
Received 23 November 2017; Received in revised form 1 May 2018; Accepted 11 June 2018
0304-8853/

both of them can cause some lattice distortion to the barrier. The influences of this lattice distortion have been investigated widely by the experiments [4,27,28]. In particular, Ref. [27] discovers that, if the MTJ is annealed, the R_{AP} will increase with raising of strain, which is much more sensitive than the R_P, and if it is non-annealed, the R_{AP} will unchange with the strain. In addition, Ref. [28] finds that the lattice distortion can modify the band gap of the MgO barrier. Based on those facts, we shall take into account the effect of the lattice distortion of the barrier upon the R_P, R_{AP} and TMR within the framework of our previous work. Our aim is to interpret theoretically the temperature dependences of the RP, RAP and TMR of MgO-based MTJs. As will be seen in the following, this effect can account for the temperature dependences of the R_P, R_{AP} and TMR of MgO-based MTJs.

2. Method

To begin with, let us consider a MTJ with a perfect single-crystal barrier. As in Ref. [15], we suppose that the atomic potential of the barrier is $v(\mathbf{r})$, and that the total number of the layers of the barrier is n. Then, the periodic potential $U(\mathbf{r})$ of the barrier can be written as

$$U(\mathbf{r}) = \sum_{l_3=0}^{n-1} \sum_{\mathbf{R}_h} v(\mathbf{r}-\mathbf{R}_h-l_3\,\mathbf{a}_3), \tag{1}$$

where $\mathbf{R}_h$ is a two-dimensional lattice vector of the barrier: $\mathbf{R}_h = l_1\,\mathbf{a}_1 + l_2\,\mathbf{a}_2$, with $\mathbf{a}_1$ and $\mathbf{a}_2$ being the primitive vectors of the atomic layers, and l_1 and l_2 the corresponding integers. The $\mathbf{a}_3$ is the third primitive vector of the barrier, with l_3 the corresponding integer. Letting $\mathbf{e}_z = \mathbf{a}_1 \times \mathbf{a}_2/|\mathbf{a}_1 \times \mathbf{a}_2|$, we shall set $\mathbf{e}_z$ pointing from the upper electrode to the lower one, which is antiparallel to the direction of the tunneling current. As pointed out in Ref. [15], it is just the periodicity of the potential of barrier that will cause strong effect of coherence to the electrons passing through it. The diagrammatic sketches of this physical picture have been shown in Figs. 1 and 6 of Ref. [15].

Now, let us consider the effect of the lattice distortion of the barrier. Physically, the periodic potential $U(\mathbf{r})$ of the barrier will be modified by the lattice distortion, as stated in Ref. [28]. In order to elucidate the effect of the distortion on the potential $U(\mathbf{r})$, we would employ the Patterson function approach, which is a standard and very powerful method for studying the diffraction by imperfect crystals [16]. Within the framework of two-beam approximation [15,16], this leads to that the Fourier transform $v(\mathbf{K}_h)$ of the atomic potential undergoes a modification as follows,

$$v(\mathbf{K}_h) = \left(1 + 2\frac{\sigma}{1-\sigma}\cos(\mathbf{K}_h\cdot\alpha)\right)(1-\sigma)v_0(\mathbf{K}_h), \tag{2}$$

where $\mathbf{K}_h$ is a planar vector reciprocal to the intralayer lattice vectors $\mathbf{R}_h$, $\sigma$is the defect concentration, α represents the effect of strain of the

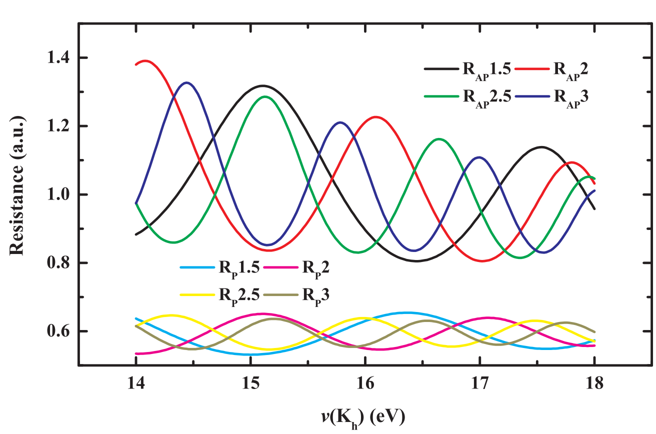

Fig. 1. R_P and R_{AP} as functions of $v(\mathbf{K}_h)$ under different barrier thickness d = 1.5 nm, 2 nm, 2.5 nm, and 3 nm.

barrier [16], and $v_0(\mathbf{K}_h)$ is the Fourier transform of the atomic potential of ideal perfect barrier,

$$v_0(\mathbf{K}_h) = \Omega^{-1}\int d\mathbf{r}\,v(\mathbf{r})e^{-i\mathbf{K}_h\cdot\mathbf{r}}. \tag{3}$$

Here, Ω is the volume of the primitive cell of the barrier: $\Omega = (\mathbf{a}_1 \times \mathbf{a}_2)\cdot\mathbf{a}_3$.

With regard to the strain α, Ref. [29] has studied it both experimentally and theoretically on some oxide heterostructures, it is found that, within the low temperature region, the strain decreases linearly with temperature T as follows,

$$\alpha = \alpha_0\left(1-\frac{T}{T_c}\right), \quad T < T_c, \tag{4}$$

where α_0 is the strain of the oxide film at zero temperature, and T_c is the recovery temperature above which the strain disappears. Generally, T_c is around 800 K. As pointed in Ref. [29], this result can be applied to other oxide heterostructures. Therefore, we would like to employ it to handle the strain of MgO barrier. As to the defect concentration σ, it should be independent of the temperature because the energy to excite defects within a lattice is too high.

Combining the Eqs. (2) and (4) above, we obtain

$$v(\mathbf{K}_h) = \left[1 + 2\frac{\sigma}{1-\sigma}\cos\left(\mathbf{K}_h\cdot\alpha_0\left(1-\frac{T}{T_c}\right)\right)\right](1-\sigma)v_0(\mathbf{K}_h). \tag{5}$$

This equation builds the relationship between the Fourier transform $v(\mathbf{K}_h)$ of the atomic potential of realistic imperfect barrier and the temperature T.

Now, according to Ref. [15], the transmission coefficient for the channel of the spin-up to spin-up tunneling reads as follows,

$$\begin{aligned} T_{\uparrow\uparrow}(\mathbf{k}) = \frac{1}{8k_z}\{&p_+^z e^{i[p_+^z-(p_+^z)^*]d} + p_-^z e^{i[p_-^z-(p_-^z)^*]d} + q_+^z e^{i[q_+^z-(q_+^z)^*]d} \\ &+ q_-^z e^{i[q_-^z-(q_-^z)^*]d} + [p_+^z e^{i[p_+^z-(p_-^z)^*]d} + p_-^z e^{i[p_-^z-(p_+^z)^*]d} - q_+^z e^{i[q_+^z-(q_-^z)^*]d} \\ &- q_-^z e^{i[q_-^z-(q_+^z)^*]d}] + \text{c. c.}\} \end{aligned} \tag{6}$$

where $\mathbf{k}$ is the incident wave vector of tunneling electrons, and k_z its z-component, d is the thickness of MgO barrier, and

$$p_\pm^z = [\mathbf{k}^2-\mathbf{k}_h^2 \pm 2m\hbar^{-2}v(\mathbf{K}_h)]^{1/2}, \tag{7a}$$

$$q_\pm^z = [\mathbf{k}^2-(\mathbf{k}_h + \mathbf{K}_h)^2 \pm 2m\hbar^{-2}\,v(\mathbf{K}_h)]^{1/2}. \tag{7b}$$

Here, $\mathbf{k}_h$ is the planar component of $\mathbf{k}$. Since $v(\mathbf{K}_h)$ is a function of T now, the transmission coefficient $T_{\uparrow\uparrow}(\mathbf{k})$ will also be a function of T. That is to say, the tunneling process will vary with temperature.

From $T_{\uparrow\uparrow}$, the conductance $G_{\uparrow\uparrow}$ for the channel of the spin-up to spin-up tunneling can be obtained as follows,

$$G_{\uparrow\uparrow} = \frac{e^2}{16\pi^3\hbar}\int_0^{\pi/2} d\theta \int_0^{2\pi} d\varphi\; k_{F\uparrow}^2\,\sin(2\theta)\,T_{\uparrow\uparrow}(k_{F\uparrow}, \theta, \varphi), \tag{8}$$

where e denotes the electron charge, θ the angle between $\mathbf{k}$ and $\mathbf{e}_z$, φ the angle between $\mathbf{k}_h$ and $\mathbf{a}_1$, and $k_{F\uparrow}$ the Fermi wave vector of the spin-up electrons. Here, we have ignored the effect of temperature on the Fermi–Dirac distribution of the electrons of ferromagnetic electrodes, which is fairly weak in the present case because $T \leqslant 400$ K $\ll T_F$ where $T_F > 10^4$ K is the Fermi temperature for either of the electrodes. Since $T_{\uparrow\uparrow}$ is a function of T, the above equation shows that $G_{\uparrow\uparrow}$ will depend on the temperature, too.

The other three conductances, $G_{\uparrow\downarrow}$, $G_{\downarrow\uparrow}$, and $G_{\downarrow\downarrow}$, can be obtained similarly. With them, one can get $G_P = G_{\uparrow\uparrow} + G_{\downarrow\downarrow}$, $G_{AP} = G_{\uparrow\downarrow} + G_{\downarrow\uparrow}$, $R_P = G_P^{-1}$, $R_{AP} = G_{AP}^{-1}$, and $\text{TMR} = G_P/G_{AP}-1 = R_{AP}/R_P-1$.

Likewise, $G_{\uparrow\downarrow}$, $G_{\downarrow\uparrow}$, and $G_{\downarrow\downarrow}$ will also depend on the temperature of the system. Physically, that arises from the fact that $v(\mathbf{K}_h)$ varies with temperature, as shown in Eq. (5). In a word, the four conductances, $G_{\uparrow\uparrow}$, $G_{\uparrow\downarrow}$, $G_{\downarrow\uparrow}$, and $G_{\downarrow\downarrow}$, as well as the TMR will all change with the