

Influence of interface termination on the magneto-Seebeck effect in MgO based tunnel junctions

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On an *ab initio* level, we investigate the recently observed magneto-Seebeck effect in MgO based tunnel junctions. In particular, we considered ordered CoFe alloys as lead material. Next to the MgO barrier, there are different possible terminations of the CoFe alloy due to the assumed ordered alloy. These results show a strong influence of the termination on the temperature dependence of the magneto-Seebeck effect. In addition, we use a simple model to account for randomly ordered alloys. We propose, that by a controlled treatment of the CoFe/MgO interface the magneto-Seebeck effect can be tuned experimentally. © 2012 American Institute of Physics. [doi:10.1063/1.3675987]

I. INTRODUCTION

The magneto-Seebeck effect is one effect in the new field of spin caloritronics,¹ which is the combination of two research fields: magnetism (spintronics) and thermoelectric. The effect describes the dependence of the Seebeck coefficient (or thermopower) in a spin valve or tunnel junction on the relative magnetic orientation of the ferromagnetic leads. This way the effect is similar to giant magneto resistance (GMR) and tunnel magneto resistance (TMR) but for the thermopower instead of electrical resistance.

The effect was experimentally observed in GMR structures² and was theoretically predicted to be high in MgO based tunnel junctions.³ Recent experiments measured the magneto-Seebeck effect in MgO based tunnel junctions with a CoFe alloy as ferromagnets.^{4,5} However, the experiments as well as the presented theoretical results for different interface terminations of the CoFe alloy were discussed at room temperature only. In this paper, we discuss the influence of the termination of the CoFe alloy on the temperature dependence of the magneto-Seebeck effect. In addition, we propose in the last section a simple model to account for disordered alloys. The different structures of the ordered alloy discussed in the following are sketched in Fig. 1. We assume ordered alloys with alternating monolayers of Fe and Co. Therefore, only the three different junctions shown in Fig. 1 are possible.

II. METHOD

We use a Korringa-Kohn-Rostoker (KKR) method based on density functional theory to calculate the electronic structure of the junctions shown in Fig. 1 self-consistently. For the transport calculation, we evaluate the transmission function $T(E)$ first. $T(E)$ is used to calculate the moments

$$L_n = \frac{2}{h} \int T(E) (E - \mu)^n (-\partial_E f(E, \mu, T)) dE, \quad (1)$$

where $f(E, \mu, T)$ is the Fermi function at a given energy E , electrochemical potential μ , and temperature T . Eventually, the conductance G and the Seebeck coefficient S are given by⁹

$$G = e^2 L_0 \quad S = -\frac{1}{eT} \frac{L_1}{L_0}. \quad (2)$$

The transmission function $T(E)$ is calculated using the non-equilibrium Green's function (NEGF) formalism implemented in KKR.⁶ The temperature dependence is considered within the Fermi function only. Although this treatment is a crucial simplification, it is justified by the experimental observation that there is only a small influence of the temperature on the TMR effect.⁷ Further, theoretical investigations of tunnel junctions with amorphous iron leads show that the transport properties are determined mainly by the crystalline iron layers next to the MgO barrier.⁸ In particular, the size and orientation of the magnetization as well as inelastic effects farther away from the MgO barrier are of second order influence. All the numerical parameters are the same like in our previous study.³ The calculation of the Seebeck coefficient is done for parallel (P) and anti-parallel (AP) alignment of the ferromagnetic leads to calculate the magneto-Seebeck S_{MS} effect by

$$S_{MS} = \frac{S_P - S_{AP}}{\min(|S_P|, |S_{AP}|)}. \quad (3)$$

III. RESULTS

A. Ordered alloy

In Fig. 2, we show the calculated magneto-Seebeck and the Seebeck coefficients for parallel and anti-parallel alignment for the junctions shown in Fig. 1 for two different barrier thicknesses. The viewgraphs clearly show that there is a strong influence of the termination of CoFe on the magneto-Seebeck effect. A similarity is that all S_{MS} are

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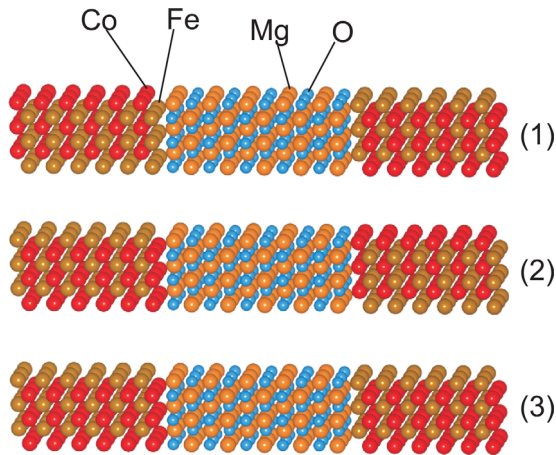


FIG. 1. (Color online) Different possible structures assuming ferromagnetic leads to alternating monolayer of Fe and Co. The thickness of the MgO barrier is 6 or 10 monolayers and of the CoFe layer is 20 monolayers. These structures are embedded between semi-infinite Cu in Fe-bcc structure, which acts as reservoirs.

positive at all temperatures, but the magnitude is quite different. In particular, the junction with different termination left and right has the highest values whereas the Co terminated junction has the smallest values.

Another common feature is the minimum of the graphs, which is around room temperature. Therefore, in experiments one has to go to larger or lower temperatures to increase S_{MS} . However, the calculations are not considering any temperature effects besides occupation. Therefore, the calculated values at higher temperatures have to be seen with caution. By making the barrier thicker, no general trend is observed. For mixed termination and for Fe termination, the

magneto-Seebeck is decreasing by increasing the barrier thickness whereas for the Co terminated junction it is the opposite behavior.

The magneto-Seebeck with Fe termination show a divergence at a temperature of about 150 K. Such a divergence can be addressed either to a vanishing Seebeck coefficient parallel or anti-parallel. Figure 2 shows that the Seebeck coefficients for the anti-parallel alignment are always negative and have an overall trend with a maximum at about room temperature. This maximum corresponds to the observed minimum in the magneto-Seebeck. Consequently, the origin of the divergence lays in a vanishing Seebeck coefficient in parallel alignment. Interestingly, at a larger barrier thickness, the divergence vanishes.

B. Disordered alloy

Up to now, we considered only ordered alloys. Experimentally, disordered alloys are more realistic. However, the discussed dependencies of the last section could be obtained by controlling the termination of the interface layer. In order to estimate the magneto-Seebeck effect in disordered alloys, we apply the simple model proposed in Ref. 10. The idea is that in a disordered alloy there are still the junctions of Fig. 1 present and we can assume that the transport through the whole junction is simply given by conducting the microscopic junctions parallel.

In particular, if we have a disordered alloy of 50% Co and 50% Fe, the probability of having junction (1) or (2) is 25% each and of having junction (3) (including the inverted one) is 50%. Conducting in parallel means that the transmission functions are just added up. Consequently, the total transmission function of a disordered alloy is

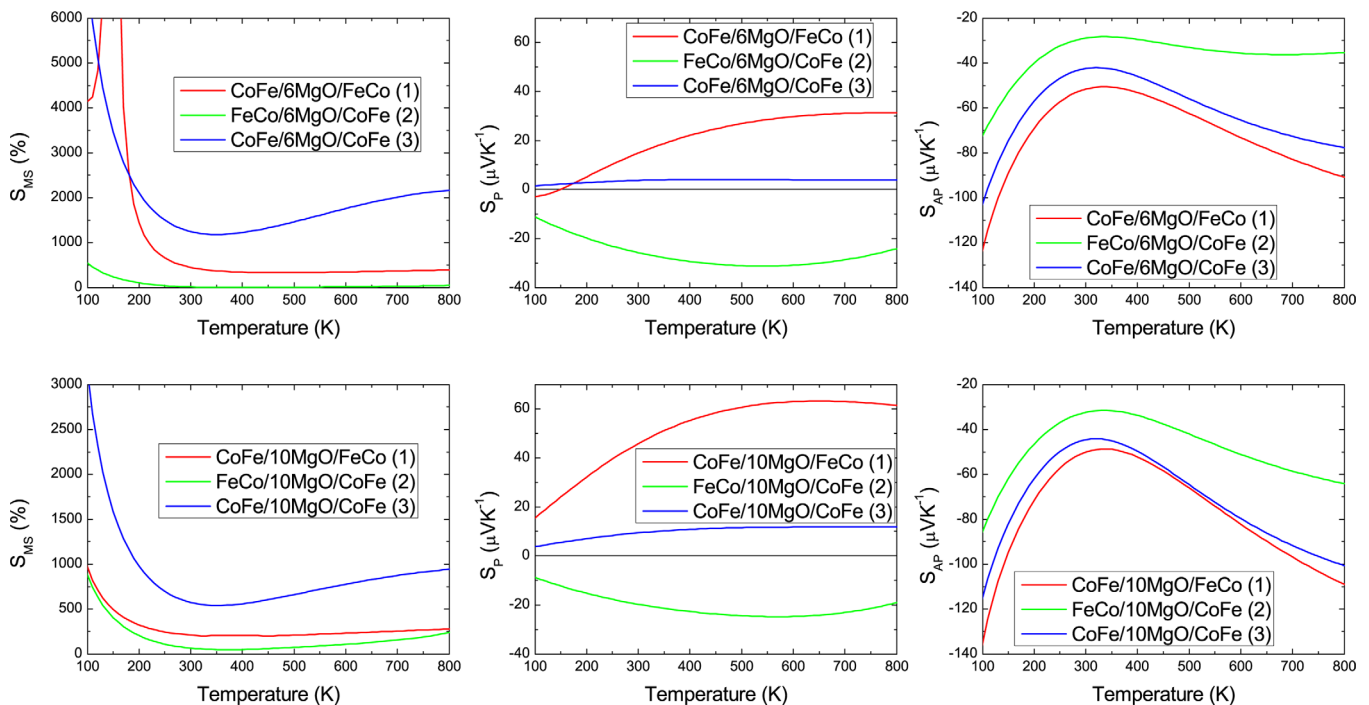


FIG. 2. (Color online) Magneto-Seebeck S_{MS} (left column) and Seebeck coefficients for parallel (middle column) and anti-parallel (right column) alignment. Top: a barrier thickness of 6 monolayers MgO. Bottom: a barrier thickness of 10 monolayers MgO. The numbering of the graphs corresponds to the junctions shown in Fig. 1.

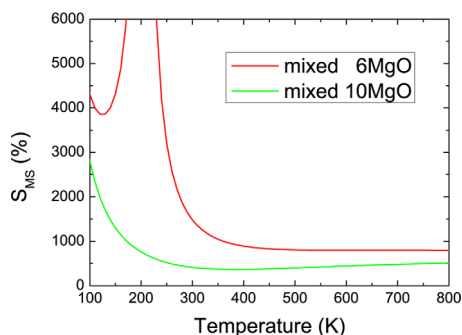


FIG. 3. (Color online) Magneto-Seebeck for disordered alloy S_{dis} (Eq. (5)) as a function of temperature. Assumed is an equal random distribution of Fe and Co at the interface, e.g., $P_1 = P_2 = 25\%$, $P_3 = 50\%$ in Eq. (5).

$$T_{dis}(E) = P_1 T_1(E) + P_2 T_2(E) + P_3 T_3(E), \quad (4)$$

where P_i is the probability to find junction i in the disordered alloy. Using this transmission function in Eq. (2) leads to the Seebeck coefficient in the disordered system

$$S_{dis} = \frac{P_1 S_1 G_1 + P_2 S_2 G_2 + P_3 S_3 G_3}{P_1 G_1 + P_2 G_2 + P_3 G_3}. \quad (5)$$

Figure 3 shows the magneto-Seebeck for the case $P_1 = P_2 = 25\%$, $P_3 = 50\%$. The important feature of this viewgraph is that the magneto-Seebeck is also always positive for all temperatures like in the case of the ordered alloys. On one hand, experiments by Liebing *et al.*⁵ show positive magneto-Seebeck effect. On the other hand, other measurements and previous calculations with an ordered CoFe in-plane supercell show negative magneto-Seebeck effect.⁴ Obviously, our proposed model Eq. (5) is too simplistic to account for a disordered alloy. Improvements could be the use of different in-plane supercells and averaging them or the use of advanced methods of alloy theory. The latter can

be achieved within KKR by using, e.g., coherent potential approximation (CPA).

IV. CONCLUSION

The termination of the CoFe alloy next to the MgO barrier influences the magneto-Seebeck effect drastically. For Fe termination at both sides of MgO even a divergence occurs for 6 monolayers of MgO. Interestingly, this divergence vanishes going to thicker MgO barrier. The proposed simple model to extrapolate from the ordered alloy to a disordered alloy was not able to capture the experimentally observed negative magneto-Seebeck effect. In the future, we plan to improve our method by using alloy theory (KKR-CPA) to account for disordered alloys.

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