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Numerical simulation of magnetization process in epitaxial Co$_2$MnSi/Cr/Co$_2$MnSi trilayers with oscillatory interlayer coupling

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Numerical simulation is carried out to investigate the magnetization process of epitaxial Co$_2$MnSi/Cr/Co$_2$MnSi trilayers with oscillatory interlayer exchange coupling. A series of the magnetization curves is successfully fitted by using a very simple model, in which the absent 180° coupling is assumed while 90° coupling and the lowest order cubic anisotropy are considered. The 90° coupling energy and the anisotropy constant can be uniquely determined, and it is revealed that the strength of 90° coupling decreases exponentially with the spacer layer thickness. © 2007 American Institute of Physics. [DOI: 10.1063/1.2713709]

Full-Heusler alloys, such as Co$_2$MnX (X=Si, Ge, etc.), were predicted as half metallic ferromagnet. These materials are characterized by a metallic density of electronic states at Fermi level ($E_F$) for one spin channel, while the states for the other spin channel display a gap at $E_F$, leading to 100% spin polarization. Such materials are expected to maximize tunnel magnetoresistance and the efficiency of spin injection in spin-electronic devices. Recent experiments demonstrated this promising improvement in tunnel magnetoresistance (TMR) junctions by using full-Heusler alloys as electrodes. Our previous work showed an enhancement of magnetoresistance and the efficiency of spin injection in polarization. Such materials are expected to maximize tunnel resistance change-area product in Co$_2$MnSi/Cr/Co$_2$MnSi trilayers. In this paper, the whole simulation results are described in detail, as well as general behavior of the calculated magnetization curves in the system without 180° coupling.

We evaluate $M_T$ (total magnetization along in applied field) versus $H$ loops by the total energy form,

$$E_T = E_K + E_Z + E_J,$$

$$E_K = K_1 t_a \sin^2 \alpha + K_2 t_b \sin^2 \beta \cos^2 \beta,$$

$$E_Z = -M_s t_d H \cos \alpha - M_s t_b H \cos \beta,$$

$$E_J = J_1 \cos(\alpha - \beta) - J_2 \cos^2(\alpha - \beta).$$

(1)

Here, $E_K$ is the anisotropy term, $E_Z$ is the Zeeman energy, and $E_J$ is the exchange coupling energy. $K$, $M$, and $t$ are, respectively, the first-order cubic magnetocrystalline anisotropy constant of CMS layers, the saturated magnetization of CMS layers, and the thickness of CMS layers. The subscripts $a$ and $b$ represent the bottom and top CMS layers, respectively. $H$ is the applied magnetic field. $\alpha$ (or $\beta$) is the angle between the magnetization and external field (or top) CMS layers. $J_1$ and $J_2$ are the first two terms of the general expansion of exchange coupling energy, which are known as the bilinear and biquadratic coupling energies. Positive $J_1$ leads to a ferromagnetic coupling state. Negative $J_1$ and negative $J_2$ stabilize 180° and 90° configurations, respectively. $M_T$ vs $H$ loops are simulated by minimizing the total energy of Eq. (1).

There are too many parameters to simplify the physical issue by the energy expression shown in the Eq. (1). However, if we temporarily neglect the 180° coupling (we found that it is reasonable for our experimental observations in CMS/Cr/CMS trilayers) with the conditions of fixed $M$, $K$, and $t$, the main features of loops are solely determined by the value of $J_2$. When $M_s=800$ emu/cm$^3$, $K_a=3 \times 10^4$ ergs/cm$^3$, $t_a=20$ nm, and $t_b=10$ nm, the corresponding $M_T$ can then be calculated and is shown in Fig. 1 for several different values of $J_2$. It is assumed that the system is
in its lowest energy configuration at each calculation field. First, one can see that there is an abrupt jump in the case of small values of $-J_2$. With a larger value of $-J_2$, the abrupt jump becomes a second order change. This transition can be understood as the result of the energy competition between the coupling energy term and the anisotropy energy term. As shown in Fig. 1, $K_t$ is 0.09 erg/cm$^2$ and the transition happens while $-J_2$ is comparable to $K_t$. In a series of samples with different thicknesses of spacer layers, even if $K$ is not determined by experiment, we can change $K$ and $J$ at the same time to evaluate two curves on both sides of the critical transition point. Since the saturation field is given by $J_2$ and $K$, and $-J_2 \approx K_t$ at the critical transition, then the $K$ can be uniquely determined for the series of samples. Second, the remanence ratio $M_r/M_s$ solely depends on the ratio of magnetic moment between top and bottom magnetic layers since the 90° alignment appears at zero field, when $M_r$ is total saturation magnetization at high field and $M_s$ is remanence of the total magnetization at zero field. As $M_a=M_b$, $M_r/M_s$ ratio can be simply determined as $t_a/(t_a+t_b)$, which is $\approx 0.67$.

The above analysis is just pure mathematics. However, we find that this quite simple analysis with $J_1=0$ gives a good agreement with our latest experiments in CMS/Cr/CMS trilayers.

Figure 2 shows the $M_T$ vs $H$ loops of the samples CMS(20 nm)/Cr(tCr)/CMS(7 nm) ($t_{Cr}=0.3–7.2$ nm). The open circles are the experiment data and the solid lines represent the simulation results based on Eq. (1) with condition of $J_1=0$, $M_a=888.9$ emu/cm$^3$, $M_b=839.1$ emu/cm$^3$, $t_a=20$ nm, $t_b=7$ nm, and $K_a=K_b=K=3 \times 10^4$ ergs/cm$^3$. There
are three kinds of loops observed in these samples. Figures 2(a), 2(e), and 2(i), are typical FM-coupling-type loops. In these cases, $J_2=0$ is reasonable. The other loops belong to NFM-coupling-type and can be classified into two cases: ones with jumps and the others without jumps, which mean that a transition happens in the magnetization process as described in the above analysis. First, it is found that samples shown in Figs. 1(g) and 1(h) have different type loops, however, they have a quite similar $H_s$ and only 0.3 nm difference of $t_{Cr}$. The transition should occur between them. The best fitting for these two curves by changing $K$ and $J$ results in $K_s=K_0=3 \times 10^4$ ergs/cm$^3$, which corresponds to $Kt=0.081$ erg/cm$^2$. Then we use this critical value to evaluate all the samples and find that it is reasonable for all the loops in this series of samples. Additionally, the value of $K$ is only a little smaller than that derived from magnetization measurements in the hard and easy axes.

In the case of sample with a 0.3 nm Cr spacer layer, a discontinuity Cr layer might form which leads to a direct coupling between CMS layers. However, as $t_{Cr}$ increases to 1.2 nm, the FM coupling behavior disappears, as shown in Fig. 2(b). $H_s$ increases up to $\sim 8000$ Oe and $M_s/M_i$ decreases from 1 to $\sim 0.75$. Further increasing $t_{Cr}$ to 2.1 nm, $M_s/M_i$ remains as $\sim 0.75$, while the value of $H_s$ decreases to $\sim 2000$ Oe, as seen in Fig. 1(c). In these two cases, the shape of loops show no abrupt jump, which means the coupling energy should be larger than anisotropy energy term $Kt=0.081$ erg/cm$^2$. The fitting results show that $-J_2$ equals 1.85 ergs/cm$^2$ for Fig. 1(b) and 0.5 erg/cm$^2$ for Fig. 1(c). In Fig. 1(d), steps appear in the loops with the same $M_s/M_i$ ratio but a much smaller $H_s$ value (30 Oe), which leads to a small value of $-J_2$ (0.018 erg/cm$^2$) compared to $Kt$. From Figs. 1(b)–1(d), for the best fitting, $-J_2$ changes rapidly from 1.85 ergs/cm$^2$ down to 0.018 erg/cm$^2$ while $J_1$ is assumed to be zero. In Fig. 1(e), FM coupling appears again. In Figs. 1(f) and (1h), jumps can be clearly seen in the loops, which are correctly reflected by the fitting results, i.e., $-J_2=0.009$ and 0.04 erg/cm$^2$, respectively. In Fig. 1(g), the loops without jumps are observed and $-J_2$ equals 0.086 erg/cm$^2$, which is just a little higher than the value of $Kt$. Figure 1(i) shows a FM-type loops in sample with $t_{Cr}=6.9$ nm. Finally, a weak 90° coupling is obtained in sample with $t_{Cr}=7.2$ nm ($-J_2=0.0085$ erg/cm$^2$), as shown in Fig. 1(j). Note that one important common feature of the samples shown in Fig. 1 is that, in all NFM coupling samples, the $M_s/M_i$ ratio remains as $\sim 0.75$, which can be explained by the ratio between top and bottom magnetizations of CMS quantitatively.

The thickness dependence of calculated $-J_2$ is plotted in Fig. 3. It is found that the 90° coupling strength decreases exponentially with $t_{Cr}$, which is in contrast to the power-law dependence commonly observed in Fe/Cr and Co/Cu systems. The exponential decay of 90° coupling strength might be characteristic of the interlayer coupling in Heusler alloy based trilayers. The long period of oscillation might be related with CMS since it has a unique electronic structure compared with the case of conventional transition metals. $J_2$ playing a dominant role in half metal based nanostructures has also been reported by Ambrose et al. in single crystal Co$_2$MnGe/NM(Mn,V)/Co$_2$MnGe trilayers. Our observation is consistent with their report and has presented the oscillation nature of the 90° coupling. It is also noted that the proximity model proposed by Slonczewski can describe the interlayer exchange coupling well especially in the case of Cr spacer layer. We have also performed numerical simulation for our data by this model. Both models show a clear 90° coupling in our series samples.

In conclusion, we have studied a quite simple simulation model for magnetization process, in which the absent 180° coupling is assumed, while 90° coupling and the lowest order cubic anisotropy are considered. $J_2$ and $K$ can be uniquely determined from the simulation, which is the result of energy competition between coupling and anisotropy energies. The calculated curves show a good agreement with the magnetization loops in CMS/Cr($t_{Cr}$)/CMS ($t_{Cr}=0.3–7.2$ nm) samples. It is revealed that the strength of 90° coupling decreases exponentially with $t_{Cr}$. This characteristic IEC behavior will be a challenge for theoretical explanation.

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