C5

Electronic structure and spin polarization of advanced CPP-GMR Heusler alloys $Co_2Fe(Si\text{-}Al)$ and $Co_2Fe(Ga\text{-}Ge)$

Oleg Mryasov[1,2], Sergey Faleev[2]
[1]Physics and Astronomy, University of Alabama, Tuscaloosa, AL, USA
[2]MINT Center , University of Alabama, Tuscaloosa, AL, USA

Recently, it has been demonstrated that GMR response can be significantly enhanced by incorporating high spin polarization ferromagnetic (FM) full Heulser alloy into spin valve nano-structures. Experimental results for two types of non-magnetic spacers (i) elemental metal [1] and (ii) non-magnetic Heusler alloy spacers [2,3] indicate promising routes towards advanced CPP-GMR. In particular, (001) textured combination of FM full Heusler alloys Co_2MnSi and $Co_2Fe(Si\text{-}Al)$ with Ag yielded MR values in excess of 28 % and ΔRA of 8.8 $m\Omega-\mu m^2$ and very recently (100) $Co_2Fe(Ga\text{-}Ge)/Ag/Co_2Fe(Ga\text{-}Ge)$ (CFGG/Ag/CFGG, $RA=30m\Omega\text{-}\mu m^2$, ΔRA = 9.5 $m\Omega\text{-}\mu m^2$ [3]. More practical (110) textured combination of Co_2MnGe (CMG) and non-magnetic Heusler alloy Rh_2CuSn (RCS) [2] have been used to build test hard disk drive reader and yielded MR of about 7 % and ΔRA of about 4.0 $m\Omega-\mu m^2$ [4]. In this work, we investigate electronic structure and spin polarization of end point of quaternary alloys $Co_2Fe(Si\text{-}Al)$ and $Co_2Fe(Ga\text{-}Ge)$ use of which as proven experimentally lead to CPP-GMR enhancement [1,3]. We employ beyond DFT-LDA method QSGW [5] for reliable calculations of minority band gaps. This approach enables accurate parameters free calculations of minority electronic structure and thus reliably predict whether material has true half-metallic features. We find that Co_2FeAl and Co_2FeGe are true half metals while Co_2FeSi has dispersed band in the direction of CPP transport for (110) textured films. Results are in a good agreement with available magnetization measurements.

References:

[1]. T. Iwase, Y. Sakuraba, S. Bosu, K. Saito, S. Mitani, K. Takahashi, Appl Phys. Express, v.2, p. 063003 (2009) ; T.M. Nakatani et.al., APL., v. 96, p. 212501 (2010)

[2] T. Ambrose and O. Mryasov, US Patent 6, 876, 522 (April 5. 2005) T. Ambrose and O. Mryasov, in "Half-metallic Alloys: fundamentals and applications", Springer Verlag Series 676, 187 (2005).

[3]. Y. K. Takahashi, A. Srinivasan, B. Varaprasad, A. Rajanikanth, N. Hase, T.M. Nakatani, S. Kasaki, T. Furubayashi and K. Hono, Appl. Phys. Lett. **98**, 152501 (2011).

[4]. K. Nikolaev, P. Kolbo, T. Pokhil, X. Peng, Y. Chen, T. Ambrose and O. Mryasov, APL., v.94, p. 222501 (2009).

[5]. Faleev, O. Mryasov, and T. Mattsson, "Quasiparticle Self-consistent GW Calculation of the Work Function of Al (111), Al(100) and Al (110)," Phys. Rev. B. 81, 205436-20542 (2010), and references therein.