First principles investigation of magnetocrystalline anisotropy at Full Heusler / MgO interfaces

RAJASEKARAKUMAR VADAPOO, ALI HAL-LAL, MAIRBEK CHSHIEV, SPINTEC, CEA/CNRS/UFJ-Grenoble-INP, INAC, 38054 Grenoble, France — Magnetic tunnel junctions with perpendicular magnetic anisotropy (PMA) have the potential for realizing next generation high density non-volatile memories and logic devices [1]. The origin of high PMA in these interfaces has been explained by orbital hybridizations at interface along with spin-orbit interactions [2]. Here we present a systematic study of PMA in Heusler alloy [X2YZ]/MgO interfaces using first principle methods with X=Co, YZ=FeAl, MnGe and MnSi. Among the interfaces studied, we found that Co terminated interface of Co2FeAl/MgO gives rise to PMA value of 1.2erg/cm2 in agreement with recent experimental observations [3]. On the contrary, FeAl terminated interfaces of the same structure shows in-plane magnetic anisotropy (IMA). We also found that the most of PMA contribution originates from dyz and d2z orbitals of Co atoms at the interface. Finally, Co2MnGe and Co2MnSi structures tend to favor IMA for any termination.