Deliverable Report

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Date: 15.09.2017

TRANSPIRE

Deliverable	**Deliverable name (Short name)**	**WP No.**	**Lead participant**	**Type**	**Diss. Level**	**Date**
D4.1	ST in devices including phonon/magnon dispersion	4	TCD	Report	Public	M9

ST in devices including phonon/magnon dispersion

Here we present the phonons, magnon and finite difference spin torque for Mn$_2$Ga and the Mn$_2$Ga/MgO junction.

In this deliverable we concentrate our efforts here on understanding the properties of Mn$_2$Ga, unlike MRG Mn$_2$Ga has a well-defined crystal structure. Mn2Ga has the D0$_{22}$ with the 2b site empty.

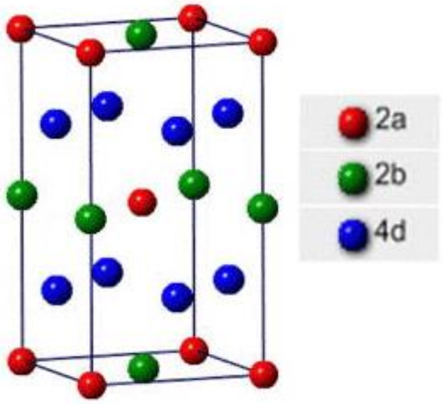	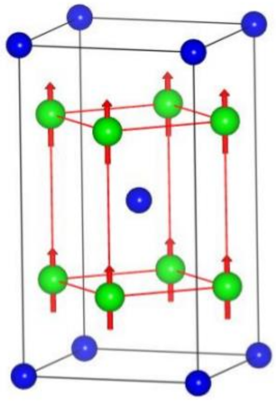
Fig 1. D0$_{22}$ structure	Fig 2. Mn$_2$Ga with Mn on 4d and Ga on 2a, 2b is empty.

Mn_2Ga

Mn_2Ga is ferromagnetic and has successfully been grown on an MgO seed layer by Kurt et al. Phys Status Solidi (b) 248 2338 (2011). We therefore assume a strain is carried though the thin film resulting in the MgO lattice parameter for the ab plane and 716pm for the c lattice parameter. Under this strain Mn_2Ga has the electronic structure shown in Fig 3. The strain of MgO slightly changes the electronic structure reducing the width of the Mn 3d manifold. The electronic structure at the Fermi level which will be responsible for the transport is largely unchanged by the strain of MgO and we still observe a large DOS for the minority spin channel as observed in the un strained structure.

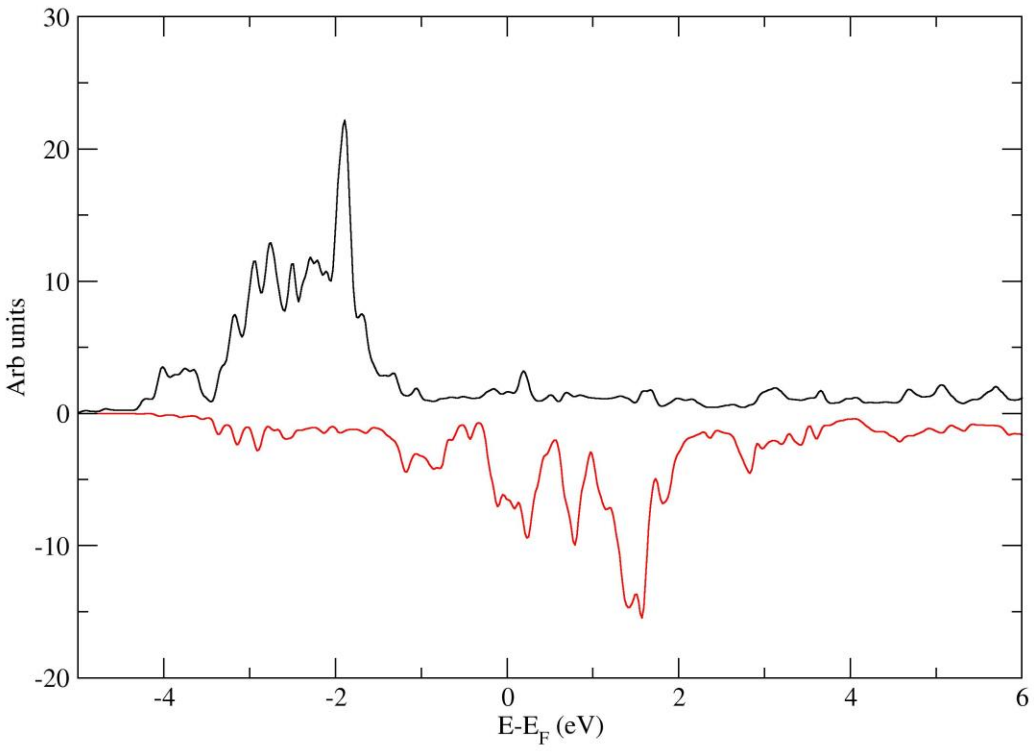

Fig 3. Mn2Ga LDOS to match the structure observed in thin film growth on MgO

The band structure of Mn2Ga and associated symmetry labels are shown in fig 4 and 5

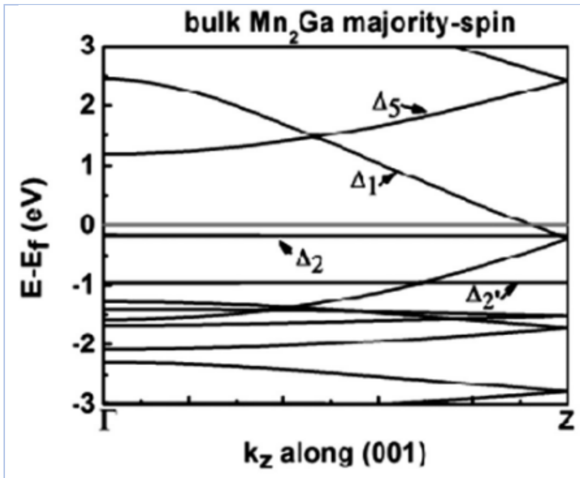

Fig 4. Mn2Ga majority spin

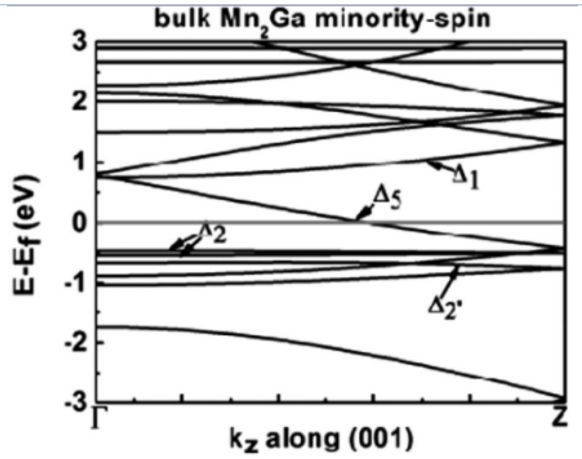

Fig5. Mn2Ga minority spin

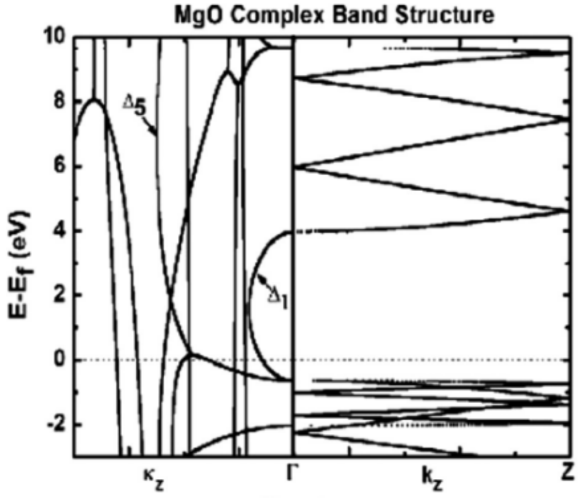

Fig 6. MgO complex band structure

With the band symmetry observed in Fig 4 and 5 coupled with the symmetry filtering characteristics of MgO we would expect that the perfect Mn2Ga/MgO/Mn2Ga junction would show a large TMR. With the largest current carried by the minority spin channel.

Mn_2Ga Magnons

To assess the magnon dispersion the code elk LAPW was used, the magnon dispersion for Mn_2Ga is shown in figure 7

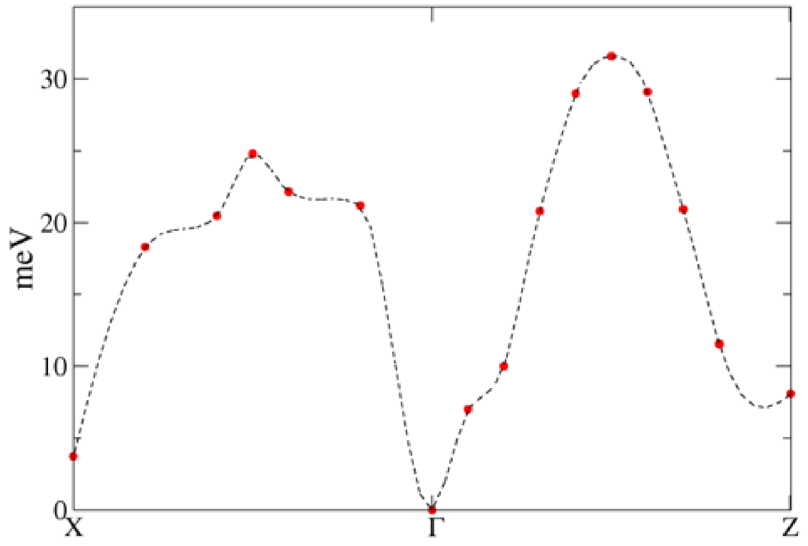

Fig 7. Magnon dispersion on Mn2Ga

The magnon dispersion can be used to evaluate the J exchange integrations and the magnetic anisotropy, these quantities will be needed to interface the ab initio calculations with the model system and the spin dynamic simulations.

Mn_2Ga Phonons

The phonon dispersion for Mn_2Ga have been calculated using the supercell finite difference approach within the Elk LAPW code show in fin Fig 8.

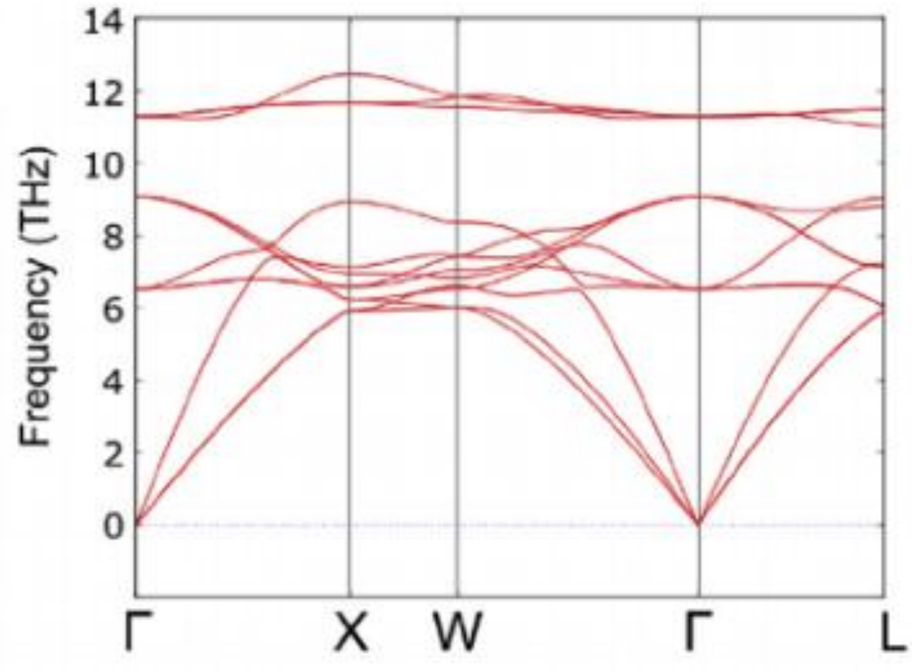

Fig 8. Mn_2Ga phonon dispersion

$Mn_2Ga/MgO/Mn_2Ga$ Junction

It is expected that the high strength of the Mn-O bond will make the termination shown in fig 9 the most stable.

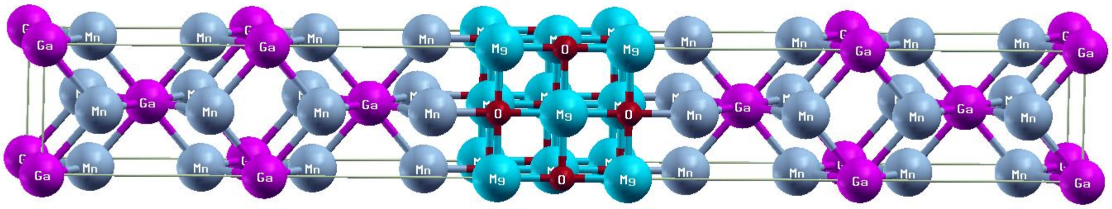

Fig 9. $Mn_2Ga/MgO/Mn_2Ga$ junction with Mn-O interface, with the junction constructed along the [001] direction of both MgO and Mn2Ga.

For the junction in Fig 9 we have used DFT with the LDA functional and the NEGF formalism to calculate the electronic structure and zero bias transmission coefficient, and the observed torque as we rotate the magnetization of the right electrode.

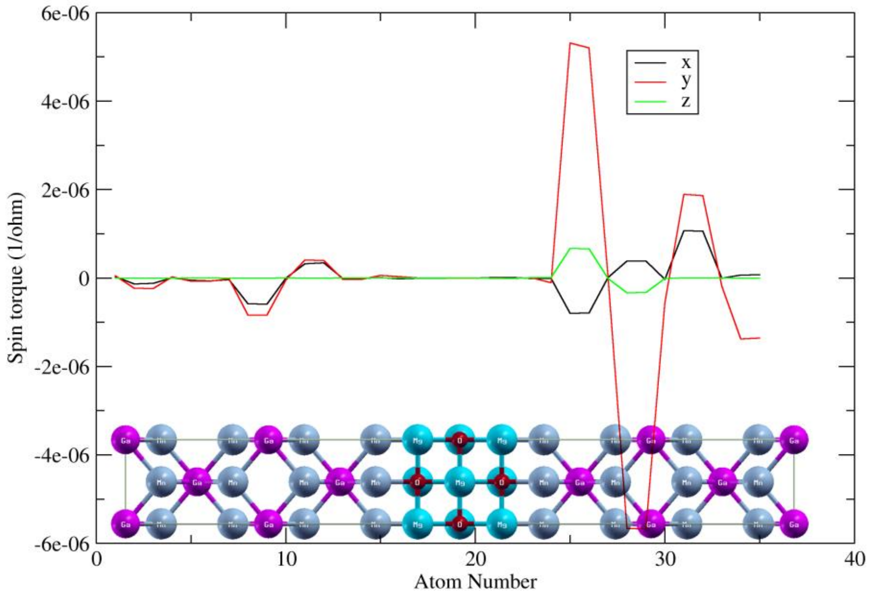

Fig 10. Spin Transfer torque due to small bias on the Mn2Ga/MgO junction, left electrode the spin points along the length of the junction, the fight electrode is rotated by 40° relative to the axis to the junction.

We have calculated the spin torque as a function of relative spin angle between the two electrodes, in Fig 9 we show an example angle of 40° from the Z direction (Z lies along the length of the junction). Fig 9 illustrates three important results which could drive the spin dynamics and will be further investigated.

1. The torque is asymmetrical on each side of the junction. Since the junction is symmetrical except the small bias applied, the fact that this material has strong spin polarization at the Fermi level is causing a significant difference between populating and emptying the different spin channels.

2. The spin-torque is concentrated at the surface, to create a predictable device will require near perfect interfaces.

3. A torque is observed on Ga, but in a different direction to Mn. The spin on Mn is in response the 40° spin polarization I.e. it is restoring the spin to a collinear spin. Ga has n in plane component as well.

Conclusion

We have calculated the phonons/magnons and spin torque for Mn2Ga and the Mn2Ga/MgO junction. These calculations are computationally heavy so full ab initio calculation for the large number of defective system to evaluate the effect of site disorder and defects is not possible.

However, the magnon spectra has proved to be valuable to evaluate the exchange interaction and anisotropy Heisenberg Hamiltonian. The spin dynamics of the Heisenberg Hamiltonians can then be simulated using the LLG equation to provide information on how MRG can be optimized for high frequency operations.