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Scope of tetragonal Manganese based Heusler alloys in context of magneto crystalline anisotropy

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Abstract

Heusler compounds are a wonderful class of materials having wide range of extraordinary multi-functionalities including halfmetallic ferrimagnets and ferromagnets, multi-ferroics, shape memory alloys, tunable topological insulators, energy technologies, and magnetocaloric and thermoelectric applications. The tunability of this class of materials is outstanding and nearly every functionality can be designed. Heusler compounds show high spin polarization in spintronic devices. Manganese-rich Heusler compounds attract much interest in the context of spin transfer torque, spin Hall effect, and rare earth free hard magnets. Most Mn_2-Heusler compounds crystallize in the inverse structure and are characterized by antiparallel coupling of magnetic moments on Mn atoms; the ferrimagnetic order and the lack of inversion symmetry lead to the emergence of new properties such as non-collinear magnetism, topological Hall effect, and skyrmions. We focus our attention on magneto crystalline anisotropy that have high values for tetragonal Heusler compounds.

Keywords: ferrimagnets, tetragonal, perpendicular magneto anisotropy, spin-transfer torque

1. Introduction

Heusler compounds are a class of materials with 1:1:1 or 2:1:1 composition comprising more than 1500 members. They were discovered by Fritz Heusler more than century ago and are still a field of active research. Novel properties and potential areas of applications emerge with time; recently the prediction of topological insulators is one of the example. The properties of many Heusler compounds can easily be predicted by the valence electron count. Their electronic structure is very flexible which allows the realization of multiple contradictory functionalities within one ternary compound. The family of Mn_2YZ Heusler compounds has attracted considerable attention for implementation as a free magnetic layer in spin-transfer torque devices such as spin-transfer torque random-access memory (STT-MRAM) [1, 2]. In these devices, a spin-polarized current is passed through a hard magnetic layer whose magnetization is switched through transfer of angular momentum. The most famous member of this group of materials is tetragonal Mn_3Ga [3]. Starting from its prediction as a compensated cubic ferrimagnet, much research in the field has been invested to promote the implementation of this compound. The reasons are [4, 5] found in its properties, namely, a low experimental magnetic moment, high perpendicular magneto-crystalline anisotropy (PMA) owing to its tetragonal structure, and a high Curie temperature of more than 700 K which ensures the thermal stability of the stored information. These properties, in combination with affordable constituent elements, make this material most attractive for high-technology utilization. Despite difficulties in the realization of such devices, other members of the Mn_2YZ family have demonstrated their potential [1, 6]. Recently, the spin-gapless semiconductor Mn_2CoAl was predicted and realized, unveiling once again the broad variety of effects to be found in Heusler materials. Peculiar transport properties were expected and have been found in such systems, making them promising candidates for room temperature semiconductor spintronics. To optimize these materials, we need a general understanding of crystal structure to design compounds with higher spin polarization and achieve compensation of the magnetization.

2. Tetragonal Crystal Structure

Apart from cubic structures of Heusler compounds, tetragonally distorted Heusler compounds have recently attracted great scientific interest in the field of spintronics, especially for spin-torque applications [7, 8]. A tetragonal distortion is observed for Mn_2YZ compounds crystallizing in the inverse Heusler structure. In this structure, the Mn atoms occupy two different lattice sites, one with tetragonal and one with octahedral coordination. Theoretical investigations by Kubler showed, that the Mn atom on the octahedral site formally possesses an oxidation state of +3 (Mn^{3+}, d^4) [9]. The electronic configuration for a single d^4 high spin ion in an octahedral environment, according to crystal field theory, is displayed in Fig. 1(a). The triple-degenerated t_{2g} orbitals and one of the double degenerated e_g orbitals are each occupied by a single electron. In fact, this electron configuration is energetically not favored, and energy can be gained by a distortion of the octahedron. Both, an elongation and a compression are possible, as shown in Fig. 1(b) and (c). These distortions lead to a lowering of the occupied orbitals resulting in an energy gain a phenomenon often referred to as Jahn-Teller distortion. Alternatively, a double degenerate van Hove singularity, i.e. a saddle point in the band structure, can lead to a tetragonal distortion since this singularity maximizes the band energy, leading to an unfavorable condition, which is avoided by a tetragonal lattice distortion.

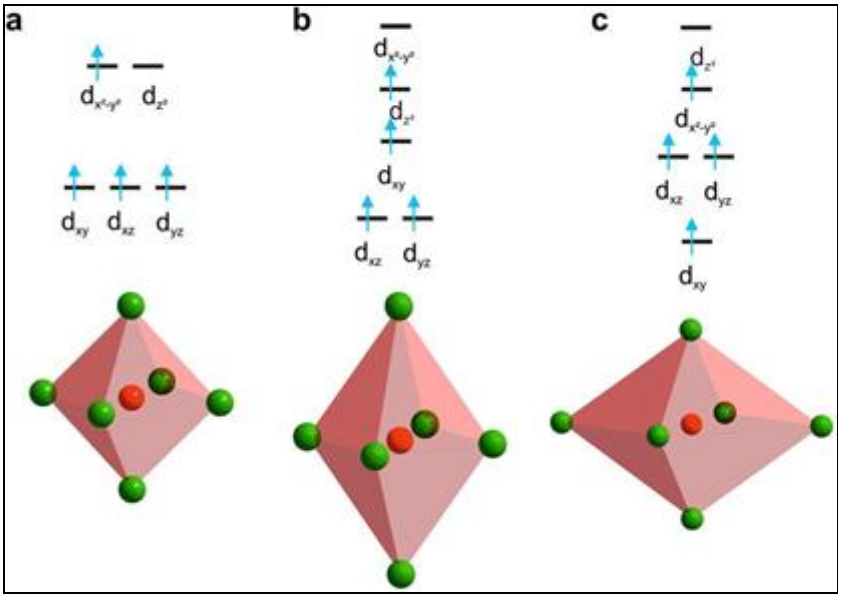

Fig 1: Crystal field splitting for a d^4 ion in an octahedral coordination sphere: (a) non distorted octahedron, (b) elongated octahedron, (c) compressed octahedron. The distortion in (b) and (c) is also known as Jahn-Teller distortion.

In the case of Mn_2YZ compounds, the cubic unit cell undergoes an elongation along the c axis, as shown in Fig. 2(a). Consequently, the symmetry of the crystal changes from the cubic space group F43m to the tetragonal spacegoup I4/mmm (space group no. 139). Fig. 2(b) and (c) illustrate the relation between the tetragonal and the cubic unit cell. The tetragonal unit cell can be derived from the cubic cell, by rotation of the cell edges by 45°. The resulting tetragonal structure is displayed in Fig. 2(d).

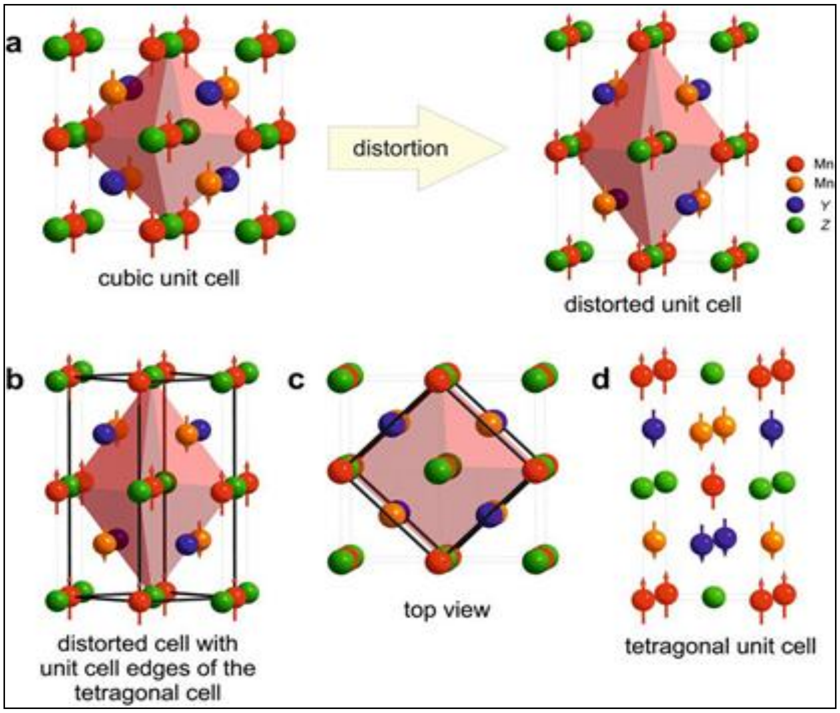

Fig 2: Relation between the cubic Heusler cell and a tetragonally distorted cell for Mn_2YZ. (a) Transition of the cubic Heusler cell to a tetragonal distorted cell with elongation along the one axis, (b) the unit cell edges of the tetragonal unit cell are marked within the cubic cell, (c) top view of the 45 rotation between the cubic and the tetragonal unit cell,(d) tetragonal unit cell with space group I4/mmm.

Similar to the Heusler structure, a regular and an inverse variant of the tetragonal cell are known (see Fig.3). The tetragonal cell derived from the Cu_2MnAl-type structure, is displayed at the bottom. The X atoms occupy the Wyckoff position 4d (0, 1/2, 1/4), the Y are placed at 2b (0, 0, 1/2) and the Z atoms are located at 2a (0, 0, 0). The prototype of this structure is Ni_2MnSn. As mentioned above, the inverse structure is frequently observed in case of Mn_2YZ materials.

Therefore, an inverse variant of the tetragonal unit cell is also possible, as shown at the top of Fig. 3. Here, the first Mn atom is located at the Wyckoff position 2b, while the second Mn atom and the Y atom are placed at the Wyckoff position 4d. Finally, the Z atom occupies the 2a position. Up to now, only few tetragonal distorted Heusler materials have been studied thoroughly, Mn_3Ga being the most prominent example [10, 11]. These materials are particularly interesting due to the perpendicular magnetic anisotropy which can be achieved in thin films [12].

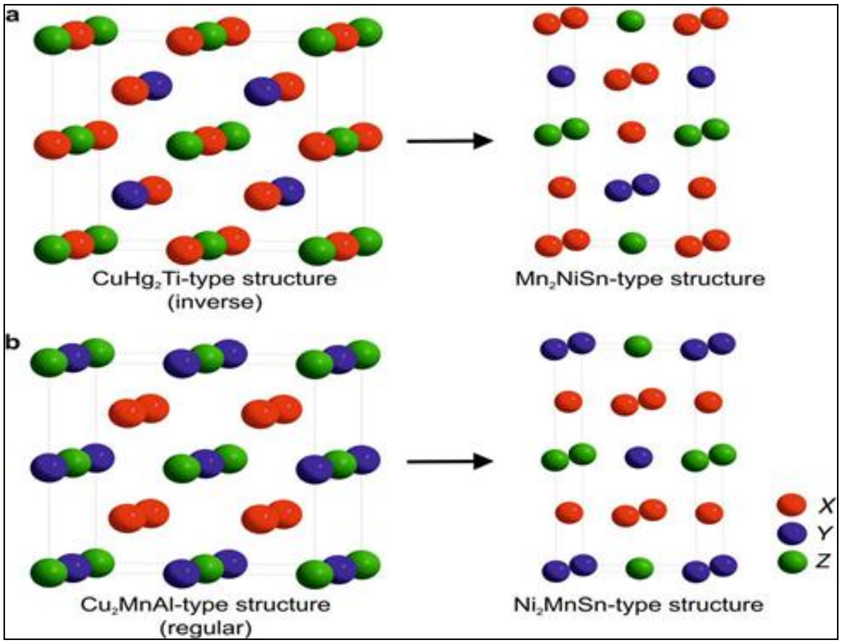

Fig 3: Comparison between the regular and the inverse Heusler structures and the corresponding tetragonally distorted unit cells.

Opening the door to spin-torque devices. Therefore, it is essential to design new materials that fulfill the corresponding criteria, i.e. low saturation magnetization, high spin polarization as well as low magnetic damping. A very intuitive route towards new tetragonal Heusler materials is sketched in. The tetragonal unit cell is closely related to the cubic fcc CuAu-type cell ($L1_0$), since doubling the cubic unit cell in one direction yields a disordered variant of the tetragonal cell. A similar relationship can be deduced for the conventional cubic Heusler materials, which can be divided into eight bcc CsCl-like subcells. These relationships make it easy to design new materials, since the combination of two materials with CuAu-type structure leads to new compounds with a tetragonally distorted unit cell. The combination of the binaries MnGa and NiMn, for example, results in the well-known shape memory alloy Mn_2NiGa. This design scheme leads to a huge variety of new materials which can be explored in future research.

3. Half-metallic ferrimagnets

Half-metallic ferrimagnetic material are appropriate candidate for the use in magnetoelectronic devices. The ferrimagnetic interactions reduce the magnetic moment due to the compensation of the moments carried by the different sublattices. These materials offer distinct advantages over their ferromagnetic counterparts which are mostly due to their small magnetic moment. The ideal compensated ferrimagnet would exhibit a total magnetic moment of zero. For such compensated ferrimagnetism which were initially named “compensated antiferromagnets” single spin superconductivity was observed by Pickett [13]. Further interesting applications can be envisioned, since they do not give rise to strong stray fields and are less affected by external magnetic fields. An ideal case for application would be a half-metallic compensated ferrimagnet since it would be a perfectly stable spin-polarized electrode in a junction device, especially for current-induced magnetic switching, which uses the spin-transfer effect. Half-Heusler compounds possess only one magnetic sublattice since only the atoms on the octahedral sites can carry a magnetic moment. So ferrimagnetic or antiferromagntic compounds do not crystallize in the Half-Heusler structures. In Heusler alloys, two magnetic sublattices allow the anti-ferromagentic coupling of the atomic magnetic moments, leading to ferrimagnetic or even completely compensated ferrimagnetic materials. In these compounds, the two atoms on the X site have to compensate the magnetic moment of the atom at the Y site (mostly Mn). The precondition for Mn to be located on the Y position is that it is the more electropositive transition metal in the compound. The only possible elements to occupy the X position are, therefore, Fe, Co, Ni, Cu, and Zn, as well as Mn itself. The two magnetic moments of the manganese atoms on the tetrahedral positions cancel the moment of the Mn^{3+} leading to zero net magnetization. The inverse Heusler structure is formed if the nuclear charge of Y is higher than the one of Mn, i.e. only for Z(Y) Mn.

4. Perpendicular magnetic anisotropy

The magnetoresistance phenomena discussed in the previous section (GMR or TMR) allows to control an electron flow through a magnetic nanostructure by its magnetic state. The reciprocal phenomenon also exists. A spin-polarized current flowing through a magnetic nanostructure can influence its magnetic state. This so-called spin-transfer torque is one of the most promising technologies today to satisfy the increasing demand for faster, smaller and non-volatile electronics. Switching the spin with a current is possible due to the exchange interaction between the spin of the incoming conduction electrons and the spin of the electrons responsible for the local magnetization, as schematically sketched in Fig. 4. A magnet usually responds to an electric current because of the magnetic field generated by the current. But if the magnet is small (typically less than 100 nm), a new force emerges [14, 15, 16]. When the electrons constituting the current pass through a magnetic conductor, their spins will become preferentially aligned to its magnetic direction, i.e. they are spin polarized. These spins may be repolarized into a new direction when they encounter another magnet (Fig. 4). In repolarizing the current, the nanomagnet experiences a torque (or turning force) associated with the change in angular momentum that occurs due to the rotation of the electron spins. This spin-transfer torque can pump enough energy into the nanomagnet to cause a precession of its magnetic moment, i.e. it moves at microwave frequencies around the symmetry axis with ever increasing amplitude until it reverses its orientation, accomplishing a magnetic switch. From an applications point of view, the thermal stability of ultra-high density magnetic memory storage devices is a crucial point. To overcome the superparamagnetic limit when decreasing the device size, thin films with Perpendicular magnetic anisotropy (PMA), i.e. with the easy magnetization axis pointing perpendicular to the film surface are advantageous. Suitable materials need to exhibit a high spin polarization, and simultaneously, a low saturation magnetization. These prerequisites make Mn_3 Ga a promising material, due to the predicted high PMA property. The ferrimagnetic coupling of the Mn atoms results in a low saturation magnetization, while the Curie temperature is higher than 770 K. The theoretical calculated spin polarization of 88% is sufficient for the desired application. The search for new materials with suitably designed properties is an active field ongoing research. Especially tetragonally distorted Heusler materials are in focus as new magnetic layers in spin-torque devices.

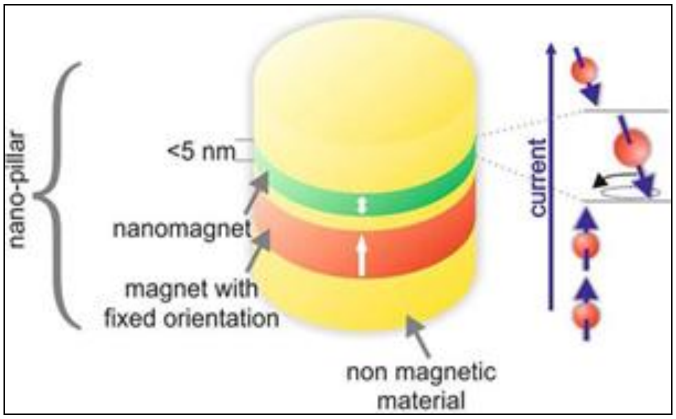

Fig 4: As conduction electrons pass a magnet, their spins preferentially align in the magnet's direction. As the electrons encounter a nanomagnet, sandwiched between layers of non-magnetic material close to the fixed orientation magnet, the direction of their spins is repolarized to match that of the nanomagnet. As a result, the nano-magnet's magnetic moment begins to precess, turning like a spinning-top about its axis.

5. Conclusion

The challenge for STT-MRAM and permanent magnets is to find tetragonal Heusler compounds with high magnetic moments, i.e., ferromagnetic coupling between the magnetic sub-lattice. Based on our knowledge today, it should be possible to design new tetragonal compounds with larger magnetic moments, but it might be difficult at first sight to design ferromagnetic Heusler compounds. Of the large number of potential tetragonally distorted Heusler compounds, including quaternary alloys, only a few are known, and the search for new compounds and a deeper understanding of the relationship between their electronic structure, magnetism, and crystal structure will likely have a high impact for all of the technological applications discussed in this article.

6. References

1. Fu L, Kane CL, Phys. Rev. Lett. 2008; 100:096407.
2. De Groot RA, Mueller FM, PGV Engen, KHJ Buschow, Phys. Rev. Lett. 1983; 50:2024.
3. Kübler J, William AR, Sommers CB, Phys. Rev. B, 1983; 28:1745.
4. Pearson's Handbook of Crystallographic Data for Intermetallic Phases, edited by Pierre Villars and Karin Cenzual, 2nd ed. ASM International, Materials Park, Ohio, 2009.
5. Nishino Y, Kato M, Asano S, Soda K, Hayasaki M, Mizutani U, Phys. Rev. Lett, 1997; 79:1909.
6. Galanakis I, Dederichs PH, Papanikolaou N. Phys. Rev. B 2002; 66:174429.
7. Wu F, Mizukami S, Watanabe D, Naganuma H, Oogane M, Ando Y, *et al.* Appl Phys Lett, 2009;94:122503.
8. Wu F, Mizukami S, Watanabe D, Sajitha EP, Naganuma H, Oogane M, *et al.* IEEE Trans Magn 2010;46:1863.
9. Kübler J, Williams AR, Sommers CB. Phys Rev B 1983; 28:1745-55.
10. Winterlik J, Balke B, Fecher GH, Felser C. Phys Rev B 2008;77:054406.
11. Balke B, Fecher GH, Winterlik J, Felser C. Appl Phys Lett 2007; 90:152504.
12. Wu F, Mizukami S, Watanabe D, Naganuma H, Oogane M, Ando Y, *et al.* Appl Phys Lett, 2009; 94:122503.
13. Pickett WE. Phys Rev Lett, 1996; 77:3185-8.
14. Slonczewski JC. J Magn Magn Mater, 1996; 159:L1-7.
15. Berger L. Phys Rev B, 1996; 54:9353-8.
16. Bazaliy YB, Jones BA, Zhang S-C. Phys Rev B, 1998; 57:R3213-6.