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Multifunctional structural and magnetic properties of Heusler compounds in relation to spintronic applications

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Abstract

Heusler compounds 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. Their electronic structure is very flexible which allows the realization of multiple contradictory functionalities within one ternary compound. Multifunctional properties based devices such as superconductivity and topological edge states has revolutionized technological applications. Heusler compounds having semiconducting properties are utilized for the development of novel materials for energy technologies. Their band gaps can easily be tuned from zero to 4eV by changing the chemical composition, so they find lot of applications in the fields of thermoelectrics and solar cell research. Heusler compounds have wide range of multifunctional properties reflected in extraordinary magneto-optical, magnetoelectronic, and magnetocaloric properties. The most prominent example is the combination of magnetism and exceptional transport properties in spintronic devices. Here we take a review of the crystal structure, the electronic structure and the relation to the magnetic properties.

Keywords: half metallic ferromagnetism, magnetoresistance, tunnel junctions, non-centrosymmetric, multifuctionality

Introduction

In the year 1903 Fritz Heusler discovered an alloy with the composition Cu_2MnAl which behaves like a ferromagnet, although non of its constituent elements is magnetic by itself [1, 2]. This remarkable material and its relatives are now known as Heusler compounds. The properties of many Heusler compounds can be predicted by simply counting the number of valence electrons [3]. Semiconducting properties of Heusler compounds are utilized as novel materials for energy technologies. As their band gaps can easily be tuned from 0 to 4 eV by changing their chemical composition. So, they attracted remarkable attention as potential candidates for solar cell and thermoelectric applications. On the basis of their calculated electronic band structures a new class of Heusler compounds was predicted called: multifunctional topological insulators, i.e. a new state of matter, in which spin-polarized edge and surface states are topologically protected against impurity scattering [4, 5]. The phenomenon of multi-functionality, i.e. the combination of two or more functionalities, like superconductivity and topological edge states in one material, is easily possible in ternary compounds. The group of magnetic X_2YZ compounds shows all kinds of magnetic behavior and multifunctional magnetic properties, such as magneto-optical [6], magneto-caloric [7] and magneto-structural characteristics [8]. The family of magneto-electrical Heusler compounds, the half-metallic ferromagnets are semiconducting for electrons of one spin orientation, whereas they are metallic for electrons with the opposite spin orientation. Such compounds exhibit nearly full spin polarized conduction electrons, and can be used as suitable materials for spintronic applications. Heusler compounds exhibits high Curie temperatures [9] and, are used in magnetic tunnel junctions [10]. Half-Heusler materials XYZ consists of a covalent and an ionic part. The X and Y atoms have a distinct cationic character, whereas Z is anionic counterpart. The most electropositive element is placed at the beginning of the formula. It can be a main group element, a transition metal or a rare earth element. Ternary Heusler compounds have the general formula X_2YZ, where X and Y are transition metals and Z is a main group element. Traditionally, the metal, which exists twice, is put at the beginning of the formula, whereas the main group element is placed at the end.

Crystal structure

There are two distinct families of Heusler compounds: one with the composition 1:1:1 and the other one with 2:1:1 stoichiometry. The compounds of the first family have the general formula XYZ and crystallize in a non-centrosymmetric cubic structure (space group no. 216, F43m, $C1_b$) which is a ternary ordered variant of the CaF_2 structure and can be derived from the tetrahedral ZnS-type structure by filling the octahedral lattice sites (Fig. 1).

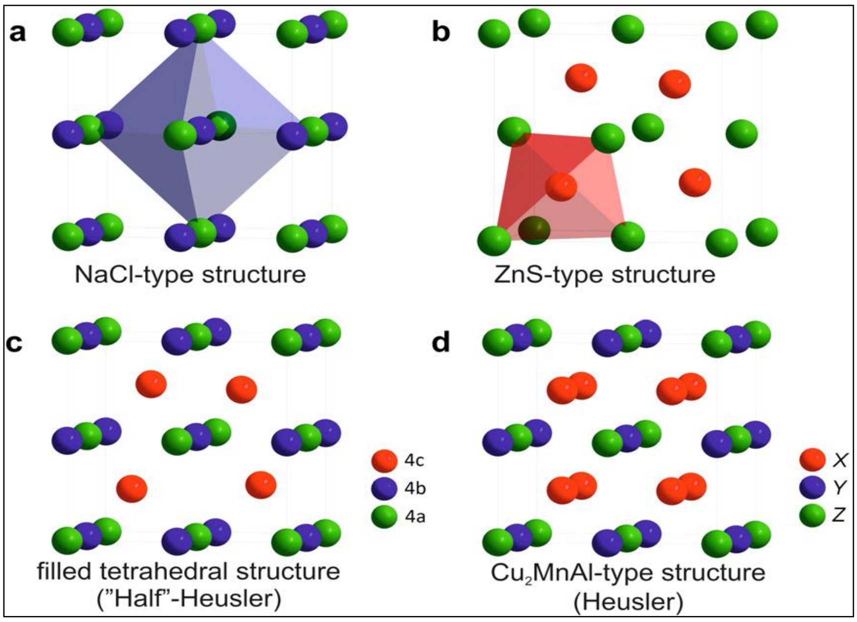

Fig 1: (a) Rock salt structure, (b) zinc blende structure (c) Half-Heusler structure (d) Heusler structure

The corresponding occupied Wyckoff positions are 4a (0, 0, 0), 4b (1/2, 1/2, 1/2), and 4c (1/4, 1/4, 1/4). The Heusler compounds X_2YZ crystallize in the cubic space group Fm3m (space group no. 225) with Cu_2MnAl ($L2_1$) as prototype [1,2,22,23]. The X atoms occupy the Wyckoff position 8c (1/4, 1/4, 1/4), the Y and the Z atoms are located at 4a (0, 0, 0) and 4b (1/2, 1/2, 1/2), respectively. This structure consists of four interpenetrating fcc sublattices, two of which are equally occupied by X. A rock salt-type lattice is formed by the least and most electropositive element (Y and Z). Due to the ionic character of their interaction, these elements are coordinated octahedrally. On the other hand, all tetrahedral holes are filled by X. This structure can also be understood as a zinc blende-type sub-lattice, build up by one X and Z, the second X occupies the remaining tetrahedral holes, whereas Y is located in the octahedral holes. These relations are illustrated in Fig. 1. In addition to the structure described above, an inverse Heusler structure is also seen, if the atomic number of Y is higher than the one of X from the same period however, it may also appear in compounds with transition metals from different periods[11]. In all cases, the element X is more electropositive than Y. The remaining X atoms and Y atoms fill the tetrahedral holes with fourfold symmetry. The structure is still described by four interpenetrating fcc sublattices and they are placed on the Wyckoff positions 4a (0, 0, 0) and 4d (3/4, 3/4, 3/4), while the Y and the Z atoms are located at 4b (1/2, 1/2, 1/2) and 4c (1/4, 1/4, 1/4), respectively. The prototype of this structure is $CuHg_2Ti$ with space group F43m (Space group no. 216). This inverse Heusler structure is frequently observed for Mn_2-based materials with Z(Y)>Z (Mn) as illustrated in Fig. 3. In case of quaternary Heusler compounds there are two different elements X and X' located at the 4a and 4d positions, respectively, Y is placed on 4b and Z on 4c. This structure has the prototype LiMgPdSn. An illustration of the inverse Heusler structure and the quaternary variant is given in Fig. 2.

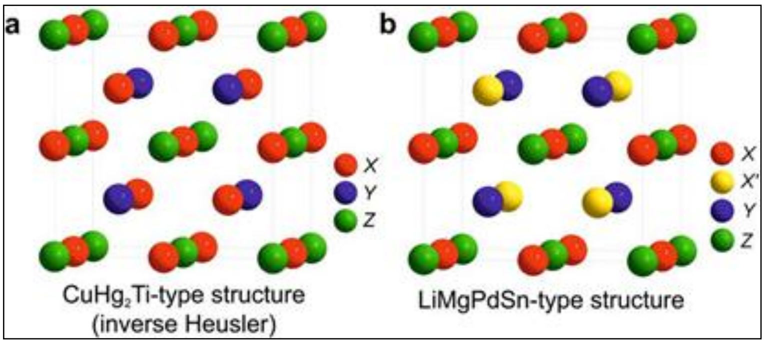

Fig 2: (a) The inverse Heusler structure $CuHg_2Ti$ and (b) the quaternary version LiMgPdSn.

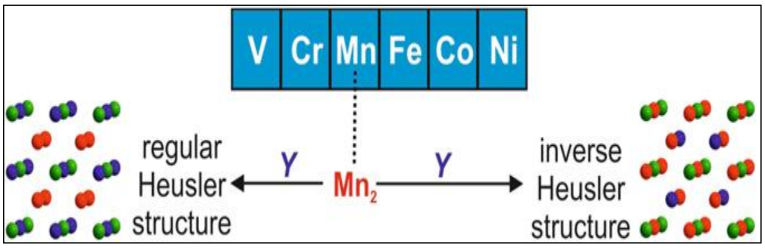

Fig 3: Mn_2-based Heusler compounds form both, the inverse and the regular structure, depending on the element on the Y position.

Magnetism and Heusler compounds

Prediction of half-metallic ferromagnetism in MnNiSb by de Groot *et al.* [12] and in Co_2MnSn by Kubler *et al.* [13] in 1983, arose scientific interest in Heusler materials. The XYZ materials exhibit one magnetic sublattice since only the atoms on the octahedral sites can carry a magnetic moment, as indicated in Fig. 4. The magnetic XYZ Half-Heusler materials exist only for X = Mn and Rare Earth(RE) because of the localized nature of the four 3d electrons of Mn^{3+} and the 4f electrons, respectively, which carry the magnetic moment. The Mn containing Half-Heusler compounds are half-metallic ferromagnets with high Curie temperatures. In the X_2YZ Heusler compounds two X atoms occupy the tetrahedral sites this allows a magnetic interaction between the X atoms and the formation of a second more delocalized magnetic sublattice (Fig. 4). Due to the two different magnetic sublattices, the X_2YZ Heusler compounds can show all kinds of magnetic phenomena like ferromagnetism, ferrimagnetism, and half-metallic ferromagnetism.

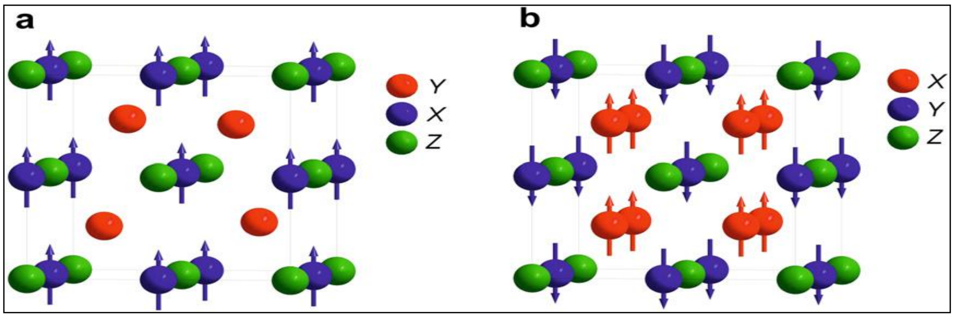

Fig 4: (a) XYZ Half-Heusler compounds exhibit only one magnetic sublattice since only the atoms on the octahedral sites carry a localized magnetic moment. (b) X_2YZ Heusler compounds have two magnetic sublattices which can couple ferromagnetically or antiferromagnetically.

Half-Metallic Ferromagnetism

Certain Heusler materials exhibit depending on the spin direction metallic as well as insulating properties at the same time, a feature called half-metallic ferromagnetism [12, 13]. De Groot and coworkers developed scheme which classified three different types of half-metallic ferromagnetism [14]. Fig. 5. displays a schematic illustration of the density of states (DOS) of (a) a metal with a finite density of states at the Fermi energy, and (b) the spin resolved representation of a metal: both spin channels are identical and equally occupied, (c) shows the DOS of a ferromagnet, in which the majority and minority states are shifted against each other, leading to a measurable net magnetization of the material, (d) a half-metallic ferromagnet (HMF) behaves like a metal for one spin direction and like an insulator for the other spin direction (e) a completely compensated half-metallic ferrimagnet. The complete spin polarization of charge carriers in a HMF is only reached in the limiting case of zero temperature and vanishing spin-orbit interactions. Since most of the Heusler compounds containing only 3d elements do not exhibit any spin-orbit coupling, they are ideal candidates to exhibit half-metallic ferromagnet.

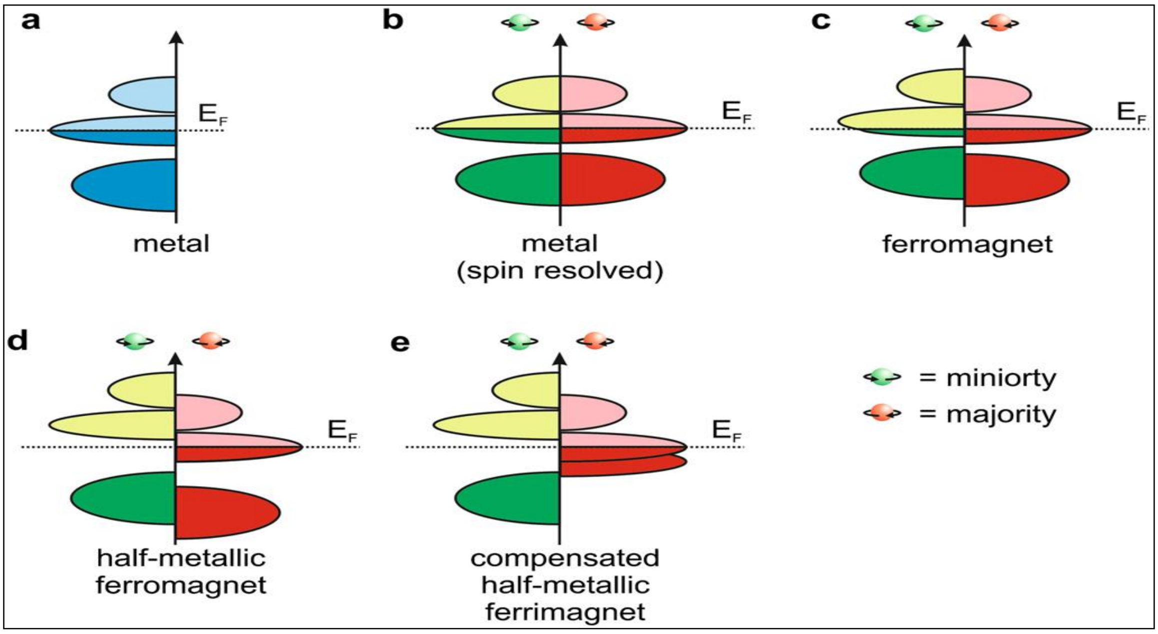

Fig 5: Schematic illustration of the density of states of (a) a metal, (b) a spin resolved metal, (c) a ferromagnet, (d) a half-metallic ferromagnet, and (e) a half-metallic ferrimagnet.

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. The ideal compensated ferrimagnet would exhibit a total magnetic moment of zero. For such compensated ferrimagnets, single spin superconductivity was observed by Pickett [15]. These materials 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 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.

Scope of Heusler alloys in devices for spintronic applications

In 1986 by P. Grünberg [16] and A. Fert [17] discovered the giant magnetoresistance (GMR) effect in magnetic multilayers which revolutionized the field of information technology and they were honored with the Nobel prize in physics in 2007. Today, spintronic devices are used in our everyday life, in form of spin valves based on the GMR effect, which form a part of magnetic hard disk drives. In such a spin valve, two magnetic layers sandwich a very thin non-magnetic metallic spacer. If the magnetization of both ferromagnetic layers is aligned in parallel direction, the resistance of the device is low, if the ferromagnetic layers are aligned antiparallel, then high resistance state is reached. GMR spin valves led to a dramatic increase in area storage density, but as emerging technologies are developed with incredibly high speed, the era of GMR is superseded by spin-dependent tunneling devices. The replacement of the metallic spacer by an insulating material lead to a rise in magnetoresistance by a factor of 10 compared to GMR spin valves. Since the effect is based on the tunneling of electrons through the insulating barrier, these new devices are known as magnetic tunnel junctions (MTJs) or as tunneling magnetoresistance (TMR) devices [18].

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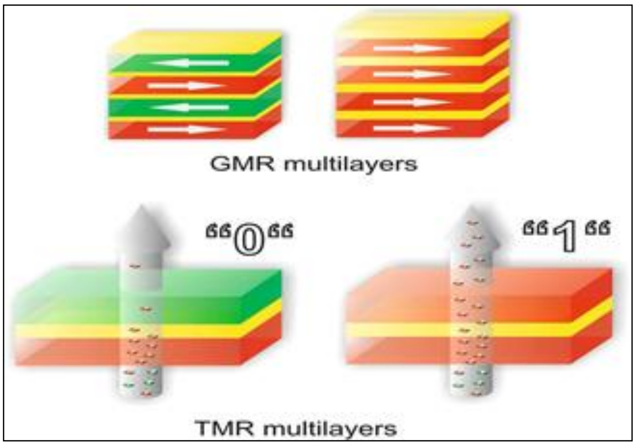

Fig 8: At the top, GMR multilayers are shown; the magnetic coupling can be adjusted by varying the thickness of the non-magnetic spacer layer. At the bottom, a TMR device is shown in which the tunneling current follows perpendicular to the film surface, experiences a high resistivity in case of antiparallel magnetization while the resistivity is low for a parallel magnetization direction.

A tunneling device with a magnetoresistance effect of several thousand percent, can be reached by two different courses: One way is to form the insulation barrier, and the other way is to develop new electrode materials with 100% spin polarization. Potential materials include half-metallic ferromagnetic oxides as well as half-metallic ferromagnetic metals, such as Heusler compounds. In the past 50 years, the only way to switch or excite magnetic moments was the use of a magnetic field, but magnetic fields are extremely harmful from a device perspective. The problem is that as devices shrink in size, larger and larger magnetic anisotropies are necessary to prevent them from being disturbed by thermal fluctuations as the superparamagnetic limit is approached. A novel method of switching magnetic tunnel junctions is the exploration of spin-transfer torque effects, which enables the scaling of magnetic random access memory (MRAM). In recent years, many business companies took notice of the outstanding research results and the vast tunability of Heusler materials. Therefore, more and more companies jump into the field of Heusler compounds and develop new products. The growing number of patents issued on Heusler-based discoveries reflects the impact of Heusler compounds for industrial research and product development. Seagate technology invented a memory cell based on spin tranfer torque effects (ST-RAM) which incorporates magnetic Heusler layers [19]. TDK designed a multilayer device with perpendicular magnetic anisotropy incorporating Heusler materials with high spin ploarization and low magnetic damping [20]. Spin-stand testing of narrow-track recording heads confirmed compatibility of these materials with the hard disk drive reader technology [21].

Conclusion

A broad overview of an outstanding class of materials, the Heusler compounds is given. Here we summarizes all important aspects concerning these amazing materials. Crystal structure and order-disorder phenomenon in relation to multifunctional tunable properties were discussed. Many fascinating research projects will certainly emerge in future which take advantage of their tunable functionalities. Heusler material based devices could be designed according to the specific needs of the corresponding application and the new, unknown multifunctional properties could be developed, all within the one material class, the Heusler compounds. Multifunctional magnetic properties explored in the field of spintronics resulted in devices of smaller size and quite high data storage density. In recent years, many business companies took notice of the outstanding research results and the vast tunability of Heusler materials. In order to meet the ever- increasing demand for ultrafast, high density data storage and processing devices the development of new concepts to commercialize nanoscale devices is need of the hour.

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