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FIRST PRINCIPLE BASED INVESTIGATION OF HEUSLER ALLOYS: A REVIEW

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Abstract
Heusler compounds generally have two categories: Half- and Full-Heusler compounds, in which former is represented by ABC, where A and B are rare-earth or transitions metals and C is from the second half of the periodic table and known as main group element and represents either non-magnetic, metals or semiconductors with $C1_b$ crystal structure. Similarly, full-Heuslers represented with the chemical formula of A_2BC with $L2_1$ structure. In this paper It is concluded that there are properties like elastic, thermoelectric and mechanical properties that has not been studied for some compounds. Mn-based, Co-based and Fe-based Heusler compounds are still to be explored so future work can be based on these compounds. Also, elastic and thermoelectric properties will be studied for different Heusler compounds.

Keywords: Heusler Alloys, Crystal Structure, Applications, Literature Review, Density Functional Theory, Structural, Electronic, Magnetic, Thermoelectric Properties.

Introduction

The Heusler compounds were revealed by Friedrich Heusler [1, 2] and were defined to have astonishing magnetic properties due to the fact of their ferromagnetic behavior after appropriate heat treatment although made up of diamagnetic and paramagnetic materials [1]. These materials are always in requirement because of attractive properties [3]. For example, Cu_2MnAl is an alloy that shows ferromagnetic behavior although not a single member is magnetic [4, 5]. The outlook scientific trends in spin/orbital electronics got improved by the refined properties of Heusler compounds [6]. The properties like high polarization at Fermi level [7], ferromagnetism, large Curie temperature [8] and thermoelectric performance [9] are making them smart materials for spintronics, magneto resistive materials, spin value generators, memory devices [10-13], topological insulators, etc. [14-16]. Many compounds are acknowledged now and called Heusler compounds. A lot of them are investigated theoretically to be half-metals. With metallic and half-metallic materials, these also embrace semiconducting, superconducting, and topological insulator substances [17, 18].

1.1 Categories of Heusler compounds

Heusler compounds generally have two categories: Half- and Full-Heusler compounds, where former is represented by ABC [19], where A and B are rare-earth or transitions metals and C is from the second half of the periodic table and known as main group element [20] and represents either non-magnetic [21], metals or semiconductors [22]. Similarly, full-Heuslers represented with the chemical formula of A_2BC [19].

1.2 Crystal structure of Heusler compounds

Half-Heuslers generally have $C1_b$ style structure and full-Heuslers have $L2_1$ type structure. Full-Heusler compounds have two structures and are represented by Cu_2MnAl and Hg_2CuTi and they are identified by their atomic positions [25]. We should be careful while providing position. These positions clearly make correct structure. Wrong position of the corresponding atoms gives wrong structure.

1.3 Applications of Heusler compounds

Growing demand of new applied sciences can assist scaling of future electronic gadgets [26-29]. It is clear that in future charge-based devices basically which depend on substances like silicon will definitely hit physical limits [30]. Among the recent technologies, where electronics of spins is involved, and it is becoming the one of the most workable choices that can replace or increase the charge-based devices [29, 31]. Giant magneto resistance (GMR) [32] is also signifying the vital interest in this field.

Literature Review

Young (1923) [3] in his work investigated Heusler compounds using molybdenum radiation and examined compounds of two different compositions from which one was face-centered cubic, while the other was a mixture of f.c.c and b.c.c structures and the latter type was more magnetic.

Leiy Harang (1927) [33] used copper radiation and found three structures, face-centered cubic, body centered cubic, and a structure similar to γ brass in his investigation. But he did not relate magnetic behavior with structure and therefore could not assign them to a single lattice.

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Elis Persson (1928) [34] radiate Heusler compounds with chromium radiations and found the structure of a ferromagnetic alloy corresponding to the formula Cu_2MnAl as body-centered cubic, with aluminum atoms forming a face-centered super lattice. The whole unit cell is made of eight body-centered cubes, and total 16 atoms from which 4 are aluminum, 4 are manganese and rest representing copper atoms. But there was no attempt to find the position of manganese atoms by X-rays.

Potter (1929) [35] in his work examined a crystal by using copper radiation and concluded that Mn atoms contain position of Al atoms. He also observed the ferromagnetic behavior when manganese atoms were placed at face-centered cubic lattice.

Persson (1929) [36] during his research tried to find out whether the crystal structure Cu_2MnAl type was solely responsible for the ferromagnetic behavior of these compounds. He examined the whole series of compounds of $(CuMn)_3$ Al after varying the proportion of elements and studied their behavior with suitable heat treatment. He also performed a quenching experiment and after all experiments, he concluded that ferromagnetism appears because of the behavior of Cu_2MnAl structure, and distribution of the manganese atoms.

Bradley AJ et al. (1933) [37] in their experiment test whether the ferromagnetism behaviour of compounds gets destroyed on changing the crystal structure by keeping the crystal composition the same. The composition of the alloy after heat treatment was checked by chemical analysis and found to be unaltered. So they concluded that ferromagnetism of the alloy is not a matter of chemical composition but of atomic arrangement.After the specification of the crystal structure of Heusler compounds advanced work has been done in this field. List of compounds investigated theoretically and experimentally.

M. Belkhouane et al. (2015) [38] had investigated Fe_2MnAl, Fe_2Mnsi, and $Fe_2MnSi_{0.5}Al_{0.5}$ theoretically by using FP-L/APW+lo where lo represent local orbitals. They considered structural, electronic and magnetic properties by means of considering muffin-tin radii as 2.0 for Fe, 2.4 for Mn, 1.95 for Al, and 2.0 is for Si with a.u. unit. Energy convergence was used to 0.1mRyd. The calculated lattice parameters are 5.680Å, 5.599Å, and 5.645Å for compounds mentioned above. All have good conformity with the calculated experimental and theoretical data. The densities of states presented in this paper confirm the half-metallic behavior of Fe_2MnAl. $Fe_2MnSi_{0.5}Al_{0.5}$ indicates half-metallic performance in electronic density of states at Fermi level with minority spin. The minority bands show a band gap of Eg=0.58 eV in case of Fe_2MnSi and 0.49 eV in case of Fe_2MnAl and hence confirmed a Half-metallic ferromagnetic (HMF) behavior.

HC Kandpal et al. (2006) [39] had examined 7 LiYZ (Where Y = Mg, Zn, Cd, Al and Z = N, P, As, Bi, Si) compounds exhibit half-Heusler structure by using FP-LAPW method and linear muffin-tin orbital (LMTO). In this paper, structural properties along with electronic properties have been investigated. They report an organized inspection of band gaps and the nature of bonding in semiconducting half-Heusler compounds with 8 and 18 electrons with first-principles density functional calculations and found the most suitable portrayal of these compounds as YZ zinc blende crystal structure stuffed with the X ion. They make it obvious that systems built up of the YZ zinc blende structure is the most informative way of taking into consideration. The affinity of the zinc blende sub lattice is to open up a semiconducting gap.

S Ouardi et al. (2011) [40] worked on crystalline structure and also studied the mechanical, magnetic, electronic properties of the polycrystalline Heusler compound Co_2MnGe. Transport properties have also been studied. The crystalline composition was examined with the help of x-ray absorption fine-structure spectroscopy and with anomalous x-ray diffraction as well. $L2_1$ structure with 2:1:1 stoichiometry confirmed with the experiment. The calculated low-temperature magnetic moment was in an agreement with the Slater-Pauling rule and showed half-metallic ferromagnetic behavior of the compound, as is defined by ab initio calculations. Transport measurements and hard x-ray photoelectron spectroscopy were done to find details about the electronic structure of the compound. The observed hardness values were consistent with a covalent-like bonding of Co_2MnGe. Band structure calculations set the half-metallic ferromagnetic behavior of the compound. The transport measurements show the metallic behavior with 0.48 μΩm resistivity and $-16\mu VK^{-1}$ Seebeck coefficient at room temperature.

J Ma et al. (2016) [41] presented first-principles density functional calculations of the electronic structure, magnetism, thermodynamic stability and structure constancy of 378 XYZ half-Heusler compounds (where X represents Cr, Mn, Fe, Co, Ru, Ni, and Rh; Y represents Cr, Fe, Mn, Ti, Ni,and V; Z represents P, Sb, Al, Si, As, Sn, In, Ge, Ga) and 6 further compounds (X=Ni, Cr; Y=Sc; Z=P, As, Sb). They found one general feature in these half-Heusler compounds which is the 'Slater-Pauling gap' within the density of states. According to them this gap between two bands for both spins meaningfully contribute to the steadiness of half-Heusler compounds. They identified some semiconductors (18-electron), half-metals, and few near half-metals with negative formation energy which follow the Slater-Pauling rule. They predicted some theretofore unknown thermodynamically steady phases that led to the experimental investigation for half Heusler structure (RuVAs, CoVGe, FeVAs) and in orthorhombic structure (MgSrSi-type).

F. Dahmane et al. (2016) [42] had used the first density functional calculations to determine structural and magnetic properties in addition to electronic properties by using FP-LAPW method to investigate Fe_2-based full-Heusler alloy with both Cu_2MnAl and Hg_2CuTi crystal types. They investigate Fe_2XAl where X=Cr, Mn, and Ni and found Cu_2MnAl crystal structure energetically more stable as compare to Hg_2CuTi with GGA approximation. The RMT for Fe and Cr was 2.18 a.u., Al designated with 20.4 a.u. in case of Fe_2CrAl, 2.20 a. u for Fe, Mn and 2.06 a. u for Al in case of Fe_2MnAl and finally 2.16 a. u for Fe, Ni and 2.03 a. u for Al in case of

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Fe_2NiAl. The full-Heusler alloy Fe_2XAl (X=Cr, Mn) was located as half-metallic in a structure type Cu_2MnAl, because of energy gap in bands for minority spin for both the compounds. Fe_2NiAl showed metallic character in both Hg_2CuNi and $MnCu_2Al$ type structures. The calculated magnetic moment is 1.0 μ_B and 2.0 μ_B for Fe_2CrAl and Fe_2MnAl respectively which are in good agreement with Slater-Pauling rule.

MK Hussain et al. (2015) [43] had used full-potential linearised augmented plane wave method for the investigation of Ti_2NiB Heusler alloy. Electronic Properties with magnetic properties are investigated in this paper and gave the information about the metallic character for spin-up electrons whereas spin-down bands show the gap of 0.62 eV resulting in stable half-metallic ferromagnetism with a magnetic moment of 3 μ_B /f.u. The total magnetic moment (Mt) and number of valence electrons (Zt) in the Ti_2NiB compound obeyed the Slater-Pauling (SP) rule of $M_t = Z_t - 18$. The magnetic moment of Ti_1 and Ti_2 demonstrate distinct behavior because of their unequal surroundings and magnetic contribution. This work also encouraged experimentalist due to the obtained value of a negative formation enthalpy. The Ti_2NiB compound maintained 100 % polarisation at the Fermi level, with its half-metallic nature present for lattice constants ranging from 5.60 to 6.50 Å that made this alloy positive for the experimental work.

A Azhar et al. (2017) [44] proposed theoretical study on a full-Heusler alloy Fe_2MnAl to identify the magnetic moment that is the way it formed microscopically. A system is modeled by constructing a tight-binding Hamiltonian and Hubbard parameter for d-orbital electrons which is based on density functional theory. After solving the model using green's function approach they treat the interaction terms within the mean-field approximation. Their next target is to formulate the computational algorithm for the overall calculation process and then to compute the total magnetic moment per unit cell. They used this method to remove the discrepancies in the magnetic moment of some Heusler compounds from Slater-Pauling rule.

L Hongzhi et al. (2007) [45] had investigated Fe2YSi (Y = Cr, Mn, Fe, Co, Ni) compounds experimentally as well as theoretically. They studied their electronic and magnetic properties. Experimentally melt-spinning method has been used for the synthesization of single phase Fe_2CrSi Heusler alloy. First principles FLAPW calculations were used to study Fe2YSi compounds theoretically. According to the results Fe_2CrSi is predicted to be a half-metallic ferromagnetic with a spin moment of $2\mu_B$/f.u. and a gap of 0.42 ev. Fe_2MnSi was found to be half-metallic in the ferromagnetic state. The saturation magnetic moments at 5K for these compounds fitted the theoretical investigations in a good manner. Specifically, the saturation magnetic moment of Fe_2CrSi was $2.05\mu_B$/cell that agreed with the value of $2\mu_B$ calculated from the Slater–Pauling rule. The Curie temperatures of Fe_2YSi compounds were crossing 500K except for Fe_2MnSi because it has a T_C below room temperature. The cause of lattice deformation on the electronic and magnetic properties of Fe_2CrSi and Fe_2CoSi was studied. It is found that Fe_2CrSi is half-metallic from −3% to +1% unvarying lattice deformation, and this nature is favored in systems like melt-spun ribbons or thin films which contain large strain.

Z Merdan and E G Ozdemir (2018) [46] had investigated structural plus magnetic properties of M_2IrSi (M = Ti, Cr and Mn) Heusler alloy. FPLAPW method is amid most precise methods were used for electronic structure calculations which are based on DFT as implemented in WIEN2k code. The generalized gradient approximation (GGA) in Perdew-Burke-Ernzerhof (PBE) was used to decide the exchange-correlation correction. They plotted electronic structures by using graphing and data analyses software of Origin Pro 8.0. The ferromagnetic states (FM) were compared to the non-magnetic states in the Hg_2CuTi and Cu_2MnAl both structures has to find the energetically more stable state using optimization curves. They figured FM states as the more stable states in Hg_2CuTi Type structure for all compounds. The electronic calculations confirmed that the majority electrons of Ti_2IrSi, Cr_2IrSi and Mn_2IrSi compounds had metallic nature whereas for Ti_2IrSi and Mn_2IrSi compounds, the minority electrons had semiconducting nature with an energy gap of 0.89 and 0.41 eV, respectively. Finally, Ti_2IrSi compound is a predictable half-metallic, Cr_2IrSi compound is metallic and Mn_2IrSi is a half-metallic ferromagnetic within 2.73, 1.0 and 3.0 μ_B/f.u. magnetic moment, respectively.

S.A Khandy et al. (2018) [6] predicted the electronic, magnetic, transport and thermoelectric properties of Co-based (Co_2TaSi and Co_2TaGe) full Heusler alloy. The observed lattice constant for Co_2TaSi is 5.88 Å and for Co_2TaGe is 5.95 Å. The stability of these compounds was confirmed in Fm-3m phase from structural optimizations and cohesive energies which gave the equilibrium lattice parameter as well. They used MBJ (Modified Beckhe Johnson) scheme for the significant electronic structure and ground state properties. This scheme gave the more efficient results as compare to GGA (generalized gradient approximation) as generalized gradient approximation underestimates the electronic structure. He found indirect band gap (spin) of 0.84 eV for Co_2TaSi and 1.04 eV for Co_2TaGe. See beck coefficient value at room temperature for Co_2TaSi and Co_2TaGe in spin-up configuration is calculated as 45μV/K and 15μv/K and in spin down configuration as 1000μV/k and 980μV/K. 3 μB value of magnetic moment was found for both of these materials.

Discussions: By the inferences drawn from literature review, it can be concluded that Heusler alloy has become thrust area for the researchers working in experimental or theoretical area. It is concluded that there are properties like elastic, thermoelectric and mechanical properties that has not been studied for some compounds. Mn-based, Co-based and Fe-based Heusler compounds are still to be explored so future work can be based on these compounds. S.A. Khandy et al. 2017 gave an idea about new Co-based compounds. Very less work has been done about these compounds also very little is known about Fe-based compounds. So, future work can be done by considering these compounds. Thermoelectric materials are becoming novel for industrial applications.

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Therefore, Heusler alloys are becoming interesting materials for them which are helping to provide new ways to the researchers. In a present work elastic and thermoelectric properties will be studied for different Heusler compounds.

Conclusion: We have studied electrical, magnetic, elastic, thermodynamic and thermoelectric properties of Heusler alloys. Ferromagnetic nature has been predicted by DOS and band structure of these alloys. Elastic constants show that the materials are stable, stiff, anisotropic, brittle and incompressible. The thermodynamic properties show that temperature and pressure have opposite influences on heat capacity. The effect of temperature on CV is more significant for both the materials and at low temperatures, the heat capacity and the thermal expansion coefficient follow T3 law. The electrical and thermal conductivity have been studied as a function of temperature. The value of Seebeck coefficient suggests that the materials can be important as thermoelectric materials. Very less work has been done about Co and Fe-based compounds. So, future work can be done by considering these compounds. We have reported a detailed and specific study of these alloys and we hope that our study will trigger more experimental study on these materials.

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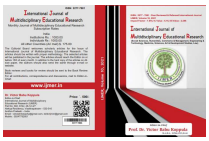
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