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PROPERTIES OF HALF HEUSLER COMPOUNDS: A CLASS OF MATERIALS FOR DIFFERENT POTENTIAL APPLICATIONS

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ABSTRACT

Half-Heusler compounds show promise in high-temperature power generation applications, such as spintronics, quantum sensors, quantum computers, and quantum resistors. These compounds have a high thermoelectric power factor and are relatively affordable. Half-Heusler compounds have piezoelectric qualities that make them suitable for a variety of applications, including SONAR detection, electromechanical resonators, and high-precision uses in microbalances and scanning probe microscopes. The half-Heusler family is one of the most varied groups of compounds, with a wide range of constituent atoms, lattice constants, and band gaps, extending its potential utility. These materials exhibit strong optical conductivity and reflectivity in the visible and infrared parts of the electromagnetic spectrum, making them attractive candidates for thermoelectrics, spintronics, and solar cells, among other uses. We looked at the features of half heusler compounds and how they can be used in a variety of technological applications. The article is broken into eight sections, including a summary and a future prognosis.

Keywords: Thermoelectrics, Spintronics, Electromagnetic spectrum, Piezoelectric properties, half-Heusler compounds, Lattice constant, Optical conductivity

1. INTRODUCTION

About 30 years ago, the hunt for novel materials in the field of spintronics led to the discovery of the Heusler compound class. Due to their tunable electronic structure, they appear to be the material of choice for many applications, allowing the design of desirable features ranging from half-metallic ferromagnets to entirely compensated ferrimagnets to nonmagnetic semiconductors and even superconductors. New fields of application have evolved in recent years, including environmental technology such as thermoelectrics and

solar cells. These compounds have a high Curie temperature as well as a high spin-polarization, both of which are important in technological applications. Heusler compounds were once thought to be intermetallic alloys, but their atomic order makes them more appropriately described as intermetallic compounds. They first piqued scientists' interest in 1903, when F. Heusler discovered that the compound becomes ferromagnetic despite the fact that none of its constituent elements are ferromagnetic on their own. Heusler and half-Heusler (or semi-Heusler) compounds are the modern names for this unique substance and its relatives (a wide array of around 1500 compounds). Surprisingly, the quantity of valence electrons in their atoms may be used to predict their qualities [1]. The half-Heusler compounds are a ternary packed variation of traditional electron closed-shell semiconductors, such as GaAs, that crystallise in a zincblende (ZnStype) lattice. Instead of two atoms, the eight valence electrons are spread among three. In the ZnS-type lattice, the third atom fills the octahedral vacancies. This fact causes a rocksalt-like sublattice to form, which is defined by ionic bonding interactions. Unusual semiconductors with 18 valence electrons are known in addition to the eight valence electron compounds, which are typically referred to as Nowotny–Juza phases [2,3]. These materials contain transition metal elements with a nearly fully filled d-electron shell, which is added to the valence electron count, resulting in a closed-shell configuration with semiconducting characteristics once again. The correct assignment of atomic locations in the crystal lattice is required to understand the properties of these materials[4].

One of the four interpenetrating fccsublattices in Heusler compounds can be left empty. Half-Heusler compounds are created by simply leaving a void in one of the two X atom positions in the X2YZ structure. Thus, these compounds are ternary, intermetallic compounds with a 1:1:1 stoichiometry and the general formula XYZ, where X and Y are s-block elements or transition or rare-earth metals, respectively, and Z is the major group element (p-block) [5]. The 'normal' atomic arrangement, which may be seen in most half-Heusler compounds, is represented by MgCuSb. The NaCl-type substructure is made up of the most electronegative element Sb and the most electropositive element Mg, while the ZnS-type sublattice is made up of the intermediate electronegativity element Cu and the most electronegative element Sb. Despite the fact that MgAgAs is the prototype for all half-Heusler compounds, it crystallises with a distinct, non-'normal' atomic order [6].

2. THE PROMINENT CHARACTERISTICS

The most prominent characteristic of these materials is that their band structure can be tuned from indirect to direct and narrow to wide-bandgap with varying constituent

elements. As these compounds' electronic structures are defined by their valence electrons count (VEC) hence, their physical properties majorly depend on their VEC. These compounds are classified into two groups based on the VEC, of which the first one has VEC = 18 and the second has VEC = 8. The half-Huesler compounds with VEC = 18 include a wide range of semiconductors and a lot of studies have been done to examine their structural, thermoelectric and optical properties , which prove them promising for thermoelectric and photovoltaic applications. However, their narrow bandgap affects their thermoelectric properties. In contrast, the half-Heusler compounds with VEC = 8 also provide a significant number of semiconductors. They fulfill the minimum environmental, technical and economic criteria for optoelectronic applications to act as a buffer layer material . Besides this, at room temperature, these compounds also exhibit excellent potential for thermoelectric application with a high thermopower value [7-11]. It will be fascinating to explore different and state-of-the-art half-Heusler alloys with VEC = 8 and 18 whether they show excellent optical and thermoelectric properties.

3. SOLER CELLS

Solar is a safe alternative that can replace current fossil fuels like coal and gas for generation of electricity that produce air, water, and land pollution. A lot of research is done using solar cells from past 25 years to improve efficiency of cell and to find material that is more suitable, which are also low in cost [12]. The p-n junction constitute of window and absorber in non-silicon solar cells with a buffer layer in between them. This layer usually with size of 50 nm to 200 nm makes the transition easier from window to absorber. To reduce the conduction band offset the thin layer made as according to band gap between window and absorber. Such offset acts like a barrier for electron flow that reduces efficiency of solar cell. Turnery copper-based chalcopyrite solar cells have CdS buffer layer of around 50 nm in between light absorbing materials like $CuInSe_2$ and ZnO type multilayer transparent window. The solar cells can optimized with an insulated contact in between CdS and transparent conducting window. In addition, buffer layers affect transient phenomena and stress induced degradation in Cu based solar cells that are useful to affect the open circuit voltage of cell. [13]. The CdS meets the entire feature for a well-optimized buffer layers except this carcinogenic compound is toxic. Half-Heusler compounds are the well-promised materials over CdS. The crystalline structure of half-Heusler is suitable to solar cell material if their lattice constants make good agreement with each other to make better surface contact with the absorber.

Kieven et al. [14] have suggested that the band gap of greater than 2 eV have less absorption losses over Cd based buffer material, although the lattice parameter must be in range of solar junction. One of the most promising approaches is the use of ternary Cu-based chalcopyrite semiconductors such as p-type CuInSe2(CISe) or Cu(In,Ga)Se2 (CIGSe) asthe light absorber materials for low-cost thin-film solar cell applications. In conventional chalcopyrite solar cells, a CdS buffer layer of around 50 nm thickness between the light absorber and the n-type ZnO window layer is used to increase the performance of the device. A record efficiency of 19.9% has been reported for the ZnO/CdS/Cu(In,Ga)Se2 heterojunction [15]. An accurate design of the heterojunction between the absorber and buffer layers is crucial to achieve a good solar cell performance. The crystal structure of the buffer layer material should ensure good contact between the absorber and buffer layers, and avoid unnecessary absorption losses. An inverted interface conduction band of the absorber close to the Fermi level at the interface, and to avoid a barrier reduction at the interface in order to minimize recombination, are important features of the buffer layer [16]. CdS seems to meet these conditions, but unfortunately it is very toxic. Thus, there is a strong interest in replacing CdS as a buffer layer in these solar cells.

Promising materials are the half-Heuslercompounds,as the rather loosely packed crystalline structure is similar to that of chalcopyrite, so that a good surface contact between the two materials is expected if the lattice constants are in the same range. Of special interest are the above-mentioned I–II–V compounds, which can be tuned by composition according to band gap size and the direct and indirect natures of the gap, respectively. For a reasonably small absorption loss, the band gap of the buffer material should not be smaller than 2 eV and the lattice constant should be around 5.9 Angstron for good[17] lattice matching with the absorber material.

4. THERMOELECTRICS

‘Thermoelectrics are materials that can generate electricity from the application of a temperature gradient, or vice versa, through the thermoelectric effect. By exploiting this coupling between thermal and electrical properties, thermoelectric devices can be made that carry heat from a cold to a hot side (refrigeration) or that generate electricity from heat flows.’

Thermoelectricity is the conversion of heat into electricity or vice versa, which occurs when heat and charge carriers in a material are coupled. Semiconductors are widely known for having the strongest coupling between these two kinds of energy and are hence the

materials of choice for thermoelectric waste heat harvesting or refrigeration [18]. The conversion of waste heat into electricity using thermoelectric devices can theoretically improve the efficiency of any heat-generating operation. However, due to low device efficiencies and a high cost per generated unit of electricity, wide-scale application is limited [19,20]. Since the 1950s, a wide range of materials has been studied, including classic thermoelectric materials such as Bi2Te3, PbTe, and Si1xGex, which have good performance near room temperature, at intermediate temperatures, and at high temperatures, respectively [21]. Over the last two decades, a lot of work has gone into finding new materials with higher energy conversion efficiencies. To understand the relationship between half heusler and thermoelectric compounds, there are many outstanding articles [22–31]. These materials, which include complicated unit cells and nanocomposite materials, provide more flexibility in terms of optimising the thermoelectric properties that underpin them. The thermoelectric figure of merit is commonly used to determine a material's efficiency: (S2/)ZT = (S2/)ZT = (S2/)ZT = (S2/)ZT S is the voltage response to a temperature gradient, is the electrical conductivity, is the sum of the lattice (lat) and electronic thermal (el) conductivities, and T is the absolute temperature. Three of the four thermoelectric factors (S, el, and el) are linked by the electrical structure and cannot be optimised independently, which is the basic challenge in reaching greater ZT values. This is shown in the frequently documented charge carrier dependence of S, and el (increases in S result in decreases in, while every increase in el is followed by an increase in el)). For most thermoelectric materials, this interdependency restricts ZT to 1. Different ways have been tried to overcome the ZT = 1 constraint, with the phonon-glass electron crystal being the most significant guiding principle (PGEC). The ideal thermoelectric material should have the electrical properties of a crystalline solid (i.e. a big S and) and the thermal properties of a glass (i.e. a low lat). [32]

To summarise, the majority of today's high-performance bulk thermoelectric materials have low thermal conductivities (1Wm1K1), which, when combined with modest power factors (S2 = 1–3mWm1K2), results in high ZT values. The half-Heuslers under consideration are unique in that they have high power factors (6mWm1K2) but are limited by 'large' thermal conductivities, which in optimised samples are typically on the range of 3–4Wm1K1, resulting in ZT 0 [44–46]. Despite the challenge of further reducing thermal conductivity, this is a viable starting point because phonon transport manipulation is more understood than enhancing the power factor beyond what can be achieved by varying charge carrier concentration. Because the phonon spectrum encompasses a wide range of

wavelengths, effective thermal conductivity reduction requires the insertion of barriers at various length scales [33]. This comprises point defects (atomic substitutions), nano-inclusions, and microstructure control through mechanical milling grain size reduction. This strategy has been labelled a 'panoscopic' approach [34, 35], in which management of the structure at all length scales is employed to lower the heat conductivity. Calculations of the minimal thermal conductivity in the half-Heuslers, assuming a disordered structure, show that values less than 1Wm1K1 should be possible, indicating that there is significant room to enhance ZT from the present reported maximum values. As a result, these materials may offer a path to ZT >> 2.

5. TOPOLOGICAL INSULATORS

All bulk materials are classified as metals or insulators based on their electronic structure. Metals have a finite electron density at the 4Fermi energy, while insulators have a band gap. A new family of materials, known as TIs, has recently been introduced. It's worth noting that the name TIs is a little deceptive. Low band gap semiconductors are used in the systems. The TI is a quantum matter state with a complete insulating gap in the bulk but topologically protected gapless surface or edge states at the boundary [36]. When doped with exogenous elements as Mn, Fe, or Cu, the currently known Tis become magnetic or superconducting. The f-shell rare-earth elements are intrinsically included in the Tis based on Heusler compounds, establishing a stoichiometric system. Aside from the chemical functions (transfer of three electrons to the zincblende lattice and determining the lattice size), the additional open f-shell element provides multifunctionality by allowing conventional ordering and the TI state to coexist, which is required to realise novel topological effects and new extended applications. [37]

6. RARE EARTH BASED HEUSLER COMPOUNDS

Rare-earth-containing compounds play a unique role among half-Heusler compounds. They are part of a large group of compounds known as REME compounds, which have a wide structural range and a variety of interesting properties such as heavy-fermion systems, heavy electron behaviour, half metallic behaviour in some Ce compounds, mixed-valent behaviour in Eu, Yb, and Ce compounds, and superconductivity. Only compounds with 18 valence electrons in this class have the half-Heusler structure. The rare-earth metal's f-electrons are strongly confined and hence are not considered valence electrons. A hexagonal form of the Heusler structure, the so-called LiGaGe structure type, can be discovered within the class of 18 valence electron REME compounds [38]. While rare-earth-containing half-Heusler compounds are mostly semiconducting, hexagonal variations

are mostly metallic, but depending on the degree of puckering of the hexagonal layers, they could become semiconducting. The localised 4f electrons are virtually entirely responsible for the magnetic behaviour and magnetic moments of rare-earth containing half-Heusler compounds. The values of the effective magnetic moments eff match the values of the free REn+ ions quite well. Half-Heusler compounds comprising antiferromagnetic rare-earth elements have fascinating transport and magnetoresistance features. Half-Heusler compounds comprising antiferromagnetic rare-earth elements have fascinating transport and magnetoresistance features. The rare-earth containing Half–Heusler compounds appear to be ideal candidates for the multifunctional Tis[39] because they are narrowgap semiconductors.

7. DILUTED SEMICONDUCTORS

The semiconductor industry has consistently reduced the size of electronic components on silicon chips over the last 40 years, enhancing computer performance. When fundamental physical restrictions preclude the smaller component size, this technology reaches its limit. Spintronics, a novel method developed in the recent decade, has changed the electronic device market. The non-volatility of data storage, faster data processing speed, high storage density, and low energy consumption are all expected benefits of this new technology. The development of new magnetic materials, magnetic semiconductors, and half-metallic ferromagnets (HMFs) is required to fully realise the potential of spintronics. HMFs meet all of the requirements of spintronics thanks to their remarkable electronic structure: electrons in one spin direction propagate like in a metal, while electrons in the other spin direction propagate like in a semiconductor. K ubler [40] shown in 1984 that the Slater–Pauling rule can be used to describe the magnetic characteristics of C1b compounds. Many XYZ compounds can be thought of as Xn+ ions stuffed in a zincblende-type [YZ]n sublattice, where the number of valence electrons associated with the [YZ]n sublattice is 18 (d10 + s2 + p6), according to Jung et al [41]. These 18-electron closed-shell compounds are nonmagnetic and semiconducting. Most magnetic and half-metallic C1b compounds, on the other hand, contain manganese or rare-earth metals. This isn't through chance, because the characteristics of manganese ions in the Y position of C1b compounds must be considered, as K ubleret al [42] explain. The production of localised magnetic moments is expected when one of the 3d metals is substituted in the 18-electron combinations. Nanda and Dasgupta or, more recently, Fukushima et al estimated the electronic and magnetic structures of several dilute magnetic semiconductors based on C1b compounds. The Cr-substituted compound's magnetic transition temperature was

discovered to be around 60 K. XRD studies, however, indicated a minor lattice misfit between pure CoTiSb and Ti–Y substituted compounds [43,44]. These substitutional series are therefore appealing for spintronic applications such as spin-LEDs and other spin-injecting devices. These materials should be able to be used to make thin-film devices, and they should be able to be grown epitaxially with clean and smooth interfaces. When depositing layer by layer, the Co planes can be used to combine the different materials without causing any interfacial damage.

8. SUMMARY AND OUTLOOK FOR FUTURE

Finally, we provide a simplified review of the Heusler family's many talents as well as their attributes. The transition from electronics to spintronics, which is mostly based on quantum effects, is now compelled by energy consumption restrictions. It all adds up to dissipationless spin currents (quantum spin-Hall effect in topological insulators), which seems like a near approximation to an ideal spintronic device. Rather than charge gradients caused by temperature, the thermoelectrics study field focuses on utilising a thermally induced spin gradient (spin-Hall, spin-Seebeck effects together with their inverse equivalents). The class of half-Heusler compounds provides a simple technique to make n- and p-type semiconductors by doping the parent component chemically. The utilisation of natural recoverable energy sources on the basis of solar cells, which is an alternative manner of energetics, has its own implementation in wide-gap Heusler insulators. The constant tendency of discovering novel physical phenomena and then realising them inside some portion of the Heusler compound family indicates that the half-Heusler materials evaluation described here will, without a doubt, be fulfilled again soon.

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