REVIEW ARTICLE

Heusler Alloys: Structural, Electronic, Magnetic, Mechanical, and Thermoelectric Features - A Review

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ABSTRACT: This review paper presents an in-depth analysis of Heusler alloys, focusing on their structural, electronic, magnetic, mechanical, and thermoelectric characteristics, and potential applications. It begins with an examination of the crystal structure and composition, highlighting how composition influences structural properties. The paper delves into the electronic aspects by analyzing band structures and Fermi surfaces through density functional theory studies. The magnetic behavior of these alloys, pivotal in spintronic applications, is also scrutinized. Furthermore, the paper discusses mechanical properties like elastic constants and shape memory effects, and thermoelectric features including phonon and electron transport. Applications in energy conversion, storage, spintronics, sensing, and actuation are explored, emphasizing the alloys' role in lithium-ion batteries, fuel cells, spin valves, and magnetic tunnel junctions. Finally, it addresses challenges and future perspectives in synthesizing and integrating Heusler alloys for enhanced performance, underscoring the need for further research to unlock their full potential in various technological fields.

KEYWORDS: Heusler Alloys, Spintronics, Thermoelectric Properties, Density Functional Theory, Mechanical and Magnetic Behavior

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1.0 INTRODUCTION

1.1 Background and History

Heusler alloys, named after Fritz Heusler who first discovered them in 1903, are intermetallic compounds with a unique crystal structure and fascinating properties [1]. These alloys are composed of three elements, typically one transition metal (X), one element from the group IIIA or IVA (Y), and one element from the group VB or VIB (Z) of the periodic table [2]. The general formula for Heusler alloys is X2YZ. Initially, Heusler alloys were primarily investigated for their magnetic properties and their potential applications in the field of magnetism and spintronics. However, subsequent research revealed their multifunctional nature, leading to explorations in various fields such as electronics, thermoelectric, and even as catalysts [3].Through this review, we aim to contribute to the understanding of Heusler alloys and their potential for various technological applications, while also identifying areas that require further research and development.

1.2 Importance and Applications

Heusler alloys have gained significant importance due to their wide range of unique properties and potential applications in several technological areas. The following are some notable applications where Heusler alloys have shown promise:

1.2.1 Magnetic Materials: Heusler alloys exhibit remarkable magnetic properties, including high magnetization, large magnetoresistance, and high Curie temperatures [4]. These properties make them suitable for applications in magnetic sensors, magnetic recording media, and spintronic devices.

1.2.2 Spintronics: The combination of excellent spin-polarized transport properties and strong spin-dependent phenomena in Heusler alloys makes them valuable for spintronics applications [5]. They have been investigated for use in spin valves, magnetic tunnel junctions, and spin-transfer torque devices.

1.2.3 Thermoelectric Materials: Heusler alloys have attracted attention as potential thermoelectric materials due to their unique electronic structure and tunable transport

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properties [6]. They offer the possibility of converting waste heat into electricity, making them suitable for energy harvesting and cooling applications.

1.2.4 Catalysis: Certain Heusler alloys have demonstrated catalytic activity, particularly in hydrogenation and dehydrogenation reactions [7]. They can be utilized in processes such as hydrogen fuel cells and hydrogen storage systems.

1.2.5 Emerging Applications: Beyond the above-mentioned areas, Heusler alloys are being explored for applications in sensors, actuators, magnetostriction, and even as novel materials for data storage and memory devices [8, 9].

Heusler alloys are a class of intermetallic compounds that exhibit a wide range of physical effects and have potential applications in various fields. Here are the key features of Heusler alloys based on the provided abstracts:

1. Structural and Electronic Properties:

- Heusler alloys have an ordered structure with a face-centered cubic (FCC) superlattice and a body-centered cubic (BCC) unit cell [10].
- The properties of Heusler compounds, such as semiconductivity and magnetic moment, can be predicted by counting the valence electrons [11].
- Some Heusler alloys exhibit half-metallicity, which makes them attractive for spintronics applications [12,13].

2. Magnetic Properties:

- Heusler alloys can exhibit various magnetic behaviors, including ferromagnetism, superparamagnetic interaction, and short-range ferromagnetic interaction [10] [14,15].
- The magnetic properties of Heusler alloys can be influenced by structural defects and disorder [15].

3. Thermoelectric Properties:

- Heusler alloys have been explored for their thermoelectric properties, with some alloys showing high power factors and low thermal conductivity [14].
- The thermoelectric response of Heusler alloys can be calculated using Boltzmann transport theory [16,17].

Heusler alloys are a class of materials that have been extensively studied for their unique properties. Here is a summary of the structural, electronic, magnetic, mechanical, and thermoelectric features of Heusler alloys based on the provided abstracts:

Structural Features:

- Heusler alloys have an ordered structure with a face-centered cubic (FCC) superlattice and a body-centered cubic (BCC) unit cell.
- The structural characteristics of Heusler alloys allow for the exploration of a range of novel material properties.
- Different types of Heusler alloys include Full Heusler, Half Heusler, Inverse Heusler, Binary, and Quaternary Heusler [18].

Electronic Properties:

- Heusler alloys exhibit unique electronic structures, including half-metallicity [19].
- The electronic properties of Heusler alloys can be predicted by counting the valence electrons [20].
- Some Heusler alloys show semiconductivity or magnetic moment based on their electronic properties [21].

Magnetic Properties:

- Heusler alloys can exhibit ferromagnetism, even though the constituent elements do not show this behaviourindividually .
- The magnetic properties of Heusler alloys can be influenced by the presence of defects and disorder [22].
- The total magnetic moment of Heusler alloys can be predicted using the Slater-Pauling rule.

Mechanical and Thermoelectric Properties:

- The mechanical properties of Heusler alloys are important for their processing and final use

- Experimental studies on the mechanical properties of Heusler alloys are limited, highlighting the need for more research in this area [19].

- Heusler alloys can exhibit good thermoelectric properties, with high power factors and low thermal conductivity [23-25].

- The thermoelectric behavior of Heusler alloys can be influenced by their electronic and structural properties.

2. Crystal Structure and Composition

2.1 Heusler Alloy Classifications

- Heusler alloys can be classified into different categories based on their crystal structures and compositions. The most commonly known types are the L2_1, X2YZ, and XYZ families [26].
- The L2_1 family, named after the Cu2MnAl prototype, has a cubic crystal structure with space group Fm-3m. Examples of L2_1 Heusler alloys include Cu2MnAl, Ni2MnGa, and Co2FeAl [27].
- The X2YZ family, named after the Heusler prototype Ni2MnGa, is characterized by a tetragonal structure with space group P4/mmm. This family includes compounds like Ni2MnGa, Co2MnSi, and Fe2VAl [28].
- The XYZ family represents a more diverse group of Heusler alloys with different crystal structures, such as hexagonal, orthorhombic, or rhombohedral. Some examples include Mn3Ga, Fe3Si, and Co2TiAl [29].

2.2 Crystal Structure and Symmetry

The crystal structure of Heusler alloys is crucial for understanding their properties and behaviour. Generally, Heusler alloys adopt a cubic, tetragonal, or hexagonal crystal structure.The cubic L2_1 Heusler alloys have a face-centered cubic (fcc) structure with a high degree of symmetry. The X and Y atoms occupy the face-centered sites, while the Z atom is located at the body-centered position. This arrangement results in a highly ordered crystal structure with strong magnetic and electronic properties [30].The tetragonal X2YZ Heusler alloys have a distorted fcc structure, where the lattice parameters in the z-direction differ from those in the x-y plane. This distortion can lead to the emergence of multiferroic properties and shape memory effects in certain Heusler alloys [31].The crystal structures of XYZ Heusler alloys vary depending on the specific compound. Hexagonal, orthorhombic, and rhombohedral structures have been observed in this family. The diverse crystal structures contribute to the versatility of XYZ Heusler alloys and their potential for various applications [32].

2.3 Influence of Composition on Structure

The composition of Heusler alloys plays a crucial role in determining their crystal structure. Substituting different elements or varying the stoichiometry can significantly influence the lattice parameters and symmetry. For example, in the X2YZ family, changing the composition of the alloy can lead to a transition from the cubic L2_1 structure to a tetragonal or even a hexagonal structure [33]. Substituting different transition metals or modifying the Y or Z elements affects the crystal symmetry and can result in variations in magnetic, electronic, and thermoelectric properties. Similarly, in the XYZ family, altering the composition can lead to different crystal structures. For instance, Co2MnTi adopts a hexagonal structure; while Co2MnAl exhibits an orthorhombic crystal structure [34].The influence of composition on the crystal structure of Heusler alloys is crucial for tailoring their properties to specific applications [35]. By understanding the relationship between composition and structure, researchers can design and engineer Heusler alloys with desired functionalities.

3. Electronic Structure and Band Properties

3.1 Density Functional Theory (DFT) Studies

Density Functional Theory (DFT) has played a pivotal role in understanding the electronic structure of Heusler alloys. DFT calculations based on the Kohn-Sham equations provide a powerful tool for investigating the electronic properties of materials [36].Numerous DFT studies have been conducted to explore the electronic structure of Heusler alloys. These studies involve calculating the band structure, density of states (DOS), and other electronic properties. DFT calculations have proven successful in predicting the half-metallic behaviour and spin-polarized properties exhibited by certain Heusler alloys [37].

3.2 Electronic Band Structure

The electronic band structure of Heusler alloys reveals valuable information about their conducting properties and energy bandgaps. It is obtained by plotting the energy eigen values as a function of momentum along high-symmetry directions in the Brillouin zone [38]. Heusler alloys often exhibit complex band structures with a combination of metallic and semiconducting features. The band structure analysis allows for the identification of energy bands crossing the Fermi level, which indicates the material's conductivity and potential for applications in electronic devices [39]. The band structure calculations also provide insights into the origin of the material's electronic properties. They help determine the energy bandgap, the presence of band crossings or bandgap, and the behaviour of the valence and conduction bands. Additionally, the band structure analysis can reveal the presence of spin-polarized states and the extent of spin-splitting in magnetic Heusler alloys [40].

3.3 Fermi Surface Analysis

The Fermi surface analysis is a crucial aspect of studying the electronic properties of Heusler alloys. The Fermi surface represents the boundary between filled and unfilled electron states at the Fermi level and provides information about the material's transport properties and electron dynamics [41].DFT calculations can determine the shape, topology, and size of the Fermi surface in Heusler alloys. Fermi surface analysis helps understand the material's response to external stimuli, such as magnetic fields or temperature variations. It also reveals important features such as Fermi pockets, nesting conditions, and the presence of Dirac cones, which can influence the material's electrical and magnetic properties [42].By studying the Fermi surface, researchers gain insights into the material's electronic transport properties, including conductivity, Seebeck coefficient, and thermoelectric behaviour. This knowledge is crucial for optimizing Heusler alloys for applications in electronic and thermoelectric devices.

4. Magnetic Behaviour

4.1 Magnetic Properties and Phenomena

The magnetic properties of Heusler alloys have been a subject of extensive research due to their potential applications in spintronics, magnetic storage, and sensing devices. Heusler alloys exhibit a wide range of magnetic phenomena, including ferromagnetism, anti ferromagnetism, ferrimagnetism, and spin glass behaviour [43].Ferromagnetic Heusler alloys are particularly interesting due to their high Curie temperatures and large magnetic moments. These alloys can exhibit half-metallic behaviour, where one spin channel shows complete spin polarization, making them ideal for spintronic applications [44]. The strong exchange interactions between localized magnetic moments result in robust ferromagnetism and high magnetic ordering temperatures [45]. Antiferromagnetic and ferrimagnetic Heusler alloys, on the other hand, possess a net zero magnetization due to the antiparallel alignment of magnetic moments. These alloys are of interest for their potential in magnetic sensors and data storage applications.Spin glass behaviour is observed in some disordered Heusler alloys, where competing magnetic interactions lead to a frustrated magnetic state with a complex magnetic structure. Understanding and controlling such behaviour is important for designing novel magnetic materials with desired properties.

4.2 Spintronic Applications

Heusler alloys have gained significant attention in the field of spintronics, which aims to utilize the spin of electrons for information storage and processing. The half-metallic nature of certain Heusler alloys makes them ideal candidates for spintronic applications, as they allow for efficient spin injection, high spin polarization, and low electrical resistance [46].Heusler alloys can be used as spin valves, magnetic tunnel junctions, and spin filters in spintronic devices. The unique combination of metallic conductivity and high spin polarization makes Heusler alloys promising for realizing spintronic devices with low power consumption, high-speed operation, and enhanced functionality.

4.3 Influence of Composition on Magnetism

The magnetic properties of Heusler alloys can be tuned by modifying their composition. The influence of composition on magnetism is particularly evident in the XYZ family of Heusler alloys, where different combinations of transition metals and elements can lead to varying magnetic behaviours. By substituting different elements or adjusting the stoichiometry, researchers can control the strength of the exchange interactions, magnetic moments, and Curie temperatures in Heusler alloys [47]. For example, replacing one transition metal element with another can result in a change from ferromagnetic to antiferromagnetic behaviour. Furthermore, the introduction of nonmagnetic elements in Heusler alloys can induce modifications in their magnetic properties. The dilution of magnetic elements or the insertion of nonmagnetic spacers can influence the magnetic ordering and spin dynamics. Understanding the influence of composition on magnetism is crucial for tailoring Heusler alloys with specific magnetic properties suitable for various applications in spintronics, magnetic storage, and sensing devices.

5. Mechanical Properties

5.1 Elastic Constants and Mechanical Stability

The mechanical properties of Heusler alloys are crucial for their structural integrity and potential applications in engineering. The elastic constants, including the Young's modulus, shear modulus, and Poisson's ratio, provide insights into the stiffness, strength, and deformation behaviour of these materials [48].Experimental techniques, such as ultrasonic measurements and nano-indentation, combined with theoretical calculations, have been employed to determine the elastic constants of Heusler alloys. The mechanical stability of Heusler alloys is assessed by evaluating the elastic constants to ensure that they satisfy the Born stability criteria [49]. The mechanical stability is essential to prevent phase transformations and maintain the structural integrity of the material under different loading conditions.

5.2 Deformation Mechanisms and Plasticity

Understanding the deformation mechanisms and plasticity of Heusler alloys is vital for their applications in structural materials. Heusler alloys can exhibit different deformation mechanisms, including dislocation glide, twinning, and martensitic transformations [50].The deformation behaviour of Heusler alloys is influenced by various factors, such as the crystal structure, composition, and temperature. The activation of specific deformation mechanisms depends on the stacking faults, grain boundaries, and alloying elements present in the material. Plasticity in Heusler alloys can be enhanced by alloy design and optimizing the microstructure to promote favourable deformation mechanisms.

5.3 Shape Memory and Super elasticity

Some Heusler alloys exhibit shape memory and super elasticity, which are unique functional properties related to reversible phase transformations. Shape memory alloys undergo a reversible martensitic transformation, allowing them to recover their original shape after deformation upon heating [51]. Superelasticity refers to the ability of a material to exhibit large recoverable strains without permanent deformation. Heusler alloys with a narrow hysteresis in their stress-strain curves can display superelastic behaviour, making them suitable for applications requiring high flexibility and damping capacity [52].The understanding and control of the deformation mechanisms, plasticity, and shape memory/superelastic behaviour in Heusler alloys contribute to the development of advanced functional materials for applications in sensors, actuators, and biomedical devices.

6. Thermoelectric Features

6.1 Thermoelectric Effect and Efficiency

Thermoelectric materials are of great interest for energy conversion applications. Heusler alloys have shown potential as thermoelectric materials due to their ability to convert heat into electricity through the Seebeck effect. The Seebeck coefficient, electrical conductivity, and thermal conductivity are key parameters that determine the thermoelectric efficiency of Heusler alloys [53].

6.2 Phonon and Electron Transport

Phonon and electron transport significantly influence the thermoelectric properties of Heusler alloys. Phonons are responsible for heat transfer, while electrons carry the electrical charge. Understanding the phonon and electron transport mechanisms is crucial for optimizing the thermoelectric performance of Heusler alloys [54].

6.3 Enhancement Strategies for Thermoelectric Performance

Various strategies have been employed to enhance the thermoelectric performance of Heusler alloys. These include alloying, doping, nanostructuring, and optimizing the carrier concentration. Alloying and doping can modify the electronic band structure and scattering mechanisms to enhance the Seebeck coefficient and electrical conductivity [55]. Nanostructuring can reduce thermal conductivity by phonon scattering, leading to improved thermoelectric efficiency [56]. The optimization of carrier concentration through doping and control of defects can further enhance the thermoelectric performance of Heusler alloys. By tailoring the composition and structure of Heusler alloys, researchers aim to achieve high thermoelectric efficiency for applications in waste heat recovery and energy harvesting.

7. Recent Advancements and Potential Applications

7.1 Energy Conversion and Storage

Heusler alloys have shown great promise in the field of energy conversion and storage. Their combination of desirable properties, such as high electrical conductivity, tunable thermal conductivity, and excellent mechanical stability, makes them suitable for various energy-related applications. For instance, Heusler alloys have been explored as electrode materials in lithium-ion batteries and fuel cells, where their high electrical conductivity and chemical stability contribute to improved battery performance and enhanced energy storage capabilities [57]. In the context of energy conversion, Heusler alloys have been investigated for thermoelectric applications. The ability of these alloys to efficiently convert waste heat into electricity through the Seebeck effect holds potential for applications in waste heat recovery and energy harvesting. By optimizing the composition and structure of Heusler alloys, researchers aim to enhance their thermoelectric efficiency and contribute to the development of more sustainable energy conversion technologies [58].

Superconductors have interesting electrocatalytic properties that make them potential replacements for expensive and scarce platinum in catalysis. High-temperature superconductors like YBa2Cu3O7 (YBCO) and Bi2Sr2CaCu2O8 (BSCCO) have been studied for their electrocatalytic potential in hydrogen evolution and oxygen reduction reactions. These superconductors can easily be synthesized and have shown impressive electrocatalytic properties [59]. Additionally, the road to implementing high-temperature superconductors in applications has seen numerous advances in materials science and manufacturing [60]. However, it is important to note that while superconductors have potential applications in catalysis, not many have become commercially viable. Challenges in commercialization and the need for further technological advancements, overall, superconductors show promise in catalysis, but further research and development are needed to fully realize their potential [61].

Superconductors have interesting electrocatalytic properties that make them potential replacements for expensive and scarce platinum in catalysis. High-temperature superconductors like $YBa_2Cu_3O_7$ (YBCO) and $Bi_2Sr_2CaCu_2O_8$ (BSCCO) have been studied for their electrocatalytic potential in hydrogen evolution and oxygen reduction reactions. These superconductors can be easily synthesized and have shown impressive electrocatalytic properties [62]. Additionally, the road to implementing high-temperature superconductors in applications has seen numerous advances in materials science and manufacturing [63]. However, it is important to note that while superconductors have potential applications in catalysis, not many have become commercially viable. Challenges in commercialization and the need for further technological advancements remain. Overall, superconductors show promise in catalysis, but further research and development are needed to fully realize their potential [64].

7.2 Spintronics and Magnetic Devices

The unique magnetic properties of Heusler alloys have opened up opportunities for their use in spintronics and magnetic devices. Heusler alloys exhibit desirable properties such as high spin polarization, tunable magnetic moments, and robust magnetism, making them attractive for applications in spin valves, magnetic tunnel junctions, and spin filters [65]. In spintronics, Heusler alloys play a crucial role in the manipulation and control of spin currents for information storage and processing. The ability to efficiently inject and transport spin-polarized electrons in Heusler alloys enables the development of low-power and high-speed spintronic devices [66]. Furthermore, the integration of Heusler alloys with other magnetic materials and non-magnetic materials has shown potential for the realization of multifunctional devices with enhanced functionality and performance.

7.3 Sensing and Actuation

Heusler alloys have also found applications in sensing and actuation devices. Their unique properties, such as shape memory effect, superelasticity, and magnetostriction, make them suitable for use in sensors, actuators, and microelectromechanical systems (MEMS). The shape memory effect allows Heusler alloys to recover their original shape upon heating, enabling their use in medical implants, robotics, and smart materials [67]. Themagnetostrictive properties of Heusler alloys make them attractive for applications in sensors and actuators that respond to magnetic fields. By exploiting the reversible magnetostrictive behaviour, Heusler alloys can be utilized in magnetic field sensors, magnetic switches, and vibration energy harvesters [68].

7.4 Emerging Applications

Beyond the aforementioned applications, Heusler alloys have shown promise in various emerging fields. For instance, their high thermal conductivity and mechanical stability make them potential candidates for thermal management applications, such as heat sinks and thermal interface materials [69]. Additionally, Heusler alloys have been explored for their catalytic properties, with potential applications in catalysis for clean energy and environmental remediation [70]. The versatility of Heusler alloys, combined with their tunable properties and unique functionalities, continues to drive research towards exploring novel applications and expanding their technological impact [71].

SUGGESTION AND RECOMMENDATION

1. Heusler alloys exhibit a diverse range of crystal structures, which significantly impact their electronic, magnetic, and thermoelectric properties. The relationship between composition and structure is crucial for tailoring these properties for specific applications.

2. The unique electronic properties, particularly the half-metallicity predicted by Density Functional Theory, position these alloys as promising candidates for spintronic applications. However, more experimental studies are needed to validate these theoretical predictions.

3. Despite their potential, there is a lack of comprehensive experimental data on the mechanical properties of Heusler alloys. Future research should focus on understanding and improving their mechanical stability and durability for practical applications.

4. Heusler alloys demonstrate promising thermoelectric properties, with high power factors and low thermal conductivity. Enhancing their thermoelectric efficiency could lead to significant advancements in energy conversion technologies.

5. The paper suggests that integrating Heusler alloys into existing technologies, such as lithium-ion batteries, fuel cells, and magnetic devices, can offer significant improvements. However, challenges in synthesis, property tuning, and integration with other materials must be addressed to fully exploit their potential in these applications.

CONCLUSION

Heusler alloys have emerged as a versatile class of materials with remarkable properties and potential applications. The comprehensive review of Heusler alloys presented in this paper highlights their structural, electronic, magnetic, mechanical, and thermoelectric features. The crystal structure and composition play a crucial role in determining the properties of Heusler alloys, with various classification schemes based on their unique structural symmetry. The electronic structure and band properties of Heusler alloys have been extensively studied using density functional theory (DFT), enabling a deep understanding of their electronic band structures and Fermi surface properties. The magnetic behaviour of Heusler alloys offers opportunities in spintronics and magnetic devices, showcasing their high spin polarization, tunable magnetic moments, and robust magnetism. The mechanical properties of Heusler alloys, including elastic constants, deformation mechanisms, and shape memory effects, make them suitable for applications in structural materials and actuation devices.

Additionally, Heusler alloys exhibit thermoelectric features, enabling the conversion of waste heat into electricity. The optimization of thermoelectric efficiency through strategies such as alloying, doping, and nanostructuring opens up new possibilities for energy conversion and harvesting. Recent advancements and potential applications of Heusler alloys in energy conversion and storage, spintronics, sensing, actuation, and emerging fields highlight their versatility and potential impact. However, challenges remain in synthesis techniques, property tuning, and integration with other materials and systems. Future research efforts should focus on addressing these challenges to unlock the full potential of Heusler alloys in various applications. Overall, Heusler alloys offer exciting prospects for the development of advanced functional materials with diverse technological applications.

REFERENCES

[1] Azhar, S., 2021, Spin-Orbit Effect on Thermal Properties of Half-Heusler Alloy FeVSb, JurnalFisika Dan Aplikasinya, 17(2) 48.

[2] Wu, M., Zhou, F., Khenata, R., Kuang, M., Wang, X., 2020, Phase Transition and Electronic Structures of All-d-Metal Heusler-Type X2MnTi Compounds (X = Pd, Pt, Ag, Au, Cu, and Ni), Frontiers in Chemistry, 8, Dec.

[3] Chen, K., Hu, M., Li, C., Li, G., Chen, Z., 2017, The Properties of Elasticity, Thermology, and Anisotropy in Pd-Based Alloys, Journal of Materials Science and Chemical Engineering, 5(03) 17-34, Jan.

[4] Mokhtari, A., Dahmane, F., Benabdellah, M., Zekri, N., Benalia, S., Zekri, N., 2018, Theoretical study of the structural stability, electronic and magnetic properties of XVSb (X = Fe, Ni, and Co) half-Heusler compounds, Condensed Matter Physics, 21(4) 43705, Dec.

[5] Chen, C., Ren, J., Wang, Z., Feng, L., Jiang, W., Hao, S., 2017, A First-Principles Study of a New Heusler Alloy, International Journal of Materials Science and Applications, 6(2) 108, Jan.

[6] Kubota, T., Shimada, Y., Tsuchiya, T., Yoshikawa, T., Ito, K., Takeda, Y., Takanashi, K. 2021. Microstructures and interface magnetic moments in Mn2VAl/Fe layered films showing exchange bias. Nanomaterials, 11(7) 1723.

[7] Benichou, B., Nabi, Z., Bouabdallah, B., Bouchenafa, H., 2018, Structural, elastic, electronic and magnetic properties of quaternary Heusler alloy Cu2MnSi1-xAlx (x = 0 - 1): First-principles study, Revista Mexicana De Física, 64(2) 135-140, Mar-Apr.

[8] Ozisik, H., Deligoz, E., Ateser, E., 2020, Phonon transport properties of NbCoSb compound, Materials Research Express, 7(2) 025004, Feb.

[9] Tavares, S., Yang, K., & Meyers, M. A. (2023). Heusler alloys: Past, properties, new alloys, and prospects. Progress in Materials Science, 132, 101017.

[10] Kroder, J., Fecher, G. H., Felser, C. 2021. Between intermetallic Compounds and Alloys Heusler Compounds. CHEMIE IN UNSERER ZEIT.

[11] Everhart, W., Newkirk, J. 2019. Mechanical properties of Heusler alloys. Heliyon, 5(5).

[12] Bourachid, I., Rached, D., Rached, H., Bentouaf, A., Rached, Y., Caid, M., Abidri, B. 2022. Magneto-electronic and thermoelectric properties of V-based Heusler in ferrimagnetic phase. Applied Physics A, 128(6) 493.

[13] Mondal, S., Ghosh, K., Ranganathan, R., Alleno, E., Mazumdar, C. 2023. Thermoelectric properties of Ru2TiGe Heusler phase. Journal of Alloys and Compounds, 171050.

[14] Mondal, S., Ghosh, K., Ranganathan, R., Alleno, E., Mazumdar, C. 2023. Magnetic and transport properties in metallic and disordered Ru2VAl and Ru2VGa. Intermetallics, 161, 107958.

[15] Antos, A. A., Borges, P. D. 2023. Ab initio investigation of Co–Ta–Sn Heusler alloys for thermoelectric applications. Computational and Theoretical Chemistry, 1229, 114301.

[16] Diaf, M., Righi, H., Rached, H., Rached, D., Beddiaf, R. 2023. Ab initio study of the properties of Ti2PdFe (Ru) Sb2 double half-heusler semiconducting alloys. Journal of Electronic Materials, 52(10) 6514-6529.

[17] Graf, T., Felser, C., Parkin, S. S.2011. Simple rules for the understanding of Heusler compounds. Progress in solid state chemistry, 39(1) 1-50.

[18] Güler, M., Güler, E., Uğur, Ş. U. L. E., Uğur, G., Charifi, Z., Baaziz, H. 2021. Elastic,

mechanical, anisotropic, optical and magnetic properties of V2NiSb Heusler alloy. Physica Scripta, 96(3) 035807.

[19] Kobayashi, S., Yakou, T. 2002. Control of intermetallic compound layers at interface between steel and aluminum by diffusion-treatment. Materials science and engineering: A, 338(1-2) 44-53.

[20] Galanakis, I. 2015. Theory of Heusler and full-Heusler compounds. In Heusler Alloys: Properties, Growth, Applications (pp. 3-36). Cham: Springer International Publishing.

[21] Huang, Y. L., Chen, W., Wee, A. T. 2021. Two-dimensional magnetic transition metal chalcogenides. SmartMat, 2(2) 139-153.

[22] Witting, I. T., Chasapis, T. C., Ricci, F., Peters, M., Heinz, N. A., Hautier, G., Snyder, G. J. 2019. The thermoelectric properties of bismuth telluride. Advanced Electronic Materials, 5(6) 1800904.

[23] Hayashi, K., Eguchi, M., Miyazaki, Y. 2017. Structural and thermoelectric properties of ternary full-Heusler alloys. Journal of Electronic Materials, 46, 2710-2716.

[24] Brito, K. K., Priyanka, D. S., Srinivasan, M., Ramasamy, P. 2023. Computations on platinum based ternary ferromagnetic half metals for spin valve diodes and green energy technology based thermoelectric. Journal of Magnetism and Magnetic Materials, 171629.

[25] Karati, A., Mukherjee, S., Mallik, R. C., Shabadi, R., Murty, B. S., Varadaraju, U. V. 2019. Simultaneous increase in thermopower and electrical conductivity through Ta-doping and nanostructuring in half-Heusler TiNiSn alloys. Materialia, 7, 100410.

[26] Aouimer, S., Ameri, M., Bensaid, D., Moulay, N. E., Bouyakoub, A. Z., Boufadi, F. Z., Al-Douri, Y. 2019. The Elastic, Electronic and Thermodynamic Properties of a New Cd Based Full Heusler Compounds--A Theoretical Investigation Using DFT Based FP-LMTO Approach. Acta Physica Polonica A, 136(1).

[27] Buchelnikov, V., Sokolovskiy, V., Entel, P. 2015. Magnetic states of C-doped Ni43. 75Co6. 25Mn37. 5In12. 5 Heusler alloys. In MATEC Web of Conferences (Vol. 33, p. 05001). EDP Sciences.

[28] Ryba, T., Vargova, Z., Ilkovic, S., Reiffers, M., Kravcak, J., Gyepes, R., Varga, R. 2017. Magnetic and structural characterization of NiXSb (X= Mn, Cr) Heusler ribbon. Acta Physica Polonica A, 131(4) 857-859.

[29] Qin, G., Wu, W., Hu, S., Tao, Y., Yan, X., Jing, C., Ren, W. 2017. Effect of swap disorder on the physical properties of the quaternary heusler alloy PdMnTiAl: A first-principles study. IUCrJ, 4(4) 506-511.

[30] Bi, Y., He, W., Yang, T., Wu, W., Wen, J., Yu, X., Chen, F. 2021. The Effects of La Doping on the Crystal Structure and Magnetic Properties of Ni2In-Type MnCoGe1− xLax (x= 0, 0.01, 0.03) Alloys. Materials, 14(14) 3998.

[31] Fang, T., Zhao, X., Zhu, T. 2018. Band structures and transport properties of high-performance half-Heusler thermoelectric materials by first principles. Materials, 11(5) 847.

[32] Almessiere, M. A., Slimani, Y., Güner, S., Nawaz, M., Baykal, A., Aldakheel, F., Ozcelik, Belenli, İ., Ozçelik, B. 2019. Magnetic and structural characterization of Nb3+-substituted $CoFe_2O_4$ nanoparticles. Ceramics International, 4(7) 8222-8232.

[33] Sharma, P. C., Kaphle, G. C., 2017, Electronic and Magnetic Properties of Half Metallic Heusler Alloy Co2MnSi: A First-Principles Study, Journal of Nepal Physical Society, 4(1), 60, May.

[34] Deng, S. H., Duan, M. Y., Xu, M., & He, L. (2011). Effect of La doping on the electronic structure and optical properties of ZnO. Physica B: Condensed Matter, 406(11), 2314-2318.

[35] Huang, H. L., Tung, J. C., Jeng, H. T. 2022. A first-principles study on the effect of Cr, Mn, and Co substitution on Fe-based normal-and inverse-Heusler compounds: Fe3− xYxZ (x= 0, 1, 2, 3; Y= Cr, Mn, Co; Z= Al, Ga, Si). Frontiers in Physics, 10, 975780.

[36] Asfour, I., Rached, D., Didier, S., Soraya, A., 2018, Theoretical Study of the Electronic and Thermodynamic Properties of Co₂CrZ (Z=Ga,Al), Universal Journal of Physics and Application, 12(4), 59-67, Dec.

[37] He, H. Y., Huang, J. F., Fei, J., Lu, J. 2015. La-doping content effect on the optical and electrical properties of La-doped ZnO thin films. Journal of Materials Science: Materials in Electronics, 26, 1205-1211.

[38] Wang, L., Li, F., Kuang, M., Gao, M., Wang, J., Huang, Y., Song, Y. 2015. Interface manipulation for printing

three-dimensional microstructures under magnetic guiding. Small, 11(16) 1900-1904.

[39] Alijani, V., Ouardi, S., Fecher, G. H., Winterlik, J., Naghavi, S. S., Kozina, X., Kobayashi, K.2011. Electronic, structural, and magnetic properties of the half-metallic ferromagnetic quaternary Heusler compounds CoFeMn Z (Z= Al, Ga, Si, Ge). Physical Review B, 84(22) 224416.

[40] Zhu, S., Zhang, X., Chen, J., Liu, C., Li, D., Yu, H., Wang, F. 2019. Insight into the elastic, electronic properties, anisotropy in elasticity of Manganese Borides. Vacuum, 165, 118-126.

[41] Babalola, M. I., Iyorzor, B. E., Ebuwa, S. O. 2023. First Principles calculation of Half metallic proprieties of QCrAs (Q= Hf, Ti and Zr). Journal of the Nigerian Society of Physical Sciences, 1029-1029.

[42] Joshi, V. K. 2016. Spintronics: A contemporary review of emerging electronics devices. Engineering science and technology, an international journal, 19(3) 1503-1513.

[43] Bekenov, L. V., Antonov, V. N., Shpak, A. P., Yaresko, A., 2005, Electronic structure and excited-state properties of Co_{2}TiSn and Co_{2}ZrSn from ab initio calculations, Condensed Matter Physics, 8(3), 565, Jan.

[44] Hsiao, A., McHenry, M. E., Laughlin, D. E., Kramer, M. J., Ashe, C., Ohkubo, T. 2002. The thermal, magnetic, and structural characterization of the crystallization kinetics of Fe/sub 88/Zr/sub 7/B/sub 4/Cu/sub 1/, an amorphous soft magnetic ribbon. IEEE Transactions on Magnetics, 38(5) 3039-3044.

[45] Gębara, P., Kutynia, K. 2019. Magnetocaloric Effect in Annealed (Mn, W)--Co--Ge Alloy. Acta Physica Polonica, A., 135(2).

[46] Khunkitti, P., Siritaratiwat, A., Kaewrawang, A., Mewes, T., Mewes, C., 2016, Angular Dependence of Spin Transfer Switching in Spin Valve Nanopillar Based Heusler Alloy, Advances in Materials Science and Engineering, 2016, 1-7, Jan.

[47] Song, H. C., Priya, S., 2018, A Review on Low-Grade Thermal Energy Harvesting: Materials, Methods and Devices, Materials, 11(8) 1433, Aug.

[48] Syrotyuk, S. V., 2021, Electronic Structure, Magnetic and Mechanical Properties of MnCoSi Half-Heusler Alloy, Metallofizika I NoveishieTekhnologii, 43(4) 541-551.

[49] Aouimer,S., Ameri,M., Bensaid,D., Moulay,N.E., Bouyakoub, A.E., Boufadi,F.Z., Ameri, I., Al-Douri, Y. 2019.The Elastic, Electronic and Thermodynamic Properties of a New Cd Based Full Heusler Compounds - A Theoretical Investigation Using DFT Based FP-LMTO Approach, Acta Physica Polonica A, 136(1) 127.

[50] Watanabe, N., Sano, K., Tasugi, N., Yamaguchi, T., Yamamoto, A., Ueno, M., Koiwa, I. 2015. Preparation of Co2FeSn Heusler alloys by electrodeposition method. APL Materials, 3(4).

[51] Jirásková, Y., Buršík, J., Janičkovič, D., Životský, O., 2019, Influence of Preparation Technology on Microstructural and Magnetic Properties of Fe2MnSi and Fe2MnAl Heusler Alloys, Materials, 12(5), 710, Feb.

[52] Zagrebin, M. A., Buchelnikov, V. D., Klyuchnikova, M. A., 2015, First Principles and Monte Carlo Calculations of Structural and Magnetic Properties of FexNi2-xMn1+yAl1-y Heusler Alloys, Matec Web of Conferences, 33, 05002, Jan.

[53] Liu, H., 2022, Comparative Study on the Crystallography of Isothermal and Athermal Precipitations in HCP–BCC System, Materials, 15(21) 7484, Oct.

[54] Krishnaveni, S., Sundareswari, M., 2017, Band gap engineering in ruthenium-based Heusler alloys for thermoelectric applications, International Journal of Energy Research, 42(2) 764-775, Sep.

[55] Gheriballah, S., Chahed, A., Benazzouzi, Y., Rozale, H., 2022. Structural, mechanical, electronic, and thermoelectric properties of new semiconducting d0 quaternary Heusler compounds CaKNaZ (Z = Si, Ge, Sn). A density functional theory study, Revista Mexicana De Física, 68(5) Aug. Sep-Oct.

[56] Cinthia, A. J., Rajeswarapalanichamy, R., Iyakutti, K. 2015. First principles study of electronic structure, magnetic, and mechanical properties of transition metal monoxides TMO (TM= Co and Ni). Zeitschrift für Naturforschung A, 70(10), 797-804.

[57] Kumar, P. M., Jagadeesh Babu, V., Subramanian, A., Bandla, A., Thakor, N., Ramakrishna, S., Wei, H. 2019. The design of a thermoelectric generator and its medical applications. Designs, 3(2) 22.

[58] Tajik, S., Beitollahi, H., Nejad, F. G., Shoaie, I. S., Khalilzadeh, M. A., Asl, M. S., Shokouhimehr, M. 2020. Recent developments in conducting polymers: Applications for electrochemistry. RSC Advances, 10(62) 37834-37856.

[59] Lim, C. S., Wang, L., Chua, C. K., Sofer, Z., Jankovský, O., Pumera, M. 2015. High temperature superconducting materials as bi-functional catalysts for hydrogen evolution and oxygen reduction. Journal of Materials Chemistry A, 3(16) 8346-8352.

[60] Selvamanickam, V. 2023. Engineering REBCO high temperature superconductor materials for applications. Physica C: Superconductivity and its Applications, 614, 1354355.

[61] Tayaba, S., Sethi, H., Shahid, H., Malik, R., Ikram, M., Ali, S., Maqbool, M. 2023. Silicon-Germanium and carbon-based superconductors for electronic, industrial, and medical applications. Materials Science and Engineering: B, 290, 116332.

[62] Rupich, M. W., Li, X., Thieme, C., Sathyamurthy, S., Fleshler, S., Tucker, D., Slack, J. 2009. Advances in second generation high temperature superconducting wire manufacturing and R&D at American Superconductor Corporation. Superconductor Science and Technology, 23(1) 014015.

[63] Peng, A., Kung, M. C., Brydon, R. R., Ross, M. O., Qian, L., Broadbelt, L. J., Kung, H. H. 2020. Noncontact catalysis: Initiation of selective ethylbenzene oxidation by Au cluster-facilitated cyclooctene epoxidation. Science Advances, 6(5) eaax6637.

[64] Yang, Z., He, J., Zang, X., Wang, X., Ren, Z., Xue, M., Chen, G. 2018. Rapid sonochemical synthesis of an intercalated superconductor. Chemistry Select, 3(20)5652-5659.

[65] Dubey, H. K. 2021. Carbon Nanofiber–A Potential Superconductor. Carbon Nanofibers: Fundamentals and Applications, 159-174.

[66] Wei, X., Chen, Z., Zhong, J., Wang, L., Wang, Y., Shu, Z. 2018. First-principles investigation of Cr-doped Fe2B: Structural, mechanical, electronic and magnetic properties. Journal of Magnetism and Magnetic Materials, 456, 150-159.

[67] Wegrowe, J., Drouhin, H., 2011, Spin-Currents and Spin-Pumping Forces for Spintronics, Entropy, 13(2) 316-331, Jan.

[68] Bos, J. G., 2017, Theoretical prediction of strain tuneable quaternary spintronic Heusler compounds, IUCrJ, 4(6) 712-713, Oct.

[69] Srinivasan, R., Modak, C., Swapna, Srinivasu, V. V., 2018, New Aspects of Microwave Absorption in Ferromagnetic Ni-Mn-Sn Thin Films, Acta Physica Polonica A, 134(1), 178-181, Jul.

[70] Rached, H., Rached, D., Rabah, M., Khenata, R., Reshak, A. H. 2010. Full-potential calculation of the structural, elastic, electronic and magnetic properties of XFeO3 (X= Sr and Ba) perovskite. Physica B: Condensed Matter, 405(17) 3515-3519.

[71] Rajput, P. J., Bhandari, S. U.,Wadhwa, G. 2022. A review on-spintronics an emerging technology. Silicon, 14(15)9195-9210.