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THE ROLE AND PRACTICAL SIGNIFICANCE OF GEYSLER ALLOYS IN MODERN MATERIALS SCIENCE

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Abstract. Heusler alloys represent an important class of functional intermetallic materials with highly tunable structural, electronic, magnetic, mechanical, and thermoelectric properties. Their scientific significance is associated with the possibility of controlling physical characteristics through chemical composition, atomic ordering, valence-electron concentration, and structural phase transformations. Full-Heusler, half-Heusler, inverse-Heusler, and quaternary Heusler systems have attracted considerable attention because of their potential applications in spintronics, thermoelectric energy conversion, magnetic refrigeration, shape-memory technologies, sensors, actuators, and emerging quantum materials. This article examines the structural characteristics, functional properties, practical applications, and research perspectives of Heusler alloys. Particular attention is paid to their half-metallicity, spin polarization, martensitic transformations, magnetocaloric behavior, and thermoelectric performance. The role of computational materials science, density functional theory, and machine-learning-assisted materials design in developing new Heusler compounds is also discussed.

Keywords: Heusler alloys, intermetallic materials, half-metallicity, spintronics, thermoelectrics, magnetic shape memory, magnetocaloric effect, materials science.

Introduction. The rapid development of modern electronics, energy technologies, information storage systems, sensors, and intelligent functional devices has increased the demand for advanced materials with controllable physical properties. Conventional structural materials are often insufficient for applications requiring simultaneous control of electrical conductivity, magnetism, thermal transport, mechanical deformation, and structural phase transitions. In this context, multifunctional intermetallic compounds have become an important research area in modern materials science. Heusler alloys occupy a special position among such materials because their physical properties can be widely modified by changing their chemical composition and atomic arrangement. The class includes full-Heusler compounds with a general composition of X_2YZ, half-Heusler compounds with XYZ composition, as well as inverse and quaternary Heusler systems. Their ordered crystal structures provide a basis for obtaining unusual combinations of electronic, magnetic, mechanical and thermal properties. The scientific importance of Heusler alloys increased significantly after the discovery of half-metallicity, in which electronic states near the Fermi level can exhibit metallic behavior for one spin channel and semiconducting or insulating behavior for the other. This feature makes appropriate

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Heusler compounds particularly attractive for spin-dependent electronic devices. At present, research on Heusler alloys is expanding beyond conventional ferromagnetic systems. Antiferromagnetic compounds, spin-gapless semiconductors, topological materials, thermoelectric Heusler compounds, magnetic shape-memory alloys, and magnetocaloric materials are also being actively investigated. Therefore, studying the role and practical significance of Heusler alloys is relevant for understanding the development of next-generation functional materials and their potential integration into advanced technological systems.

Literature review. Heusler alloys have attracted sustained scientific interest because of their remarkable combination of structural, electronic, magnetic, mechanical, and thermal properties. Since the early discovery of anomalous magnetic behavior in Heusler-type intermetallic compounds, research has gradually expanded from fundamental crystallographic studies toward the development of multifunctional materials for advanced technological applications. Contemporary investigations emphasize that the properties of Heusler compounds can be systematically modified through chemical composition, atomic ordering, valence-electron concentration, and structural phase transformations [1]. One of the fundamental contributions to the understanding of Heusler compounds was provided by the development of electronic-structure-based classification principles. Graf, Felser, and Parkin demonstrated that relatively simple relationships between valence-electron concentration, crystal structure, and magnetic moment can be used to understand and predict important properties of many Heusler compounds [4]. Their work established a theoretical framework for explaining the magnetic behavior of these materials and subsequently contributed to the development of composition-based strategies for materials design. A particularly important direction in Heusler alloy research is associated with the concept of half-metallicity. In ideal half-metallic compounds, electronic states exhibit metallic behavior for one spin channel and a band gap for the opposite spin channel. This characteristic can result in high spin polarization and makes such materials attractive for spintronic applications. According to Hirohata and co-authors, Heusler alloys are promising candidates for spin-dependent electronic devices because their electronic and magnetic properties can be tailored through compositional engineering and atomic ordering [2; 3]. The literature also demonstrates the importance of Heusler alloys in the development of spintronics. Unlike conventional electronics, spintronic technologies exploit both the charge and spin of electrons. Heusler compounds with high spin polarization have consequently been investigated for magnetic tunnel junctions, spin valves, spin-transfer-torque devices, magnetic sensors, and non-volatile memory technologies. Palmstrøm emphasized that the combination of high Curie temperatures and favorable electronic structures makes Heusler compounds particularly attractive for room-temperature spintronic applications [5]. Another significant research direction concerns the thermoelectric properties of Heusler materials. Half-Heusler compounds have received considerable attention because their electronic structures and transport properties can be modified through elemental substitution and defect engineering.

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Research into martensitic transformations and shape-memory effects has considerably expanded the practical significance of Heusler alloys. Ni–Mn-based systems are among the most intensively studied materials because they can undergo reversible structural transformations between austenitic and martensitic phases. These transformations may be accompanied by changes in magnetization, strain, and mechanical properties. Consequently, Heusler alloys have been investigated for magnetic shape-memory actuators, sensors, microelectromechanical systems, and smart-material applications [6]. Therefore, the existing literature demonstrates that Heusler alloys constitute a highly versatile materials platform rather than a single-purpose class of intermetallic compounds. Their tunable electronic, magnetic, structural, and thermal properties provide a strong foundation for applications in spintronics, thermoelectric energy conversion, magnetic refrigeration, shape-memory technologies, sensing, and emerging quantum devices. At the same time, the integration of experimental methods with first-principles calculations, high-throughput screening, and artificial intelligence represents a promising pathway for overcoming existing limitations and accelerating the discovery of next-generation Heusler materials.

Materials and methods. The theoretical analysis presented in this article is based on a review and comparative analysis of scientific publications concerning Heusler alloys. Particular attention is given to studies addressing crystal structure, electronic properties, magnetism, phase transformations, thermoelectric behavior and technological applications.

The main methodological approaches include:

- comparative analysis of full- and half-Heusler structures;
- analysis of structure–property relationships;
- examination of electronic and magnetic characteristics;
- assessment of potential technological applications;
- analysis of density functional theory (DFT)-based materials design;
- comparative evaluation of recent developments in functional Heusler materials.

Modern research frequently combines experimental characterization with first-principles calculations. X-ray diffraction is particularly important for determining crystal structure and atomic ordering, while magnetic, electrical and thermal measurements provide information about functional behavior.

Results and discussion. The distinctive properties of Heusler alloys originate largely from their ordered intermetallic structures. Full-Heusler compounds generally have the X_2YZ composition, while half-Heusler compounds have XYZ composition. Depending on composition and atomic arrangement, inverse and quaternary structures can also be formed. The degree of atomic ordering is particularly important. Structural disorder can modify electronic states, magnetic moments and transport properties. Consequently, controlling synthesis conditions, composition and thermal treatment is essential for obtaining the desired functional characteristics. In Ni–Mn-based Heusler systems, for example, changes in temperature and composition can lead to transitions between ordered austenitic and

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martensitic structures. Such transformations are closely related to magnetic and shape-memory behavior.

Electronic and magnetic properties. One of the most significant characteristics of selected Heusler alloys is half-metallicity. In an ideal half-metallic system, one spin channel exhibits metallic conductivity while the opposite spin channel possesses a band gap. This creates a high degree of spin polarization that is highly desirable for spintronic applications. The magnetic properties can be controlled through elemental substitution. Changes in valence-electron concentration influence the electronic structure and magnetic moment, which provides a practical strategy for designing materials with predetermined magnetic characteristics. This tunability is particularly important for magnetic tunnel junctions, spin valves, magnetic sensors and other devices in which the control of spin-polarized current is essential.

Role in spintronics. Spintronics is one of the most important technological areas in which Heusler alloys have demonstrated considerable potential. Conventional electronics primarily uses the charge of electrons, whereas spintronic technologies exploit both charge and spin. Heusler alloys with high spin polarization can serve as efficient spin sources. Their use in magnetic tunnel junctions and related structures may contribute to the development of non-volatile memory, magnetic logic and low-power information-processing technologies. The combination of high spin polarization and potentially low magnetic damping is also attractive for high-speed magnetization switching. Consequently, Heusler alloys are being investigated for spin-transfer-torque and spin-orbit-torque devices.

Thermoelectric applications. Another important field is thermoelectric energy conversion. Thermoelectric materials transform temperature differences into electrical energy and can therefore contribute to waste-heat recovery and solid-state cooling. Half-Heusler compounds are particularly interesting because their electronic structures can be modified through chemical substitution while maintaining relatively stable crystal frameworks. Research on transport properties demonstrates that Heusler compounds can exhibit tunable electrical conductivity, thermopower and thermal transport characteristics. The practical challenge is to achieve an optimal combination of high electrical conductivity, high Seebeck coefficient and low thermal conductivity. Elemental substitution, nanostructuring and defect engineering are among the approaches used to improve these parameters.

Magnetic shape-memory effect. Certain Ni–Mn-based Heusler alloys exhibit martensitic transformations accompanied by significant changes in magnetic and mechanical behavior. These materials can demonstrate magnetic shape-memory effects, in which deformation can be controlled through an external magnetic field or temperature variation. Such properties create opportunities for developing compact actuators, sensors and smart mechanical systems. Recent structural studies indicate that the phase composition, atomic ordering and crystallographic defects strongly influence these functional properties.

Magnetocaloric applications. Heusler alloys are also investigated as magnetocaloric materials. The magnetocaloric effect involves a temperature or entropy change associated with the application or

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removal of a magnetic field. Such materials have potential for solid-state refrigeration technologies. The advantage of magnetocaloric Heusler systems is associated with their ability to combine magnetic transitions with structural phase transformations. Proper control of composition and phase stability can therefore be used to optimize caloric responses.

Topological and quantum materials. An especially promising direction is the investigation of Heusler compounds as topological materials. Their electronic band structures can exhibit nontrivial characteristics, making some members of this materials family potential candidates for topological insulating and semimetallic states. This research direction is important because topological materials may provide new physical principles for electronic and spintronic devices. Combining topological properties with magnetism or superconductivity could further expand the functionality of Heusler-based systems.

Computational design and artificial intelligence. A major contemporary trend is the use of computational materials science for predicting new Heusler compounds before experimental synthesis. Density functional theory can be used to investigate electronic structures, magnetic moments, formation energies, phase stability and mechanical characteristics. High-throughput computational screening enables researchers to analyze large numbers of potential compositions. More recently, machine-learning methods have been incorporated into materials discovery workflows, allowing researchers to identify relationships between composition, structure and desired properties more efficiently. This approach is particularly important for Heusler alloys because the number of possible elemental combinations is extremely large. Therefore, computational screening combined with experimental verification can reduce the time and resources required for the discovery of new functional materials.

Practical significance of Heusler alloys. The major practical areas of Heusler alloys can be summarized as follows:

Property	**Potential application**
Half-metallicity and high spin polarization	Spintronics, magnetic tunnel junctions
High thermoelectric performance	Waste-heat recovery, thermoelectric generators
Magnetic shape-memory effect	Sensors, actuators, smart devices
Magnetocaloric effect	Solid-state refrigeration
Tunable magnetic properties	Magnetic storage and sensing
Topological electronic states	Advanced quantum electronics
Controlled thermal/electrical transport	Energy-conversion technologies
Multifunctional behavior	Intelligent and adaptive materials

The practical significance of Heusler alloys is therefore determined not by a single property but by their multifunctionality. Their composition and structure can be engineered to achieve specific combinations of properties required for particular applications.

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Conclusion. Heusler alloys have evolved from scientifically interesting intermetallic compounds into an important platform for the development of advanced functional materials. Their unique combination of electronic, magnetic, structural, thermal and mechanical properties provides opportunities for applications in spintronics, thermoelectric energy conversion, magnetic refrigeration, shape-memory devices, sensors and emerging quantum technologies. The analysis demonstrates that the most important advantage of Heusler alloys is their high degree of tunability. By changing chemical composition, valence-electron concentration, atomic ordering and structural phase, it is possible to control their functional properties. This makes them especially attractive for materials-by-design approaches. Future development of the field is closely connected with the integration of experimental research, density functional theory, high-throughput calculations and machine-learning methods. Such integration can accelerate the discovery of stable, efficient and environmentally sustainable Heusler compounds. Consequently, Heusler alloys can be regarded as one of the promising material classes for next-generation technologies. Their further investigation and optimization may contribute significantly to the development of energy-efficient electronics, intelligent functional devices, advanced sensors and sustainable energy-conversion systems.

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