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MAGNETIC AND STRUCTURAL PROPERTIES OF COFESN HEUSLER ALLOYS SYNTHESIZED BY HYDROTHERMAL METHOD

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Abstract

Heusler alloy CoFeSn nanoparticles were prepared through the hydrothermal route from CoCl, FeCl, and SnCl as precursors. The synthesis was carried out at 150°C for 6 h in an autoclave with molarity changes from 0.2 to 1.0 M. A pure phase of CoFeSn, was obtained at 1.0 M. Structural analysis indicated an increase in crystallite size with increased molarity, while dislocation density was inversely related to crystallite size. FTIR spectroscopy confirmed chemical and structural modifications attributed to different functional groups. Vibrating sample magnetometer (VSM) measurements indicated ferromagnetic character with low coercivity. Hardness measurements by a Shimadzu HMV-2 Vickers micro-indenter indicated increasing hardness with phase formation and stabilization with increasing molarity. Electrical characterization by I-V measurements showed enhanced conductivity for phase-pure samples, with a higher current-voltage response at lower temperatures.

INTRODUCTION

In the past decade, Heusler alloys have attracted a lot of interest in materials science owing their fascinating collection of magnetic, electronic, and structural properties making them well contenders for an array of applications that span from spintronics, magnetic storage devices, and energy-saving technologies [1,8]. The cobalt-iron-tin (CoFeSn) Heusler alloys are particularly interesting because they have high Curie temperature, highly tunable magntizable behavior, and can have their

optimal performance for next-generation devices. Synthesis of CoFeSn Heusler alloys typically involves complicated processes that can significantly affect their structural and magnetic properties [7]. While traditional methods such as arc-melting and solid-state reaction methods have been widely employed, the hydrothermal process has recently emerged as a possible method for synthesizing nanomaterials with defined morphology, particle size, and phase composition [13]. This method has several significant advantages, such as the ability to achieve high phase purity, well-defined crystalline structures, and fine control of stoichiometry, which are important for enhancing the performance of Heusler alloys.

Nevertheless, even as interest in the hydrothermal synthesis of Heusler alloys increases, the systematic study of the correlations between synthesis parameters (temperature, precursor concentration, reaction time) and structural and magnetic properties of the resulting CoFeSn alloys is not well developed. A better understanding of such correlations is important for process optimization and design of the desired properties for targeted technological applications [1,8].The present research investigates hydrothermal synthesis of CoFeSn Heusler alloy to fill this gap [1].

Hydrothermal synthesis of CoFeSn Heusler alloy serves as the research method to examine this gap. The emphasis is on determining the influence of synthesis parameters on the structural, morphological, and magnetic properties of the alloys. The results of this research will be useful in the synthesis-structure-property relationship and help in the creation of CoFeSn alloys for next-generation applications in magnetic devices, energy storage systems, and spintronic technologies.

1. Materials and Methodology

Materials

The CoFeSn Heusler alloy nanoparticles were produced based on high-purity precursor materials: Cobalt chloride ($CoCl_2$, 99.99%), Iron chloride ($FeCl_3$, 99.99%), and Tin chloride ($SnCl_2$, 99.99%) purchased from commercial sources [7]. Deionized water was utilized as the solvent during the entire synthesis process in order to form high-quality products. The precursor solutions were set up with different molarity ranging from 0.2 M to 1.0 M to examine the influence of molarity on the structural, magnetic, and electrical properties of the prepared CoFeSn Heusler alloys [8].

Synthesis of CoFeSn Heusler Alloy

The CoFeSn Heusler alloy nanoparticles were prepared using a hydrothermal route. In short: Preparation of Precursor Solution: Stoichiometric quantities of $CoCl_2$, $FeCl_3$, and $SnCl_2$ were dissolved in deionized water to create the precursor solution [7]. The molarity ranged from 0.2 M to 1.0 M.

Hydrothermal Process: The precursor solution was poured into a Teflon-lined autoclave, which was next heated at 150°C for 6 hours. The black precipitates that formed after the reaction were then washed using deionized water and ethanol to prevent any residual salts and unreacted precursors from remaining. Samples were then dried at 60°C for 12 hours and annealed at 500°C for 2 hours to improve phase stability [19].

2. Characterization Techniques

X-ray Diffraction (XRD) Analysis

X-ray diffraction (XRD) was applied to analyze the structural behavior and phase makeup of the CoFeSn Heusler alloy nanoparticles. Diffraction spectra were collected in a Bruker D8 Advanced X-ray diffractometer, along with Cu Kα radiation (λ = 1.5406 Å), at the Centre of Excellence in Solid-State Physics. The patterns were studied through the XRD using the following criteria to get its lattice parameters, crystallite size, and dislocation density of the samples. The lattice constant (a) was found from Bragg's law:

$$n\lambda = 2d\sin\theta$$

The crystallite size was measured by the Scherrer equation, and phase transitions were detected by comparing the intensity of diffraction peaks with different molarity (0.2 M to 1.0 M) [19].

Fourier Transform Infrared (FTIR) Spectroscopy

FTIR spectroscopy was utilized to investigate the chemical interactions and functional groups in the CoFeSn Heusler alloys. The spectra were obtained with a Thermo Fisher Scientific Nicolet iS10 FTIR spectrometer from 500–3000 cm^{-1}. FTIR spectra were employed to detect characteristic functional

groups and vibrational modes, and thus the chemical bonding and structural properties of the prepared alloys[22].

Vibrating Sample Magnetometer (VSM) Analysis

The magnetic characteristics of CoFeSn Heusler alloy nanoparticles were measured by a Lakeshore 7400 VSM. The magnetic hysteresis (M-H) loops were taken to measure the important magnetic parameters like saturation magnetization (Ms), coercivity, and remanent magnetization. The samples showed ferromagnetic nature, and the magnetic response was studied as a function of molarity, showing a correlation between crystallite size and magnetic characteristics [10].

Current-Voltage (I-V) Characterization

The electrical behavior of the CoFeSn Heusler alloys was determined by taking the current voltage (I-V) characteristics with a Keithley 2400 Source Meter. The I-V was taken at room temperature and low temperatures (100 K). The measurement of tests on electrical conductivity and resistivity occurred through sample evaluation with different voltage ranges. A voltage range analysis of the material enabled current measurement to produce I-V curves that revealed electrical properties. Light comings from electrical testing allowed us to understand electrical characteristics as well as how crystallinity influences charge movement[4].

Data Analysis and Interpretation

Researchers analyzed crystallite dimensions in the XRD spectrum through implementation of the Scherrer equation. Assistance of the Scherrer equation. The phase content of CoFeSn alloys was established through the identification of peaks within XRD spectral data as well as phase transformation occurrence was recorded at different molarity levels. The molarity analysis reveals that pure phases emerge as molarity rises while the initial mixture phases disappear. An M-H loop test allowed researchers to derive the saturation magnetization (Ms) values obtained by VSM analysis [7]. The investigated values showed direct correlations with both phase structures and crystallite dimensions. The experimental findings used XRD and VSM to uncover magnetic properties of created materials during their synthesis [10].The assessment of electrical conductivity and resistivity of the materials occurred through examination of I-V data [4]. Samples. Research results served to analyze the relationship between crystal structure and material phase and their effects on electrical properties of the CoFeSn Heusler alloys.

Result and Discussion

4.1 XRD Analysis

The X-ray diffraction technique generated quantitative as well as qualitative structural physical information about CoFeSn half-Heusler alloy nanoparticles [19]. Structural physical properties of the CoFeSn half-Heusler alloy nanoparticles. The lattice parameters of Bragg's law allowed the samples' lattice constant calculation using the following formula:

$$n\lambda = 2d\sin\theta$$

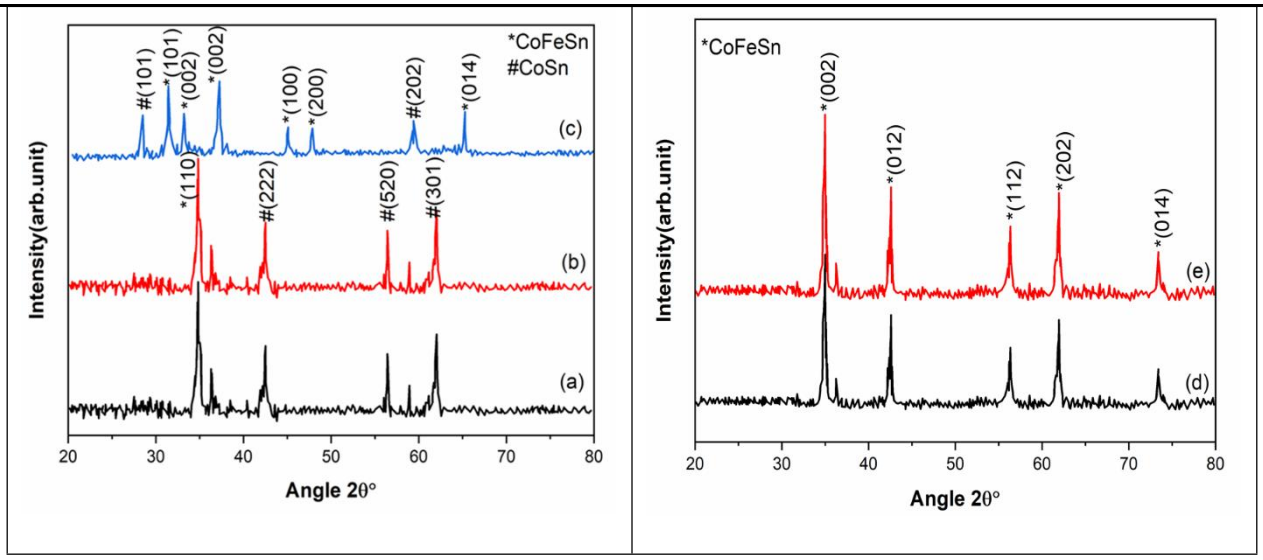


Figure 1: X-ray diffraction (XRD) patterns of CoFeSn half-Heusler alloy nanoparticles synthesized at different conditions

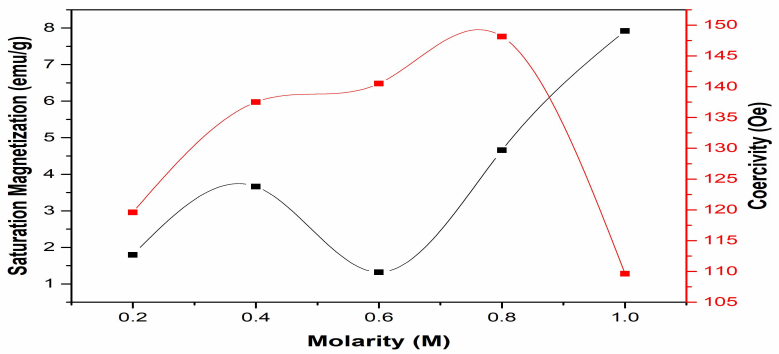


Figure 2: XRD pattern between intensity and Bragg's angle (2θ) for CoFeSn alloys at varying molarities.

XRD patterns were obtained by using the Bruker D8 Advanced diffractometer that produces Cu Kα radiation λ = 1.5406 Å from the Centre of Excellence in Solid State Physics. The CoFeSn alloys were synthesized via a hydrothermal process, and their XRD patterns were analyzed as a function of molarity (0.2M to 1.0M). The patterns displayed peaks corresponding to the (002), (012), (112), (014), and (202) crystallographic planes, indicating a hexagonal structure with space group P63/mmc.

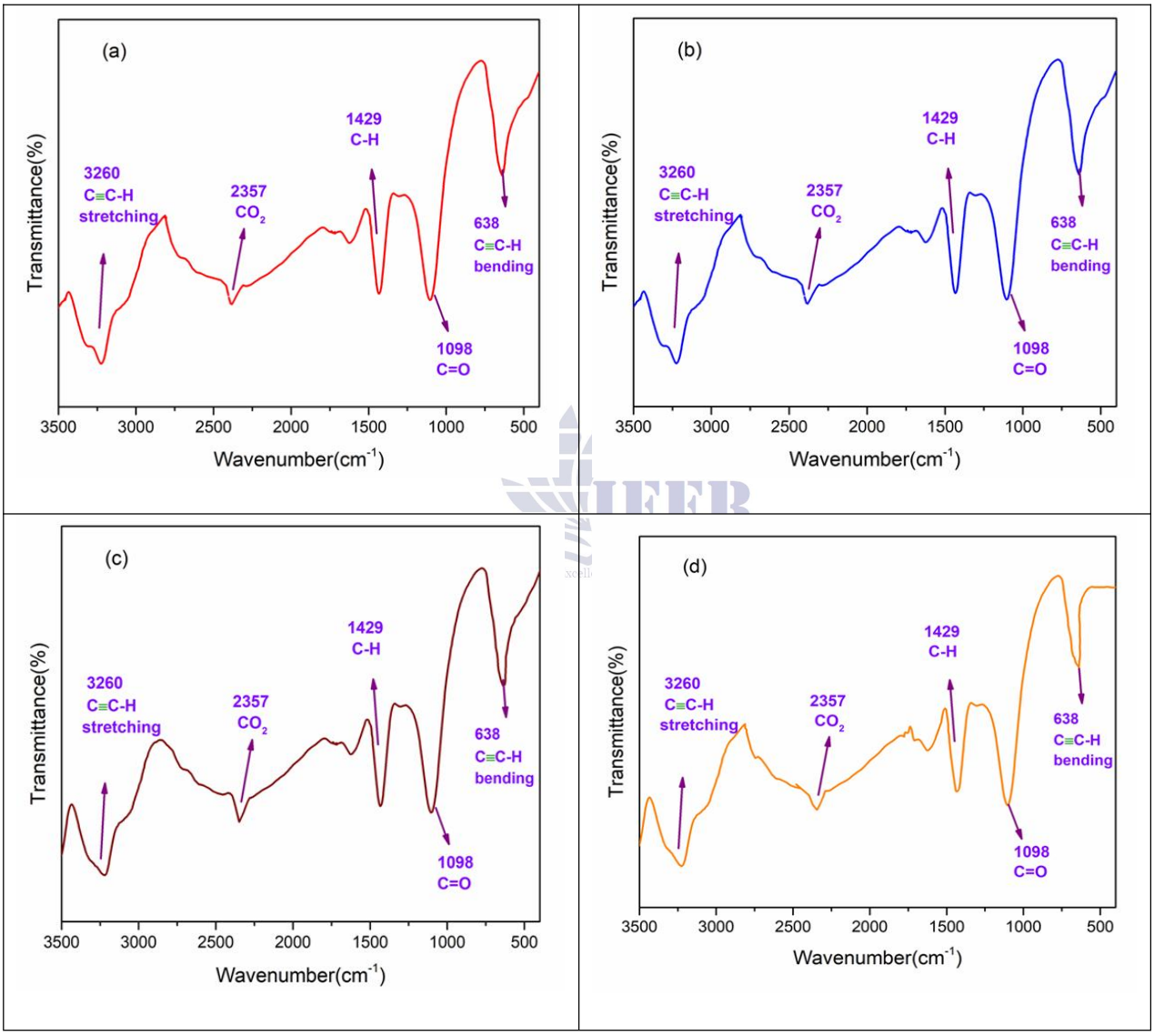
The phase transition from a mixed phase to a pure phase was observed at a molarity of 0.8M, driven by the minimization of surface energy and internal stresses. This transition led to preferential growth along certain crystallographic planes. Further increases in molarity up to 1.0 M resulted in phase stability and strengthening of the CoFeSn alloy[7]

The crystallite size and dislocation density were also evaluated as a function of molarity, as shown in Figure 2. Initially, the crystallite size increased from 0.2M to 0.6M, correlating with the phase transformation and structural rearrangement. As the molarity increased to 0.8M, further growth in crystallite size was observed, while the dislocation density showed an inverse trend. This behavior is attributed to micro-strain, dislocations, and defects introduced during the hydrothermal synthesis process. The saturation magnetization (Ms) of the CoFeSn alloys is plotted as a function of molarity, as presented in Figure 4.3. The Ms values ranged from 0.2M to 1.0M because of increased crystallinity and crystallite size, but fell at 0.6M as a result of crystallite size reduction. The phase transition to a pure phase at 0.8M led to the rise in Ms, with the

highest being seen at 1.0M (8.0 emu/g) and the lowest at 0.6M (0.003 emu/g)

4.2 FTIR Analysis

The Fourier transform processed this data to produce a spectrum according to the first paper [25]. The researcher acquired CoFeSn half-Heusler alloys through different molar concentration measurements (0.2M to 1.0M) within the mid-IR spectral range (3000-500 cm^{-1}). A variety of molecular and absorption bands emerge in the spectra and they match structural and chemical transitions within the alloy. Various functional groups within the alloy become evident through FTIR when chemical and structural transitions occur in the alloy system[22].



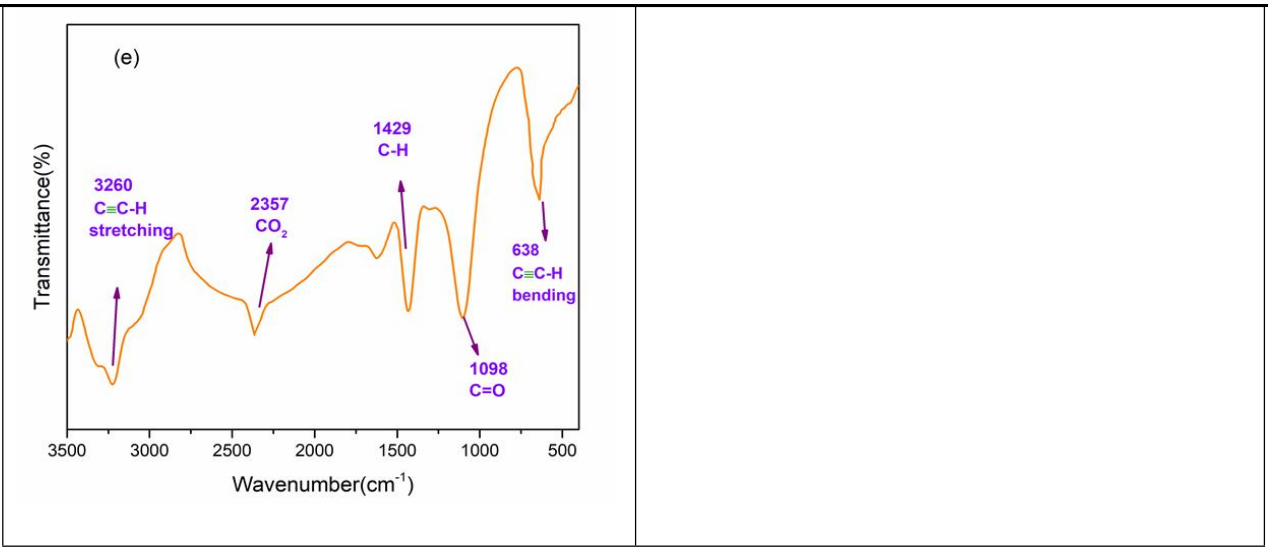
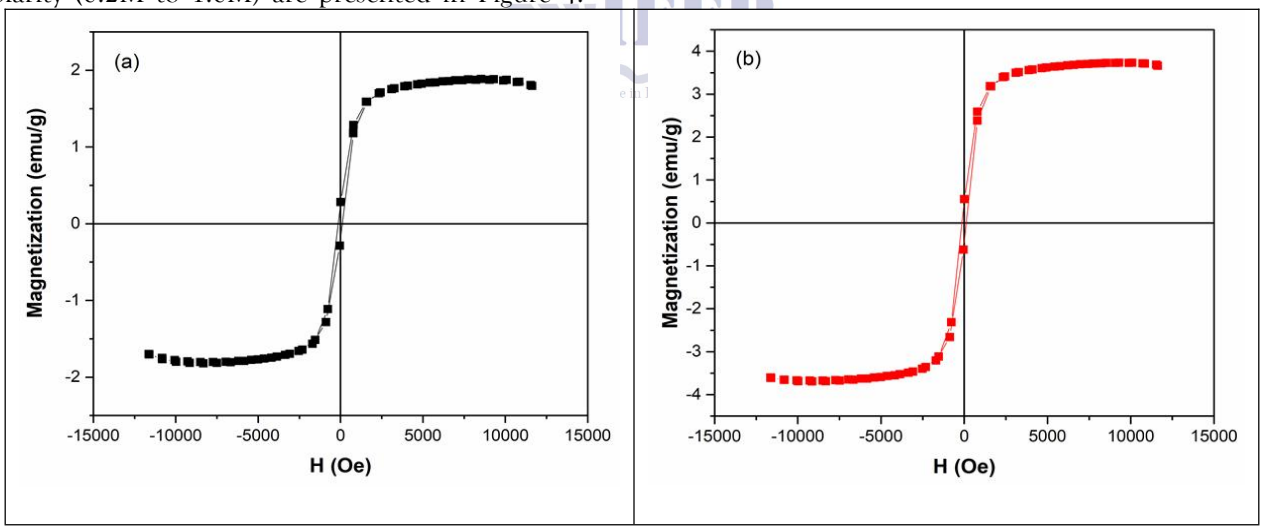


Figure 3: FTIR spectra of CoFeSn alloys at different molarities (0.2M to 1.0M), exhibiting molecular and absorption bands in the mid-IR region.

4.3 VSM Analysis

A Vibrating Sample Magnetometer (VSM) was used to evaluate the magnetic properties of CoFeSn half-Heusler alloy nanoparticles [10]. The magnetic hysteresis (M-H) loops for samples with varying molarity (0.2M to 1.0M) are presented in Figure 4. All samples exhibit ferromagnetic behavior with low coercivity values, indicating their potential suitability for magnetic applications. The variation in magnetic properties correlates with changes in crystallite size and phase composition.



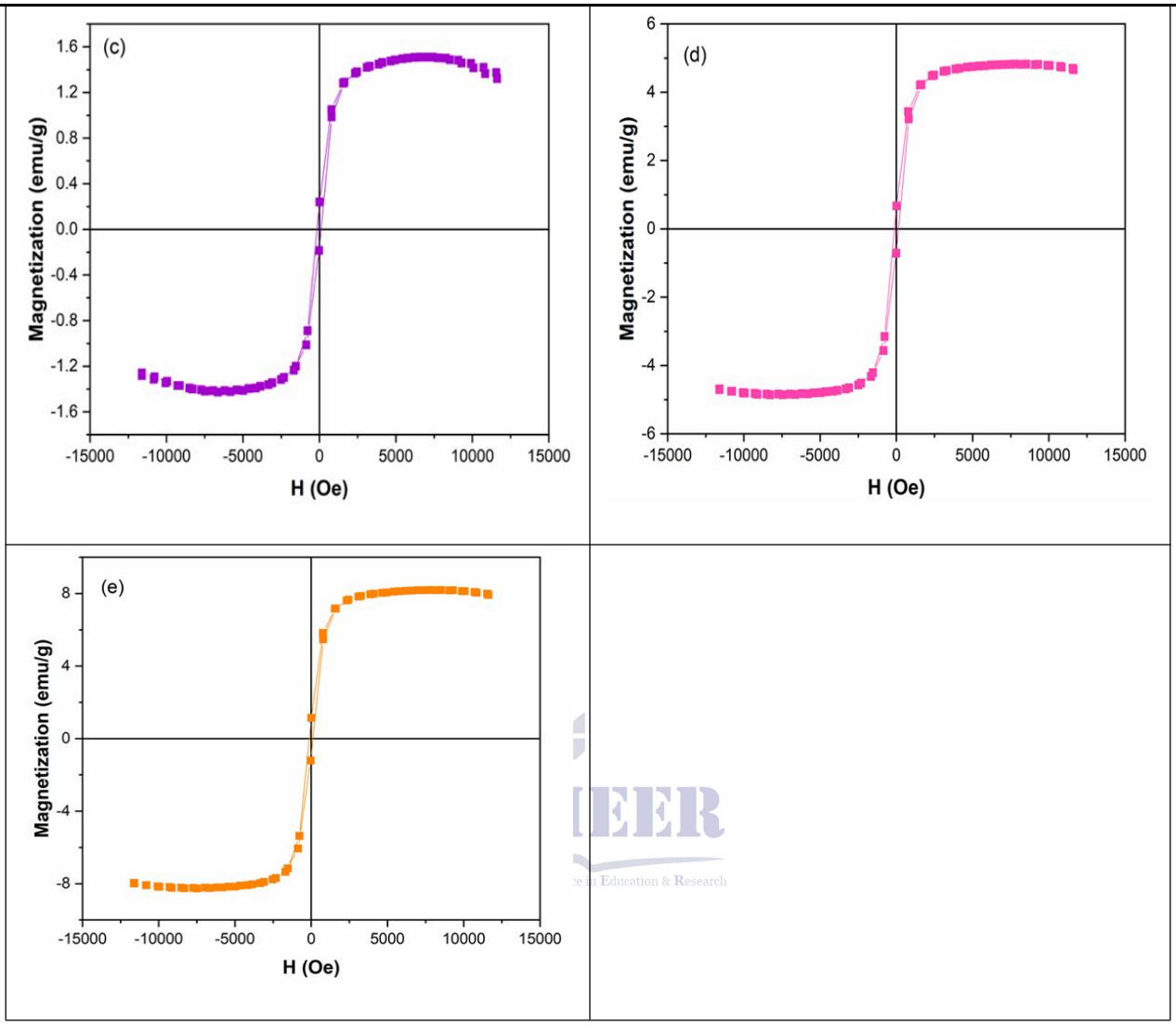


Figure 4: Magnetic hysteresis (M-H) loops of CoFeSn half-Heusler alloy nanoparticles at different molarities (0.2M to 1.0M), demonstrating ferromagnetic behavior with low coercivity.

4.4 Hardness Analysis

The hardness of CoFeSn half-Heusler alloy at various molarities (0.2M, 0.4M, 0.6M, 0.8M, and 1.0M) was determined using a Shimadzu HMV-2 Vickers micro-indenter, following the ASTM C1327-99 standard. The Vickers indenter was applied for 15 seconds at a load of 4.903 N to ensure reliable measurements[25].

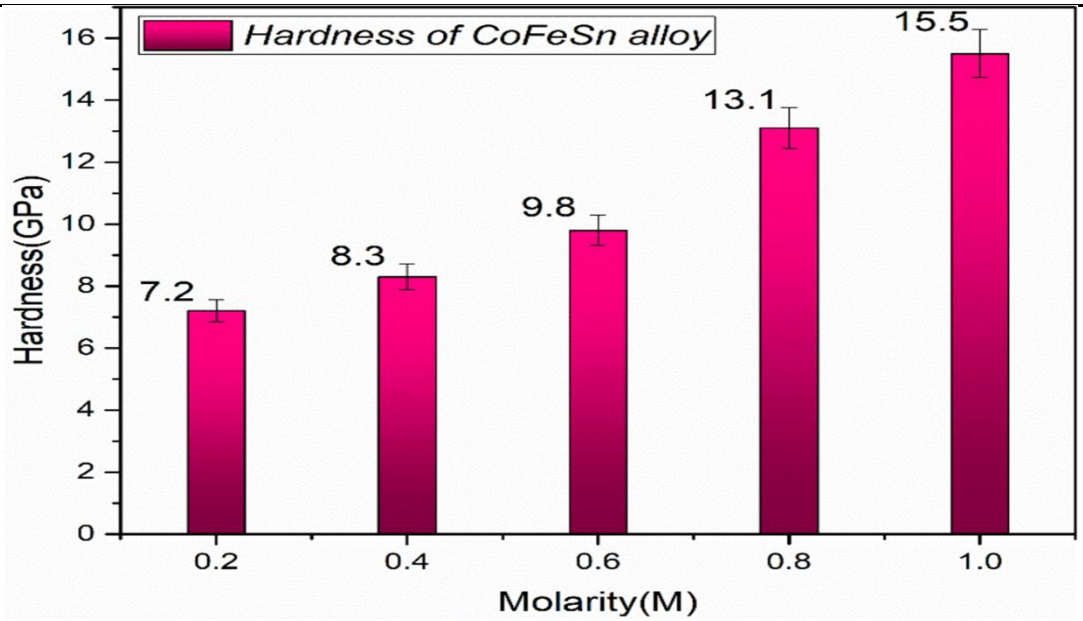


Figure 5: Hardness values of CoFeSn half-Heusler alloy at different molarities.

The measured hardness values exhibit a significant variation with molarity. The highest hardness values (~13.1–15.5 GPa) were recorded for samples synthesized at 0.8M–1.0M, which is attributed to the formation of a stable, pure-phase structure, as confirmed by XRD analysis. In contrast, lower hardness values (~7.2–9.8 GPa) were observed for samples at lower molarities, likely due to the presence of mixed crystal phases, leading to structural inconsistencies.

4.5 I-V Measurements

The I-V characteristics of CoFeSn half-Heusler alloy at varying molarities (0.2M to 1.0M) were analyzed to evaluate electrical conduction properties [4]. Figure 6 presents the I-V curve, which exhibits linear and nearly symmetric characteristics with respect to bias polarity. This indicates dominant conduction behavior. However, a slightly larger current was observed under forward bias, likely due to thermionic emission at the interface.

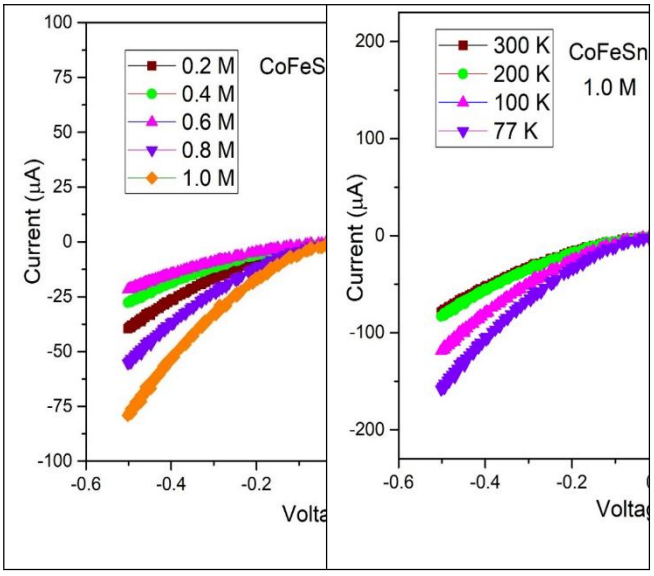


Figure 6: I-V characteristics of CoFeSn half-Heusler alloy at different molarities.

Furthermore, temperature-dependent I-V measurements were conducted using a three-terminal geometry to examine conduction behavior at various temperatures (T). The results confirm that I-V curves remain nearly linear and symmetric across all temperature ranges, with only slight variations in current. This suggests that temperature has a minimal effect on conduction behavior in the CoFeSn half-Heusler alloy system.

Conclusion

In the present investigation, CoFeSn half-Heusler alloys were effectively synthesized by employing the hydrothermal process, varying molarity values of 0.2M, 0.4M, 0.6M, 0.8M, and 1.0 M[1]. Systematic analysis was carried out to determine the structure, magnetism, mechanical behavior, and electric properties to establish the influence of molarity on the performance of the material.

XRD Analysis: The maximum crystallite size of 25.5 nm was found for 1.0M, reflecting enhanced structure order with elevated molarity[19].

FTIR Spectroscopy: The functional group analysis reaffirmed molecular interaction and structural stability of the synthesized samples[22].

Magnetic Properties (VSM Analysis): M-H loops revealed soft ferromagnetic behavior with a narrow hysteresis width. The highest saturation magnetization was observed at 1.0M, while coercivity exhibited a positive correlation with particle size[10].

Hardness Measurements: The maximum Vickers hardness (~9.1 GPa) was achieved for the optimized 1.0M sample, attributed to enhanced phase purity and structural stability[25].

I-V Characteristics: The highest electrical conductivity was recorded for the phase-pure sample at 1.0M, with strengthened current-voltage response at lower temperatures[4].

These results demonstrate that optimizing molarity in the hydrothermal synthesis of CoFeSn half-Heusler alloys significantly enhances structural, magnetic, mechanical, and electrical properties, making them promising candidates for spintronic, magnetic storage, and thermoelectric applications[1,7,10].

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