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UNVEILING THE VIBRATIONAL FINGERPRINTS OF TRANSITION METAL-DOPED NICKEL FERRITE NANOPARTICLES VIA FTIR SPECTROSCOPY

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Abstract

Because of their distinct structural, magnetic, and electrochemical characteristics, nickel ferrite ($NiFe_2O_4$) nanoparticles are particularly noteworthy and show promise as materials for energy storage applications. The synthesis and structural analysis of nickel ferrite nanoparticles doped with transition metals for use in super capacitors are the goals of this study. In order to investigate how the substitution of transition metal ions into the Ni ferrite lattice can alter the structure and electrochemical activity of Ni ferrite. An adequate preparatory chemical reaction can be used to synthesize the nanoparticles, and the necessary material can then be produced by the right processing. FTIR can be used to characterize structures and morphologies. While FTIR spectroscopy is used to examine metal-oxygen interactions and their distinctive vibrations. Additionally, electrochemical methods including cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy can be utilized to evaluate the produced nanoparticles' suitability for usage in super capacitor devices. Establishing a relationship between transition metal doping, structure, and electrochemical characteristics is the aim of the research. The findings may be helpful in creating an effective ferrite-based electrode material for cutting-edge energy storage uses.

Keywords:
Nanoparticles, Super capacitors, Electrochemical Properties, Structural characterization, FTIR Transition metal doping, Nickel ferrite

INTRODUCATION

Recent advances in nanotechnology have opened up new possibilities for the creation of sophisticated materials with improved optical, chemical, electrical, magnetic, and structural qualities. Because of their nanoscale size, which can provide their material properties different features from those of bulk materials, nanoparticles have attracted a lot of attention. Their huge surface area to volume ratio, size-dependent behaviors, and easily adjustable chemical composition make them suitable for use in biological sciences, electronics, sensors, environmental cleanup, catalysis, and energy storage. The characteristics of nanoparticles can be altered by a number of variables, including their size, shape, chemical makeup, crystallinity, and synthesis circumstances. Therefore, obtaining nanomaterials with desired properties requires the synthesis of suitable synthesis procedures and a methodical investigation of structural properties. (Altammar, 2023; Anu Mary Ealia & Saravanakumar, 2017).

Metal oxide nanoparticles are an important class of functional nanomaterials with excellent chemical and physical characteristics. Among these materials, ferrite nanoparticles have garnered a lot of scholarly attention due to their magnetic properties, chemical stability, and potential uses in technology and industry. Usually, ferrites consist of iron oxide plus one or more metal cations. Metal cations are accommodated into both tetrahedral and octahedral positions of the oxygen lattice in the crystal structure of the spinel Fe_3O_4, which is characteristic of the spinel ferries and is represented by the generic formula MFe_3O_4.The distribution of the cations between these sites has a major impact on the material's structural, magnetic, and electrical characteristics. Thus, it is advantageous to modify the composition of spinel ferrites in order to customize their properties according to certain uses (Houshiar et al., 2014; Astafyev et al., 2020). Nickel ferrite, also known as $NiFe_2O_4$, is a significant member of the Spinel ferrite family and has been thoroughly studied because of its chemical stability, magnetic characteristics, and prospective industrial uses. Because the iron and nickel cations are located in separate crystallographic locations, it is commonly referred to as an inverse spinel.These structural characteristics affect nickel ferrite's electrical and magnetic characteristics. Nickel ferrite nanoparticles have been researched for a variety of uses, including sensors, magnetic devices, catalysis, and electrochemical energy storage. According to Houshiar et al. (2014) and Ilayas et al. (2023), they can be customized by modifying the solved synthesis circumstances or incorporating additional metal ions into the crystal's structure.The substitution of some of the Fe ions in the host crystal structure with Cr3+ or Al3+ is one of the most common methods of ferrite structural modification. Lattice characteristics, crystallite size, ion distribution and defect concentration, and electron interactions can all be impacted by doping. The kind and concentration of the dopant, as well as its ionic size, oxidation level, and propensity for particular crystallographic sites, all affect how much of these changes occur.As a result, doping is now a crucial tool for researching how ferrite nanoparticle behavior is altered depending on composition. Research on modified ferrite systems has demonstrated the ongoing interest in the connection between these materials' structural features, chemical makeup, and functional attributes (Ghayour et al., 2017; Hamza et al., 2025; Iliyas et al., 2023).Because zinc dopant provides an example of how to modify the structural and magnetic properties of nickel ferrite, zinc doped $NiFe_2O_4$ nanoparticles are intriguing. Zinc-substituted Ni-Fe oxide typically has the chemical formula $Ni_{1-x}Zn_xFe_2O_4$, where x is the ratio of Ni to Zn ions. As the concentration of zinc varies, so can the distribution of metal cations inside the spinel structure. As with the general situation of tetrahedrally coordinated spinel type structures, the

distribution of the cations depends on the composition or preparation circumstances. Zinc ions in spinel type ferrites are tetrahedrally coordinated.The lattice parameters, crystallite formation, magnetic interactions, and other characteristics of the material may be impacted. In order to determine how zinc affects the characteristics of nickel ferrite nanoparticles, it would be useful to investigate different zinc concentrations.

The structural and magnetic characteristics of ferrites containing zinc were examined in earlier research. Ghayour et al. (2017) have looked into the usage of Zn-doped $NiFe_2O_4$ nanoparticles for magnetic hyperthermia and found that the Zn inclusion matter in $NiFe_2O_4$ ferrite nanostructured materials shows its importance in a particular application.In conclusion, our study of Ni-Zn ferrite-based nanoparticles is noteworthy due to its wider implications in modifying spinel ferrite materials through composition modification. Their morphological and structural characteristics can be quantitatively assessed to provide direction for more research and to identify the ideal composition for a certain technological application. The impact of zinc incorporation in $NiFe_2O_4$ and how it aids in the creation and description of functional ferrite nanoparticles will be examined in this work.

Synthesis Procedure

Zinc-doped NiFe nanoparticles are produced using a straightforward and inexpensive technique (co-precipitation method) that has been demonstrated to be viable for ferrite nanoparticle creation (Houshiar et al., 2014). In distilled water, the salts of the predecessors of Ni, Zn, and Fe were first individually dissolved. Solutions: To create a homogenous mixture, these were made by stirring for a considerable amount of time. To create a very alkaline solution that might aid in precipitation, NaOH solution was then added dropwise. The resulting mixture was constantly agitated and allowed to settle so that the precipitate might develop. To clean it, they centrifuged the precipitate and repeatedly washed it with distilled water. Following oven drying, the material was crushed into a fine powder and kept in a dry, clean container for additional analysis. The analytical methods for characterizing produced. They would require additional electrochemical testing to determine their application in super capacitors.

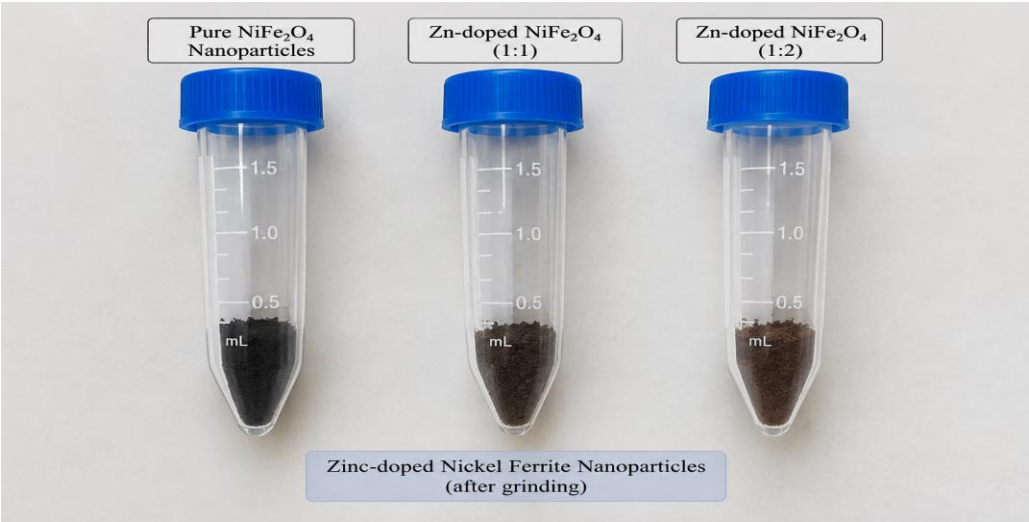


Figure 1: Nanoparticles after grinding Zinc doped Nickel Ferrites Nanoparticles with different ratios

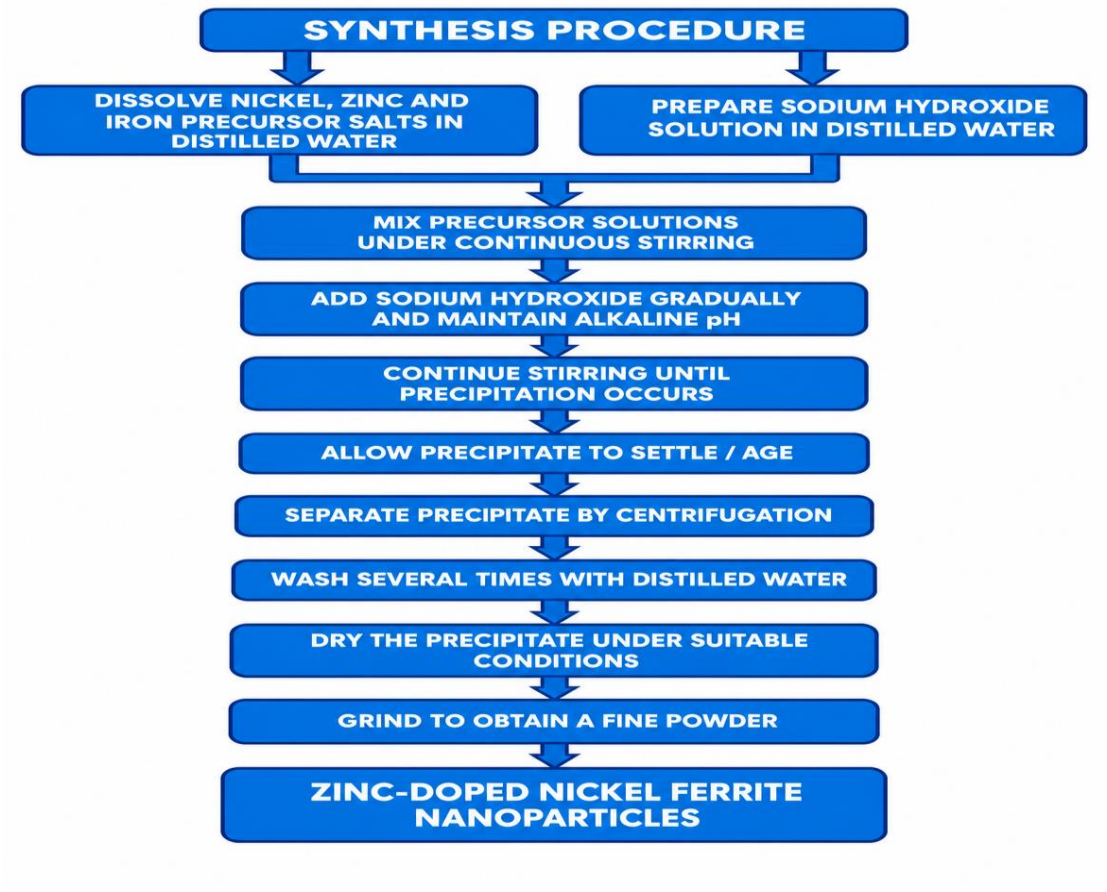


Figure 2: Flow chart for of Zinc doped Nickel Ferrites Nanoparticles

Result and Discussion

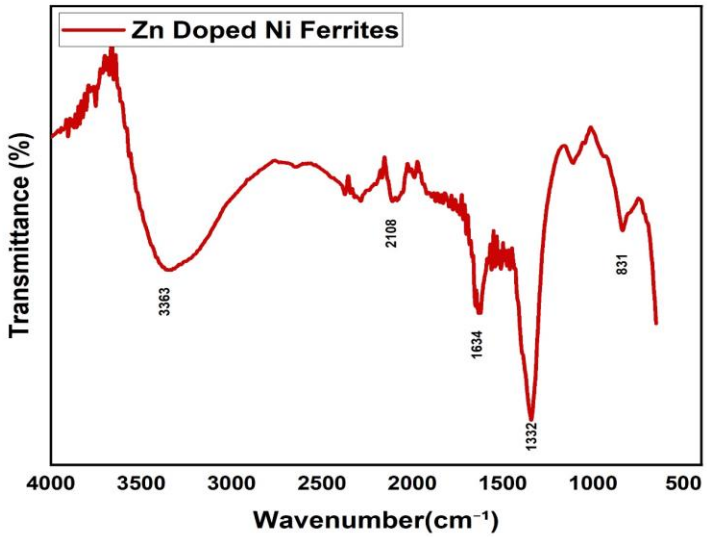


Figure 3: FTIR spectra of Zinc doped Nickel Ferrites Nanoparticles

FTIR spectroscopy was used to examine the produced zinc-doped $NiFe_2O_4$ nanoparticles in order to determine their vibrational characteristics and the functional groups involved. Absorption bands at around 3363, 2108, 1634, 1332, and 831 cm^{-1} are visible in the FTIR spectrum. Ferrite nanoparticles' bonding properties and metal-oxygen vibrations can be examined using FTIR spectroscopy, which provides important details about the nanoparticles' chemical structure (Anu Mary Ealia & Saravanakumar, 2017; Houshiar et al., 2014).

The broad absorption band that appears at about 3363 cm^{-1} can be attributed to the stretching vibration of O–H groups, either because of the presence of hydroxyl ions on the surface or because of the adsorbed water. These kinds of nanoparticle samples frequently show bands because moisture sticks to the particle's surface. This band may therefore be associated with the existence of hydroxyl-containing compounds that remain in the produced material even after drying.Because of the absorption property displayed, vibration of any single species at 2108 cm^{-1} is achievable. This is not characteristic of the primary vibrations of the spinel structure's metal–oxygen bonds. As a result, it is best to precisely assign its spectrum by comparing it to reference spectra and considering the precursor chemicals and synthesis conditions. The vibrational and structural characteristics of Fe_3O_4 nanoparticles need to be investigated in addition to other characterization data, according to Houshiar et al.'s investigation of the structural characteristics of ferrite nanoparticles produced by various synthesis techniques. The band seen at about 1634 cm^{-1} may be related to the bending of the water molecules that have been adsorbed on the nanoparticle surface. The big, featureless O–H band found at 3363 cm^{-1} is consistent with this. According to Anu Mary Ealia and Saravanakumar (2017), the FTIR spectra of the nanoparticles are also understood in relation to harmonic atomic vibrations connected to their surface. At 1332 cm^{-1}, a prominent absorption characteristic is observed. Other surface functional groups and trace amounts of precursor-related species may be present in this band. However, it is challenging to identify a single vibration in the spectrum with confidence. To determine its origin, a more thorough analysis of the initial materials and comparison with reference spectra are required. This assignment should not be taken for granted. The absorption band at about 831 cm^{-1} may be connected to a lattice vibration or other vibrations related to the presence of O-Me complexes. Due to the presence of the distinctive metal oxygen vibrational bands, spinel ferrites are often examined in the lower wavenumber range. Therefore, it is necessary to carefully examine the 400–700 cm^{-1} range in order to find frequencies that may indicate ferrite lattice vibrations.Houshiar et al. (2014) It provide background information on the structural characterization of ferrite nanoparticles.The entire FTIR spectrum provides details about hydroxyl-related groups and other potential species that might be present on the surface of the artificially produced zinc-doped nickel ferrite nanoparticles. However, the identification of the spinel ferrite structure requires careful consideration of data and metal–oxygen vibrations at lower wavenumbers. Furthermore, FTIR is the sole method that can validate the effective inclusion of Zn into the $NiFe_2O_4$ lattice.

Conclusion and Future Perspective

This study uses the co-precipitation approach to synthesize and characterize zinc-doped nickel ferrite nanoparticles for potential use in supercapacitors. The co-precipitation approach has been extensively researched for the manufacture of ferrite nanoparticles due to its straightforward methodology, low cost,

and good control over synthesis conditions. Since then, it has been observed that a number of experimental factors, including temperature, pH, stirring settings, and precursor concentration, affect the structural and morphological characteristics of the resulting nanoparticles.(Houshiar et al., 2014; Anu Mary Ealia & Saravanakumar, 2017).

These investigations demonstrate the importance of the relationship among material qualities, crystal structure, and dopant concentration. However, it is crucial to use experimental characterisation to confirm the impact of the zinc doping in the current samples. Because the materials' electrochemical characteristics can be used as supercapacitor electrodes, ferrite materials based on nickel have also attracted study interest for their usage in energy storage. The concept of altering ferrite materials' composition to make them more electrochemical was pioneered in the realm of research on doped nickel ferrite electrodes.(Ilayas et al., 2023). For upcoming research on electrode materials for energy storage applications, zinc-substituted nickel ferrite nanoparticles can serve as a potential model. However, based solely on structural characterizations, they are not always appropriate for supercapacitors; instead, electrochemical techniques must be used to evaluate them. Therefore, the co-precipitation approach provides a practical way to get zinc-doped nickel ferrite nanoparticles ready for further study.It is emphasized that a thorough investigation should be conducted to clarify the impact of zinc inclusion and their potential for application in supercapacitors. This investigation should encompass structural, morphological, compositional, and electrochemical characterisation of the synthesized material.The effects of different zinc concentrations on the morphological, structural, and electrochemical characteristics of nickel ferrite nanoparticles require more investigation. A correlation between the performance of the material and the amount of zinc would be possible if nickel ferrite samples were taken before and after the addition of various zinc levels.Previous research has examined the importance of composition and electrode properties for enhanced electrochemical materials in doped ferrite materials for energy storage applications (Ilayas et al., 2023; Hamza et al., 2025). FTIR can be used to study characteristic bonding vibrations, This different technique will provide a deeper understanding of the relationship between the structure and characteristics of Ni-ferrite nanoparticles based on zinc.Electrochemical characterisation of zinc-doped nickel ferrite as a supercapacitor electrode material is a crucial subject for future research. These kinds of measurements enable the comparison of material properties with other ferrite-based electrode systems and are essential for assessing electrode performance.Moreover, zinc-doped nickel ferrite could be combined with conductive fillers like graphene, reduced graphene oxide, or carbon nanotubes to perform a functional investigation of the electrochemical characteristics. These composites can facilitate the transfer of charges and enhance electrical conductivity. Therefore, in order to get superior performance, different ideal circumstances of dopant concentration, composite composition, electrolyte selection, and preparation technique should be improved.The stability, repeatability, and usefulness of the electrodes based on zinc-doped nickel ferrite for longer cycle lifespans must also be further investigated. Comparisons of the performance of reported electrode materials and modified nickel ferrite could be useful in understanding the benefits and limitations of zinc incorporation. Studying the doped ferrites, which have been explored for energy storage applications, may also be helpful in examining these compositional changes (Hamza et al., 2025).

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