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**ANALYSIS OF THERMAL BEHAVIOUR OF UNDOPED AND DOPED
CADMIUM SULPHIDE NANOMATERIALS FOR ENERGY APPLICATIONS**

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Abstract

Undoped Cadmium sulphide and doped cadmium sulphide nanomaterials with copper and silver are effectively synthesized using ethylene glycol as a capping agent by the chemical precipitation process. Scanning electron microscopy and x-ray diffraction studied the composition and crystalline structure of materials. These techniques have estimated the average particle size of such nanomaterials to be between 4-8 nm. Energy Analysis Dispersive X-Ray reveals the components present in these materials. Using UV-visible absorption spectrums, the nanoparticles were calculated in the band gap, resulting in significantly blue values being moved from the large Cadmium Sulphide Band Gap values. The thermal properties of the nanomaterials were analysed by Thermogravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC).

Keywords: Cadmium Sulphide, Chemical Precipitation, XRD, TGA, DSC

1. Introduction

The thermal behavior of undoped and doped cadmium sulphide (CdS) nanomaterials was analyzed in several studies. CdS nanofilms were synthesized and characterized for photovoltaic cell applications, and their thermal properties were investigated [1]. CdS nanoparticles were synthesized through polyol synthesis method using a novel ligand and its Cadmium (II) complex, and their thermal behavior was characterized [2]. Control-sized CdS quantum dots and cellulose nanocrystals grafted polyvinylpyrrolidone doped CdS quantum dots were synthesized, and their thermal properties were studied [3]. CdS thin films were deposited using chemical bath deposition technique, and their thermal behavior was analyzed [4]. Nanostructured europium doped CdS thin films were grown using spray pyrolysis, and their thermal properties were investigated [5]. These studies provide insights into the thermal behavior of undoped and doped CdS nanomaterials, which is important for their applications in various fields. Due to their specific optic, electronic and catalyst properties [6-9], nanomaterials semiconductors have been intensively investigated over the past few years. The strong surface-to-volume ratio and the measuring impact is both due to these properties. II – VI category nanomaterials of semiconductors are particularly valued in Optics because of their strongly optical properties based on scale [10]. Many methods were developed to produce nanomaterials such as chemically reduced semiconductors, fluid reaction methods, slaughter template method, hydro-thermal and Solv thermal methods [11, 12]. The Solv thermal process recently has potential benefits of fairly low-cost, standardized measurements, good purity, and regulated morphology across all these methods [13]. Solvents are the main problem in this method for processing Solv thermal nanomaterials for CdS purposes. To order to produce outstanding CDS semi-conductive nanomaterials, mixed solutions are required. Due to their optical and semiconductor capabilities, cadmium sulphide (CdS) nanoparticles are popular in energy applications. In solar cells, CdS nanoparticles are essential. CdS nanoparticles absorb or sensitize electrons in quantum dot-sensitized solar cells. CdS quantum dots in the photoactive layer improve light absorb and electron transport in these devices. This increases photoconversion efficiency and solar power output. CdS nanoparticles' variable bandgap allows them to match the solar spectrum on absorption, making them adaptable photovoltaic device enhancers. Additionally, CdS nanoparticles show photocatalytic activity. Solar radiation can make them effective photocatalysts for water splitting and pollutant degradation. Their ability to form electron-hole pairs when exposed to light converts solar energy into chemical energy, decomposing organic pollutants and producing hydrogen gas from water. Photocatalytic energy conversion and environmental remediation could be sustainable and ecologically beneficial.

2. Methodology

Various essential components are involved in the synthesis process of cadmium sulphide (CdS) nanoparticles. Initially, it is worth noting that cadmium chloride (CdCl₂) or cadmium acetate (Cd(CH₃COO)₂) are frequently employed as cadmium precursors in order to furnish a supply of cadmium ions for the purpose of nanoparticle generation. In addition, a sulphur source is utilised in the process, commonly sodium sulphide (Na₂S) or thiourea (CS(NH₂)₂), to provide sulphur ions that undergo a reaction with cadmium ions, resulting in the formation of CdS nanoparticles. Furthermore, the utilisation of a solvent such as distilled water is employed to facilitate the dissolution of these precursors, thereby establishing the

appropriate reaction media. In certain instances, the inclusion of capping agents or stabilising agents, such as thioglycolic acid, polyvinylpyrrolidone (PVP), or sodium dodecyl sulphate (SDS), can be employed to regulate the dimensions and durability of the CdS nanoparticles. These materials collectively enable the precise production of CdS nanoparticles with adjustable characteristics, rendering them highly desirable for various applications in fields like optoelectronics, catalysis, and solar energy conversion.

Multiple techniques exist for the synthesis of cadmium sulphide (CdS) nanoparticles, each presenting distinct benefits and enabling precise manipulation of the nanoparticles' dimensions, morphology, and characteristics. Chemical precipitation is a frequently employed technique in which cadmium and sulphur precursors are combined in a solution to initiate the creation of nanoparticles via precipitation. An alternative technique is the hydrothermal method, wherein the synthesis of CdS nanoparticles is facilitated by subjecting the reaction system to elevated temperatures and pressures. The sol-gel synthesis method is an alternative methodology that employs a sol-gel transition process to achieve the controlled formation of nanoparticles. Furthermore, the utilisation of microwave-assisted synthesis involves the application of microwave radiation as a means of expediting the heating process, resulting in accelerated reaction kinetics. In contrast, sonochemical synthesis employs ultrasonic vibrations as a means to enhance the creation of nanoparticles. Each of the aforementioned approaches offers unique benefits in terms of controlling particle size, scalability, and ease of implementation, rendering them appropriate for a range of applications, spanning from optoelectronics to catalysis and photovoltaics. The selection of the appropriate methodology is mostly influenced by the specific criteria of the planned application and the desired characteristics of the CdS nanoparticles.

The chemical precipitation technique utilised in the synthesis of cadmium sulphide (CdS) nanoparticles is a simple and economically efficient process. The process entails the creation of precursor solutions through the dissolution of cadmium chloride or cadmium acetate in water, as well as the inclusion of sulphur sources such as sodium sulphide in a distinct container. Subsequently, the aforementioned solutions are combined with continuous agitation, resulting in the progressive generation of CdS nanoparticles by the process of precipitation. The manipulation of reaction parameters, such as temperature, pH, and reaction time, enables the regulation of both size and characteristics of nanoparticles. Following the completion of the reaction and the regulation of nanoparticle growth, purification is commonly carried out by means of centrifugation or filtration. The resulting nanoparticles are then collected, subjected to a washing process, and subsequently dried. The chemical precipitation process presents several benefits, including the capacity to scale up production, achieve high yields, and customise the characteristics of CdS nanoparticles to meet diverse application requirements. Nevertheless, it is imperative to exercise prudence when utilising cadmium precursors that possess toxic properties. This necessitates the implementation of appropriate safety protocols during the synthesis procedure. Additionally, the attainment of nanoparticle purity and stability may entail the inclusion of supplementary procedures.

The synthesis of CdS nanoparticles was based on cadmium chloride (CdCl_2) and sodium sulphide (Na_2S) and ethylene glycol as a capper. The beaker was treated with the introduction of a single mole of cadmium chloride solution and a sodium sulfide (Na_2S) mole concentration (0.1 mole of capping agent) solution in another beaker. At a temperature of 380rpm, beaker solutions are stirred continuously and added with a magnetic stirrer and stirred again with a magnetic stirrer for 30 minutes. The solution colour is converted into light yellow.

The solution was centrifuged at a room temperature of 12,000rpm after mixing. The rainfall sample was eventually collected and dried 3 times with methanol. The above preparatory method to get fine powder for prepared samples was repeated by 1 mole of cadmium sulphide, added with 1 mg silver nitrate (AgNO_3) and Cadmium sulphide doped with 1 mg of copper fillings added with a 1 mole. In the structural process of the samples, Powder XRD diffraction experiments were conducted with copper radiation. The calculations of grain size were made on the basis of the scherrer equation using half the normal diffraction time, which was adjusted for extension of the instrument axis. Unoped Cadmium sulphide, copper doped cadmium and silver doped Cadmium sulphide nanomaterials are 6 nm, 4 nm and 8 nm respectively Scanning electron microscopy, energy scanning spectroscopy (EDAX) tests conducted for morphology analysis and sample proofing of the elements presented.

3. Results and Discussion

Thermogravimetric analysis (TGA) examines the thermal characteristics of undoped and doped CdS nanomaterials. The thermal decomposition of Cadmium sulphide (CdS), Copper doped CdS (CdS: Cu) and Silver doped (CdS: Ag) nanomaterials is used for TGA processing. The synthesized materials had been heated by synchronized thermal systems from

room temperature up to 1300°C, rising by 100°C/min. Figure 1 shows the TGA test of Pure CdS. The weight loss is determined by TGAs and the heat flow as endogenously.

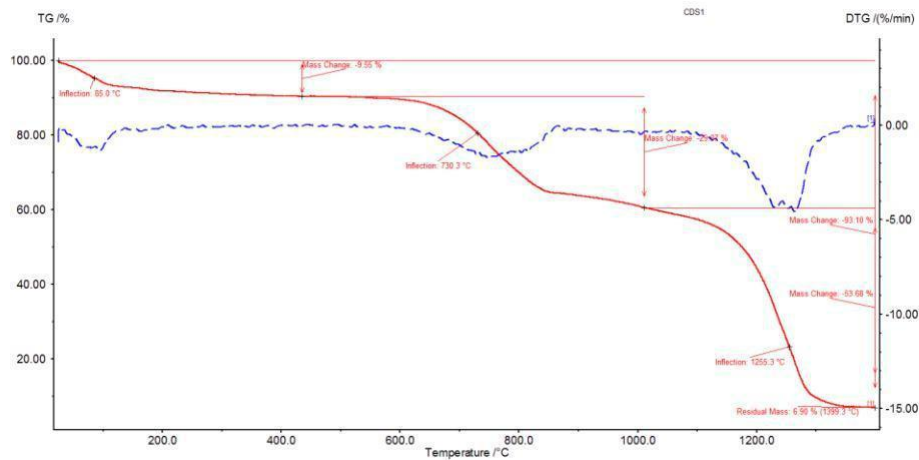


Fig.1 TGA and DTG of Pure CdS

With a slight endothermic peak of about 85°C and two other at 730°C and 1255°C, the Pure CdS is thermally stable. In general the evaporation of dissolved water on the surface of the substance is liable for a very slight weight loss below 1300°C. Due to this evaporation, the material has a very small weight loss. Therefore, the sample is up to 1300°C thermally stable. Due to evaporations of organic components on the surface of the material, there is an exothermic peak at 85°C. So between 100°C and 500°C a weight reduction of 9.55 percent is reported. During the change, weight loss is about 29.87% from 600°C and 1000°C. It is accompanied by a substantial weight loss from 1000°C and 1300°C of about 63.68%. Around 600°C and 1300°C the total process transition was 93.1%. The DSC curve for pure CdS nanoparticles was also investigated between 50°C and 1300°C.

figure 2 shows the DSC curve of the pure CdS nanomaterials. It is observed from the graph that, there is a peak around at 505°C, 823°C and 899.8°C

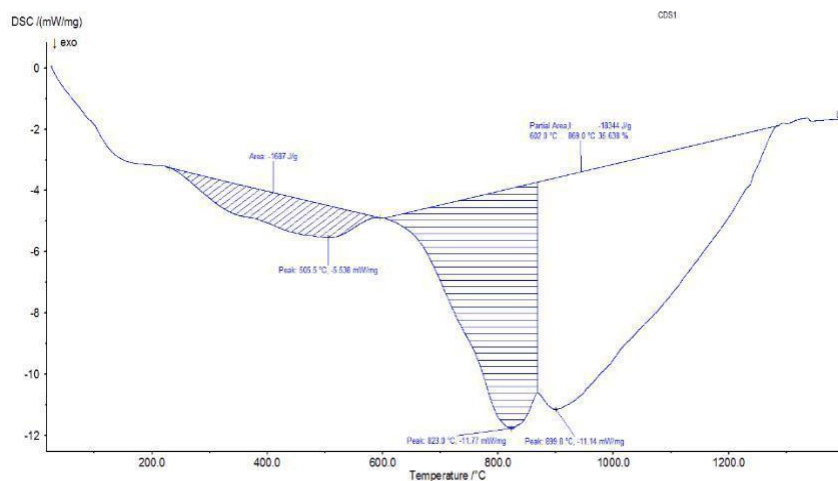


Fig.2 DSC of Pure CdS

Similarly figure 3 shows the case of Copper doped cadmium sulphide there is a peak at 66.3°C due to the evaporation at 50°C to 150°C and the phase transformation is at 729°C, 786°C and 1218°C with weight loss of 19.30%, 9.86% and 52.05% with a temperature of 650°C to 1250°C. The overall weight loss for the phase transformation is 93.03%.

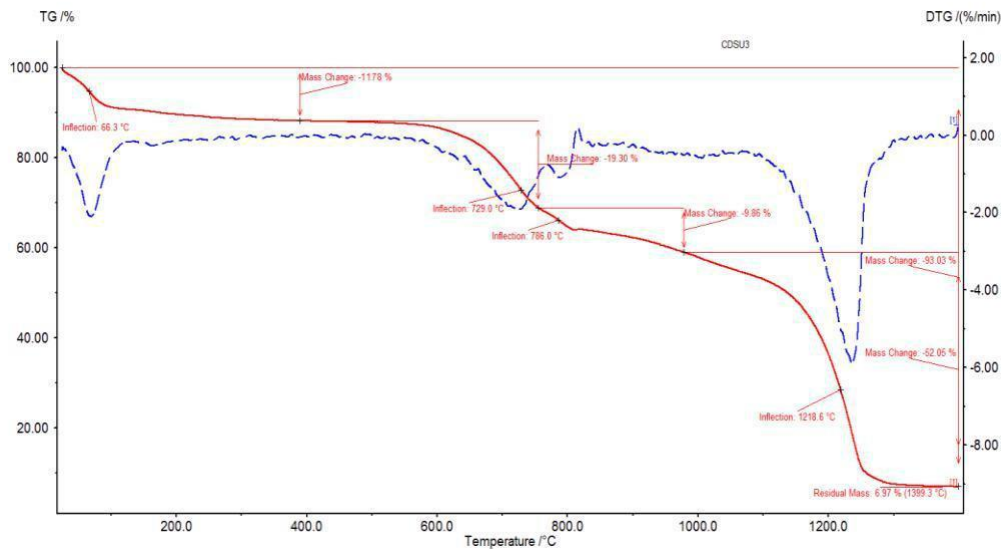


Fig.3 TGA and DTG of Copper doped CdS

figure 4 shows the DSC curve of the Copper doped CdS nanomaterials. It is observed from the graph that, there is a peak around at 489^oC, 807^oC and 878^oC

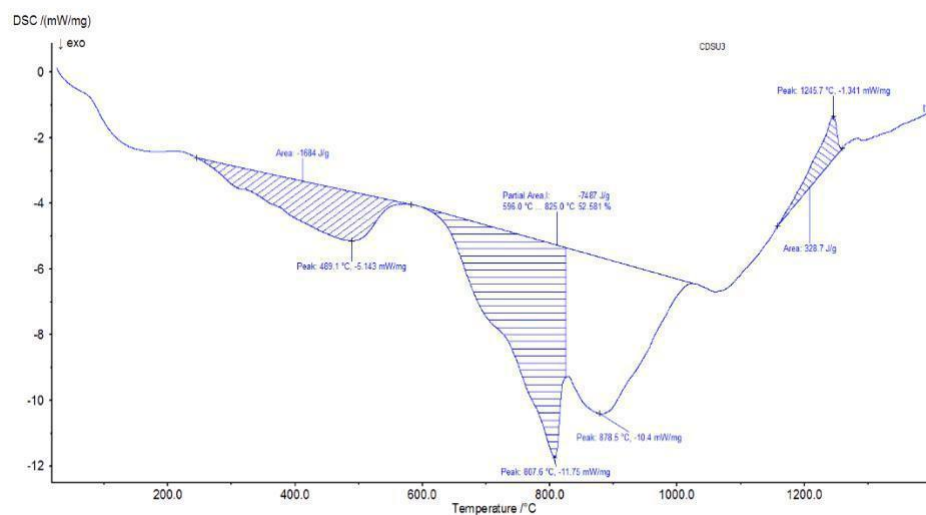


Fig.4 DSC of Copper doped CdS

Similarly figure 5 shows the case of Copper doped cadmium sulphide there is a peak at 82.1^oC due to the evaporation at 50^oC to 175^oC and the phase transformation is at 669^oC, 778.3^oC and 1283.1^oC with weight loss of 15.19%, 8.06% and 60.99% with a temperature of 650^oC to 1250^oC. The overall weight loss for the phase transformation is 93.11%.

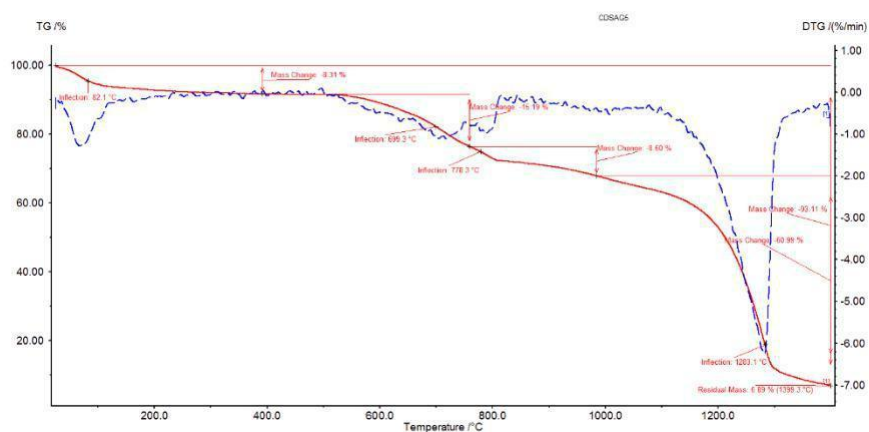


Fig.5 TGA and DTG of Silver doped CdS

figure 6 shows the DSC curve of the Silver doped CdS nanomaterials. It is observed from the graph that, there is a peak around at 384⁰C, 801⁰C and 925.4⁰C

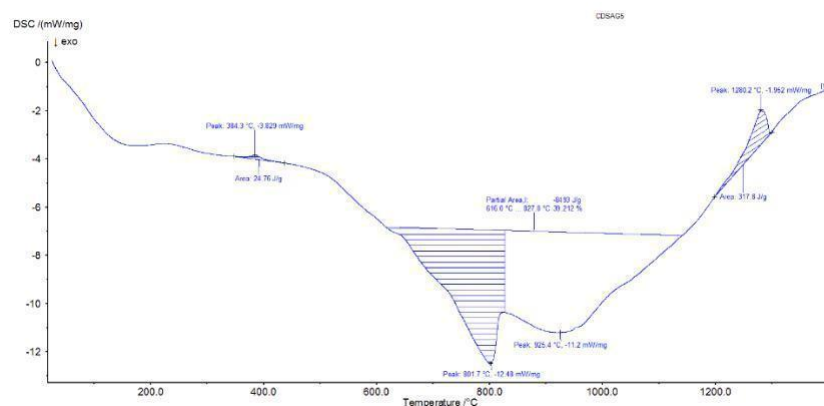


Fig.6 DSC of Silver doped CdS

The thermogravimetric analysis (TGA) traces, at that temperature, the presence of water molecules on the surface of the material. Another exothermic rise has been identified, and the evaporation of organic materials on the material surface may be related to this commonly. In all CdS nanomaterials, the TGA curve also shows a 93 percent weight loss. The samples do not impact on the thermal stability of cadmium sulphide nanomaterials due to the addition of the dopant is clear. The intermediate materials will only alter the electrical and optics properties.

4. Conclusion

The thermal conductivity of pure and doped cadmium sulphide nanoparticles is assessed using thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) at various temperatures. The introduction of cadmium sulphide, copper, and silver doping will have a substantial impact on the endothermic peaks observed in the samples. However, the overall phase of material conversion remains unaffected. Furthermore, it is worth noting that in all cadmium sulphide (CdS) nanomaterials, the thermogravimetric analysis (TGA) curve exhibits a weight loss of approximately 93 percent. The introduction of a dopant into cadmium sulphide nanomaterial samples does not appear to have an impact on their thermal stability. The alteration in electric and optical characteristics can solely manifest when the transitional materials undergo a process of doping. Due to their optical and semiconductor capabilities, cadmium sulphide (CdS) nanoparticles are popular in energy applications. In conclusion, CdS nanoparticles show great promise in solar cells and photocatalysis, where their unique properties improve energy conversion and environmental remediation, enabling cleaner, more sustainable energy solutions.

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