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Development of nanocrystalline multilayer Ni–Fe alloy coatings: characterization and its corrosion behaviour at elevated temperature

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Abstract. The present work deals with the galvanostatic fabrication of Ni–Fe nanostructured composition-modulated multilayer alloy (CMMA) coatings on steel panel from the newly optimized acid-sulphate bath solution. The recurring cathode current density combination (RCCC) and the number of layers have been optimized for enhanced performance of the coatings against corrosion. Corrosion behaviour of the nanostructured multilayered coatings was evaluated by Tafel extrapolation and electrochemical impedance spectroscopy (EIS) methods in 3.5% NaCl solution. Under optimal conditions, the CMMA coatings developed were more corrosion-resistant than the monolithic alloy coatings obtained from the same bath. Least corrosion rate (CR) was witnessed at 300 layers, above which saturation of corrosion resistance at a high temperature was found, which is attributed to a shorter relaxation time for redistribution of metal ions during multilayer deposition. Hardness and roughness of the coatings were evaluated using Vickers hardness test and atomic force microscope, respectively. Phase structure of the coatings was discussed using X-ray diffraction technique. The cross-sectional view of the coatings was characterized by scanning electron microscope. CR analysis and the surface morphology of the optimized coatings exposed to high temperature revealed the better performance of CMMA coatings at the elevated temperatures compared to the monolithic coatings.

Keywords. CMMA; Ni–Fe; corrosion resistance; XRD; AFM; SEM.

1. Introduction

The electrodeposited Ni–Fe alloys as sacrificial coatings are studied widely for its excellent corrosion protection action on steel substrates. Nanostructured Ni–Fe alloy coatings on mild steel are the prevalent method for its high magnetic permeability. Ni–Fe alloys due to their distinctive nature and a wide range of unique properties have gained considerable attention for their practical applicability in modern industries, such as in rocketry, computers, space technology, etc. [1,2]. The early researchers have reported that development of Ni–Fe alloy coatings has enhanced the corrosion resistance to a greater extent when compared to pure nickel coating, further innovative methods for the development of even better protective coatings than the monolayer coatings are of distinct scientific and industrial interest [1–5].

It was known that the compositionally modulated multilayer coatings (CMMA) like Ni–Fe, Ni–Zn, Ni–Co, Ni–P has the superior corrosion protection ability in comparison to monolayer alloy coatings of the same [6–10]. The CMMA coatings can be obtained by various electrochemical deposition methods. These methods can be broadly classified as electrodeposition by (1) dual bath technique (DBT) [11,12], (2) single bath technique (SBT) either by potentiostatically or galvanostatically [1–5,13] and (3) single bath by pulse plating technique [14,15]. However, DBT has its own drawbacks even though pure metals or alloys can be deposited by this method. It is laborious and there is fear of bath solution loss during the transfer of substrates within the baths. Development of CMMA coatings by pulse technique was not preferable due to the complexity in achieving the modulation in composition and thickness variation [16–18]. Whereas in SBT by galvanostatic method, high deposition rate of the coatings with modulation in the composition can be accomplished in lesser time compared to DBT.

The excellent corrosion resistance observed from CMMA coatings was due to the improved barrier effect with the increase in the number of layers [19,20]. The Zn–Fe CMMA coatings developed by Venkatakrishna and Chitharanjan Hegde [21] and Yogesha and Chitharanjan Hegde [22] have reported that they have better corrosion resistance than its monolayer coating of same thickness. It is reported that in the CMMA coatings, with the increase in number of

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Characterization and Corrosion Analysis of Electrodeposited Nanostructured Zn–Fe Alloy Coatings

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Abstract
Eight distinct Zn–Fe alloy films have been galvanostatically electrodeposited with a current density ranging from 1 to 8 A dm^{-2}. The surface morphology, chemical composition, phase structure and microhardness of these coatings were examined using scanning electron microscope coupled with energy dispersive x-ray spectroscopy (SEM-EDX), X-ray diffraction (XRD) and Vickers Microhardness Tester. XRD results suggest the formation of metastable crystal structure in all the electrodeposits and formation of η phase confirms the higher content of Zn in the coatings. To evaluate the corrosion resistance, the developed coatings were immersed in 3.5 wt% NaCl solution followed by the application of potentiodynamic polarization and electrochemical impedance spectroscopy (EIS) tests on each sample. The results indicated the greater impact of the coating characteristics on the corrosion resistance of electrodeposited Zn–Fe alloy.

Keywords Zn–Fe alloy · Electrodeposition · Microhardness · Corrosion behavior

1 Introduction

Surface modification is a remarkable technique among the continuous development in the field of production and manufacturing processes for the corrosion protection of steel [1–3]. Several investigations were carried out to enhance the coating characteristics through chemical passivation, superhydrophobic treatment, and nanostructured electrodeposition techniques [4, 5]. Among these, Surface modification by nanocrystalline alloy electrodeposition is a convenient technique as it does not require additional postprocessing compared to other methods [6]. Zn was widely used for steel applications in the aerospace, automotive and electric sectors due to its outstanding corrosion resistance and mechanical properties [7–9]. Zn alloy coatings like Zn–Ni, Zn–Co, and Zn–Fe, however, provide high corrosion resistance on steel compared to pure Zn [10–12]. The Zn–Fe alloy coatings are distinguished by its excellent resistance to corrosion, good weldability, and formability. They have numerous significant applications in the automotive and aerospace industries, such as in chemical and galvanic processes [13]. The development of the Zn–Fe alloy follows the nucleation and subsequent growth mechanism. It was found that Zn^{2+} ions in the electrolyte inhibit the deposition of Fe, while Fe^{2+} ions promote the deposition of Zn. Moreover, Zn and Fe co-deposition exhibits anomalous behavior [14]. Yang et al. developed Zn–Fe alloy coatings by electrolytic bath containing sulfate and showed that the interfacial pH governs the kinetics of deposition [15]. During electrodeposition of Zn–Ni and Zn–Fe alloys in the acidic medium by Hegde et al. [16], the metal alloy transition exhibits anomalous co-deposition arising from changes in the applied current density. It was concluded by Eliaz et al. [17] that deposition of iron group metals shows good corrosion resistance compared to pure metal deposition.

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TECHNICAL ARTICLE—PEER-REVIEWED

Electrodeposition of Zn–Ni Monolithic Coatings, Characterization, and Corrosion Analysis

D. Rashmi · G. P. Pavithra · B. M. Praveen · Deepa Devapal · K. O. Nayana · G. Nagaraju

Submitted: 11 October 2019 / in revised form: 19 February 2020

Abstract Bright Zn–Ni coatings were developed by using thiamine hydrochloride as a brightener. Hull cell was used for the optimization of bath constituents and parameters. Galvanostatic electrodeposition from zinc sulfate and nickel sulfate with additives results in Zn-rich solid solution of nickel in zinc η-phase. Surface morphology was observed by scanning electron microscopy, chemical and phase composition determined by X-ray diffraction, and corrosion investigations by electrochemical techniques. Coatings obtained at 5 Adm^{-2} exhibited more corrosion resistance.

Keywords Zn–Ni alloy · Corrosion · XRD · AFM · SEM

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Introduction

In the 1980s, Zn–Ni alloy coatings were developed for the automotive industry as a corrosion protective coating [1]. Electrodeposited Zn coatings are widely used to protect steel from corrosion due to their barriers and sacrificial characteristics [2]. The high consumption rate of pure Zn coatings has been resolved by alloying components with Fe group elements such as Ni, Co, and Fe, which also improves their corrosion resistance [3, 4].

Among the Zn alloys, more attention has been paid to Zn–Ni alloy coatings as they have been widely used for steel protection in the aerospace and automotive industries [5]. The coarse-grained Zn–Ni alloy coatings lead to bad resistance of the coatings to corrosion, mechanical and electrochemical characteristics, thus reducing the life of the deposits. Several investigators have tried to enhance the coating characteristics through chemical passivation, superhydrophobic treatment, and nanostructured electrodeposition techniques [6, 7].

Electrodeposition parameters such as bath composition, current density, temperature, and pH significantly influence the coating quality. These parameters should be optimized in order to obtain finer morphological coatings that enhance the micromechanical and corrosion resistance properties [8–10]. In this regard, the present work deals with optimizing electrolytic bath for the development of fine-grained nanostructured corrosion-resistant Zn–Ni alloy coatings.

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Development of Nanostructured Ni–Fe Alloy Coatings; Characterisation and Corrosion Analysis

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Abstract—The present investigation deals with the electrofabrication of nanostructured Ni-Fe alloy coatings on a mild steel using sulfate bath. The electrolytic bath composition and the current density of the coatings were optimized. Composition analysis by energy dispersive X-ray spectroscopy revealed that the Ni–Fe alloy coatings are of anomalous type. Potentiodynamic polarization corrosion test and electrochemical impedance spectroscopy methods in 3.5% NaCl solution direct towards the lowest corrosion rate at 4 A dm^{-2}. Hardness and roughness of the coatings were evaluated using Vickers hardness test and atomic force microscopy, respectively. The surface morphological analysis of the coatings was characterized by scanning electron microscopy with energy dispersive X-ray spectroscopy. The phase structure, the texture coefficient, and the crystallite grain size of the coatings were calculated and studied using X-ray diffraction.

Keywords: nanostructured Ni-Fe electrodeposition, energy dispersive X-ray spectroscopy, scanning electron microscopy, atomic force microscopy, X-ray diffraction, corrosion behavior

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INTRODUCTION

The property of a material initiates from its surface and thus it becomes the most important engineering part of the material, solely dependent on its thermal, mechanical, chemical, and electro-chemical interaction with the external environment. The surface of the material is always under the threat of damage either by corrosion or by any other destructive phenomena [1]. The surface modification of steel is the breakthrough in the production engineering process since it is widely used in industrial applications. Steel often undergoes corrosion causing huge damage to environment as well as industries. The resulting damage will be irrecoverable if the corrosion phenomena are not controlled [2]. The corrosion process can be controlled by numerous techniques, among which electrodeposition is one of the best [3, 4].

Electrodeposition of nanostructured metals and alloys finds a wide range of applications in various low and high technology areas so as to introduce new and better-quality materials into the market. Likewise, the nanostructured coatings of nickel-based alloys have gained an extra attention among the researchers due to their ability to produce coatings that possess excellent physical and mechanical properties [5, 6]. Bright Ni–Fe coatings were strongly promoted as a substitute for pure Ni coatings as they decrease the cost of production and exhibit good microstructural parameters like grain size, crystallographic texture, thermal stability, and microhardness [7–10].

Nanostructured Ni–Fe alloy electrodeposited on mild steel is a prevalent method for its high magnetic permeability and small coercive force [10]. The effect of a smaller crystallite grain size of these nanostructured alloys enhances the material properties such as strength, hardness, wear resistance, electrical resistivity, and thermal conductivity [11]. There arises an unusual kind of electrodeposition, namely, anomalous co-deposition within the iron group binary alloys: Ni–Fe, Zn–Fe, Co–Fe [12–14], which allows an intrication between the electrodeposit characteristics, the bath composition and operating parameters. The coatings fabricated in each bath will be distinct with respect to the bath composition and its operating parameters [8, 10, 15, 16]. In our present investigation, an attempt was made to optimize the deposition condition of a new electrolytic bath for the development of corrosion resistant Ni–Fe alloy deposited at various current densities. Efforts were made to correlate the deposition current density. with the surface morphology, phase structure, roughness, and the corrosion rate. An additive effect on the coatings was also inves-

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PAPER

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Development of nanofibrous scaffolds by varying the TiO_2 content in crosslinked PVA for bone tissue engineering

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The use of ceramic and metal nanoparticles is widely being proven as a preferred candidate for tissue engineering owing to their excellent properties such as their high penetration ability and high surface area with tuneable surface properties. In view of this, the effect of bioinert TiO_2 incorporation into the polymer matrix is studied in the present study. Crosslinked poly(vinyl alcohol) (PVA) was used as the main polymer base and different weight percentages of TiO_2 (0.1 to 0.3 g) were incorporated into the crosslinked PVA matrix by varying the ratio of PVA : TiO_2. Nanofibrous scaffolds were then fabricated using the electrospinning technique. The physicochemical properties of the developed nanofibrous scaffolds were analysed systematically. Scanning electron microscopy images demonstrated the good interconnected porous structure with uniform fibres in the range of several hundreds of nanometres. The effect of TiO_2 incorporation was observed in terms of an increase in the hydrophilicity of the scaffolds required for cellular infiltration. The mechanical characterization of the developed scaffolds demonstrated an improved mechanical strength for a reduced amount of TiO_2 incorporated scaffolds. The degradation study revealed the slow rate of degradation with an increase in the TiO_2 content in the PVA matrix of the scaffolds. Cell viability was studied using MG-63 bone osteosarcoma cells for 24, 48, 72 and 96 h, wherein the PT1 scaffold with a content of 0.1 g of TiO_2 exhibited the highest cell proliferation of 99.2%. The results thus clearly show that the TiO_2 incorporated PVA scaffolds could be potential candidates for bone tissue engineering.

1. Introduction

The multidisciplinary field of tissue engineering and regenerative medicine is in increasingly high demand in the present decade owing to the many drawbacks of tissue and organ transplantation, such as limited donor availability, the need for immune-suppression and insufficient success rate (rejection of the transplant). Tissue engineering is the development of artificial constructs known as scaffolds that can mimic the natural extracellular matrix (ECM), resembling natural tissues or organs provided with appropriate mechanical strength.[1] Scaffolds specifically developed for bone tissue engineering must possess a good-interconnected porous network with a large pore volume in order to ensure viable cell infiltration and attachment, and transportation of nutrients and waste products.[2,3] The geometry of scaffolds thus plays an important role in improving the overall properties. In order to incorporate the required physical properties into the scaffolds many advanced scaffold fabrication techniques have been employed.[1] Recently, electrospinning has been found to be an amazing method for the development of scaffolds in the form of nanocomposite fibres possessing nano structures.[4–7]

The material intended for scaffold development should be highly biocompatible with favourable surface properties for bone cell attachment and a large surface area-to-volume ratio for cell infiltration.[8,9] There are many biocompatible and biodegradable polymers used for bone tissue engineering applications, including (poly(L-lactic acid), poly(L-lactic-*co*-glycolic acid), poly(ε-caprolactone), poly(vinyl alcohol) (PVA) and poly(D,L-lactic acid)).[10] Among these, PVA is a biodegradable, biocompatible, nontoxic, and non-carcinogenic polymer which makes it an excellent biomaterial for bone tissue engineering. However, in addition to these properties, the highly hydrophilic PVA lacks the intrinsic mechanical properties that favour cell attachment, cell growth and differentiation. In order to overcome this, PVA was crosslinked with the minimum ratio of a non-toxic tetraethylorthosilicate (TEOS) crosslinker in the present study. The crosslinking of the PVA solution

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ORIGINAL PAPER

Development of novel 3D scaffolds using BioExtruder by varying the content of hydroxyapatite and silica in PCL matrix for bone tissue engineering

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Abstract

Polycaprolactone (PCL) is considered as a most widely used biodegradable polymers in tissue engineering. But, PCL is also associated with certain limitations like, low stiffness, hydrophobic nature and limited cell affinity. These drawbacks are addressed in the present study by incorporating different wt% of silicon dioxide (SiO_2) and hydroxyapatite (HAp) in the PCL matrix. 3D scaffolds were developed using a novel BioExtruder. The physicochemical properties, thermal stability and wettability of the composite scaffolds were studied systematically. Optical and Scanning Electron Microscopic images were analysed for morphological evaluation of the scaffolds. The pore size of the developed scaffolds increased from 290 to 315 μm with increasing SiO_2 content, as examined by scanning electron microscope. An improved compressive modulus of 68.82 MPa was observed for 15 wt% SiO_2 incorporated composite scaffold. The in-vitro degradation study of the composite scaffolds demonstrated an increase in the degradation rate for PCL/HAp scaffolds, while no significant change was observed for SiO_2 incorporated scaffolds. Further, the cytotoxicity and cell proliferation studies were carried out using L929 Mouse Fibroblasts and MG-63 Osteoblasts respectively. The developed scaffolds revealed no toxic effects towards the cellular response and an increase in cell proliferation of ≥90% was observed during 7 days of cell culture. Thus, the scaffolds were proved to be potential candidate for bone tissue engineering application, particularly the scaffold with 10 wt% SiO_2 incorporation into PCL/HAp (75/15) composite has resulted into higher cell proliferative % and improved mechanical strength.

Keywords Biodegradable · Scaffold · Bone tissue engineering · Three dimensional · Wettability · Biocompatibility

Introduction

Bone tissue repair is one of the widely emerging areas under the field of tissue engineering and regenerative medicine. Bone has a hierarchical structure at multiple length scales which provides multiple functions such as, structural support, protection and storage of healing cells, and mineral ion homeostasis [1–3]. Under a variety of clinical situations the natural bone regeneration fails and it is necessary to undertake an interventional therapy. Bone grafting was one of the earlier methods for bone tissue repair. The grafting of bone in reconstructive surgery is based on the principle of replacing defective tissues with viable and functioning alternatives. It provides the structural stability and osteogenic behaviour to the defective site. But the method was not proved to be 100% effective because of some immunogenic responses to the foreign tissue as well as leading to some inflammatory reaction [4, 5]. To overcome this, a new approach of bone tissue engineering (BTE) has come to picture which includes the use of

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REVIEW

Dynamic mechanical properties of natural fiber composites—a review

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Abstract
Natural fiber composites have become a new tradition as an alternative to conventional materials. To meet this new tradition material testing, newer techniques have been set up that are termed as dynamic mechanical analysis (DMA), which is an adaptable methodology that accompanies the more traditional techniques. Through these techniques, it is summarized that interconnected bonds between reinforced natural fibers within different matrix materials will affect the dynamic variables like storage modulus (E′), loss modulus (E″), and damping factor (tan δ), and also, it was stated that these are temperature dependent. The dynamic variables were unfavorably affected by the improvement in the length of fibers and fiber loading, but geometric changes (developments) were not considered. Frequent uncertainties in the dynamic loading in any structure are because of noises, shocks, winds, tides in the ocean and some of the live and imbalanced loads, etc. Much importance was given to vibration damping parameters for structural applications in order to have an improvement in the effectiveness, performance, and freeness in some of the building constraints. In this review, the employability of different natural fibers in forming composites with different matrix materials and the impact of fiber length, chemical treatment, and compositions on the dynamic mechanical characteristics were discussed in detail.

Keywords Natural fiber · Dynamic mechanical analysis (DMA) · Storage modulus (E′) · Loss modulus (E″) · Damping factor (tan δ) · Chemical treatment

1 Introduction

Natural fiber-reinforced composites have turned out to be well known for a diversity of uses due to their improved specific strength, specific modulus, bio-degradability, eco-friendly, and eco-efficiency natures [1–6]. Biodegradability is one of the important criteria which are gaining the concentration of all the sectors, and this special property of natural fibers/filaments plays an essential part in the increased future use of natural fiber composites [7]. With the utilization of a different variety of fibers used (artificial (man-made)/natural), life cycle of a composite component is shown in Fig. 1.

Also, natural fiber strengthened ecofriendly polymer composites materialized to have an extremely brilliant features for a wide scope in future applications [8]. Figure 2 demonstrates the type of biocomposites available with their biodegradability. Also, it shows the type of matrix and natural fiber available to prepare different combinations of bio-composites [8]. Many of the natural filaments, such as Sisal (*Agave sisalana*), Banana (Musa sepientum) and Roselle (*Hibiscus sabdariffa*), Sisal and banana (hybrid), Roselle and banana (hybrid), and Roselle and sisal (hybrid), were incorporated in the powder format along with the polymer(s) and are utilized in the fabrication of composites using molding method. And many more types of natural fibers and bio-polymers have benefits in the field of composites [9].

Usually, composites rely on the use of manmade fibers, but many of the researches showed us that natural fibers can be easily replaced with these manmade fibers and the use of naturally available fibers is of current interest.

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The significant role of molecular dipole arrangements on the second and third-order nonlinear optical properties of a furan based chalcone

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ABSTRACT

In this article, we report an experimental investigation on second and third-order nonlinear optical (NLO) properties of an efficient chalcone material 1-(5-methyl furan-2-yl)-3-(4-nitrophenyl) prop-2-en-1-one (MFNP) along with other characterization techniques. The synthesized material is confirmed through FT-IR and FT-Raman spectroscopic techniques. Single-crystal XRD study showed that the crystal belongs to the triclinic crystal system crystallizing in the P1 space group which is a non-centrosymmetric crystal form. From UV-VIS-NIR spectroscopy, the crystals were found to possess less absorbent in the visible region. Furthermore, the crystal exhibits excellent thermal stability up to 136 °C. The intermolecular interactions in the crystal were identified by obtaining the Hirshfeld surface and the related 2D finger plots. The second harmonic generation (SHG) efficiency of MFNP is three times the standard KDP crystals. Using a continuous-wave laser beam z scan experiment was performed and the "nonlinear refractive index (n_2)", "third-order nonlinear absorption coefficient (β)" and "second-order molecular hyperpolarizability(γ_h)" were calculated for MFNP. The estimated threshold value for optical limiting was found to be 1.85 kJ/cm^2. The excellent experimental results show that MFNP is a very useful material especially in the field of optical power limiting applications.

1. Introduction

Organic nonlinear optical (NLO) materials have attracted much attention in recent times due to their ease of synthesis, manipulation of molecular structure and large NLO responses which makes them suitable for various technological applications such as optical computing, optical data storage, optical limiting, frequency modulation, electro-optic devices, etc [1]. Among the different types of organic NLO materials subjected to investigation, chalcones have proved to be potential candidates for device applications as these materials exhibit a high degree of nonlinearity. A chalcone molecule consists of two phenyl rings interconnected by a conjugation bridge [2]. The electronic delocalization in the chalcone molecule can be altered to the highest degree by substituting suitable electron donor and/or acceptor groups at the end of this highly polarizable conjugated bridge. This structural modification will help to establish noncentrosymmetric crystal structures that are considered necessary for the second harmonic generation (SHG) [3]. In addition to this, the replacement of the benzene ring at the benzoyl arm of the chalcone by pyridine ring or thiophene ring has proved to be a wise move in altering the electronic delocalization and thus improving the second and third-order optical nonlinear response of these molecules [4–7]. Among these, several molecules with thiophene ring at the benzoyl arm crystallized in centrosymmetric crystal form and hence did not show any second-order nonlinearity [6–8]. It is well understood that the strength of the electron donor groups at the end of the conjugated bridge plays an important role in the formation of enantiomorphic crystal structures. Another crucial factor in increasing the optical nonlinearity of the chalcone molecules is a change in direction of charge transfer through the molecule [9,10]. Further, Satheeshchandra et al. reported a furan based bromo substituted chalcone, BBP with good SHG response of 2.03 times that of KDP with considerably good third-order nonlinearity [11] whereas the thiophene based bromo and nitro substituted chalcones, 2AT4B and 2AT3N did not show any SHG [8]. Considering the above facts and since furan is a sturdy electron donor than thiophene [12], a furan based chalcone is designed with a nitro group placed at the para position of the phenylene moiety. To increase the conjugation length and to increase the electron-donating strength of furan, a methyl group is attached to the furan ring. This strategy forms a molecule with

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A novel bromo-substituted thiophene based centrosymmetric crystals: Thermal, mechanical, and third order NLO properties for the optical limiting applications

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Abstract

A thiophene based bromo substituted novel chalcone derivative (E) -3-(4-bromophenyl)-1-(thiophen -2yl) prop-2-en-1-one (2AT4B) is synthesized and crystals are grown using solution slow evaporation method at ambient temperature. The single crystal XRD analysis is accomplished to confirm the three dimensional structure of the grown crystals and 2AT4B crystallizes with orthorhombic crystal system

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Role of UV irradiation of Nafion membranes on ionic groups responsible for proton conduction and mechanical strength: A FTIR spectroscopic analysis

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Abstract

This work presents an evidence of why proton conductivity of Nafion increases with increase in UV-radiation dosage and drops beyond ultraviolet radiation dosage of 198 mJ cm^{-2}. FTIR spectroscopic analysis is used to analyse the shifting of the peaks of groups responsible for proton conduction (i.e. sulfonic acid ($-SO_3H$) and hydronium (H_3O^+) ions) of Nafion irradiated by various dosages of UV-radiation. The analysis showed that crosslinking of $-SO_3H$ increases up-to UV-radiation dosage of 198 mJ cm^{-2}. Beyond this optimum UV-radiation dosage the chain-scission of these groups takes place. On the other hand, UV-radiation has significant degradation effect on H_3O^+. FTIR spectra of H_3O^+ show that even with slightest dosage of UV-radiation, chain-scission takes place. Further, the effect of UV-

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Investigation of structural, physical, linear, and nonlinear optical properties of two novel thiophene centred D-π-A type push-pull organic derivatives for nonlinear optical applications

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Abstract

The aim of the present study is to investigate the different key parameters of two novel thiophene based D-π-A type push-pull organic chalcone derivatives; 3-(4-nitrophenyl)- 3-hydroxy-1-(thiophen-2-yl) propan-1-one (2ATN) and 3-(4-nitrophenyl) -3-hydroxy -1-(thiophen-3-yl) propan-1-one (3ATN) through various experimental techniques. The 2ATN and 3ATN single crystal are grown at ambient

04

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Significant effect of film thickness on morphology and third-order optical nonlinearities of $Cd_{1-x}Zn_xO$ semiconductor nanostructures for optoelectronics

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Abstract

The work presented here reported the thickness dependent structural, linear and nonlinear optical properties of nanostructured $Cd_{1-x}Zn_xO$ thin films. Thin films were prepared with two different thickness (≈ 0.5μm and 1μm) by employing a spray pyrolysis (SP) technique for different Zn-doping levels ($Cd_{1-x}Zn_xO$ with the x value of 0.00, 0.01, 0.05 and 0.1). X-ray diffraction studies confirm the polycrystalline nature having a cubic crystal structure. In terms of an aspect ratio of the columnar structure and dispersion in hexagonal (1 1 1) basal plane orientation, a thickness dependency of structural evolution was discussed. The Scherrer rule was employed to determine the crystallite size

03

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Novel nitro based chalcone derivative single crystals: characterization on structural, linear optical, thermal, and third-order nonlinear optical properties

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Abstract

Crystals of "(2E)-1-(4-nitrophenyl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one" (NPTMP) are grown by slow solvent evaporation technique. The compound purity and presence of functional groups elements in the material were identified from the spectroscopic techniques (FT-IR and ^{1}H-NMR). The single-phase formation in the bulk powder crystalline sample has been confirmed from powder XRD analysis. The intermolecular interaction and structure-related parameters were obtained and analyzed by utilizing single-crystal XRD data. Using single-crystal XRD data (CIF file), display of the intermolecular interactions and contribution of H···H and H···O/O···H interaction have been obtained. The molecule is mapped over dnorm, de, di, curvedness, shape index, and electrostatic potential by generating the Hirshfeld's surface of NPTMP molecule. The linear optical absorbance and optical bandgap of the material have been confirmed by UV–VIS–NIR spectroscopic technique. The thermal stability of the crystal NPTMP is obtained from TGA/DTA/DSC techniques. The surface morphology of the crystal is collected from scanning electron microscopy (SEM) and the electronic contribution of

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Direct and integrated radial functions based quasilinearization schemes for nonlinear fractional differential equations

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Abstract

In this article, two radial basis functions based collocation schemes, differentiated and integrated methods (DRBF and IRBF), are extended to solve a class of nonlinear fractional initial and boundary value problems. Before discretization, the nonlinear problem is linearized using generalized quasilinearization. An interesting proof via generalized monotone quasilinearization for the existence and uniqueness for fractional order initial value problem is given. This convergence analysis also proves quadratic convergence of the generalized quasilinearization method. Both the schemes are compared in terms of accuracy and convergence and it is found that IRBF scheme handles inherent RBF ill-condition better than corresponding DRBF method. Variety of numerical examples are provided and compared with other available results to confirm the efficiency of the schemes.

Keywords Nonlinear fractional ordinary differential equation · Direct and integrated radial basis functions · Collocation · Quasilinearization · Convergence analysis

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Regularization of Highly Ill-Conditioned RBF Asymmetric Collocation Systems in Fractional Models

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K. S. Prashanthi, G. Chandhini

Chapter
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Abstract

While attempting to approximate differential equations using Kansa's radial basis function (RBF) collocation, we need to solve a non-symmetric, highly ill-conditioned system. There are