

Identifying bioactivity of pseudo-natural products using the Cell Painting assay

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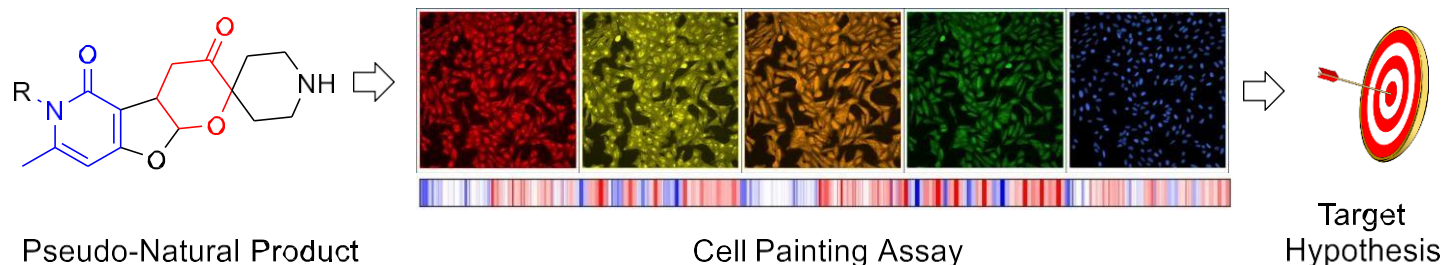
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Abstract

Natural Products (NP) are a major source of inspiration to develop novel bioactive substances. Various strategies were developed to make use of the relevance of NPs in drug design strategies. It has been shown that NP-derived fragments may still be of biological relevance. Thus, combining various different NP-derived fragments may result in new biologically relevant molecules. These compounds retain some physicochemical properties of NPs but are not accessible through biosynthesis and were therefore termed pseudo-NPs. Since it is not possible to infer the bioactivity of pseudo-NPs from their NP-derived fragments, it is not straightforward to identify their potential targets. Hence more general, morphological phenotypic screens may be the best methods to identify impacted pathways. We highlight the potential of the pseudo-NP approach combined with a recent morphological-, image-based screening technology termed Cell Painting.



Keywords: Pseudo-natural product, cell painting, biological target, biological activity

Chemical synthesis of palmitoylated histone H4

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Dedicated to Prof. Horst Kunz on the occasion of his 80th anniversary

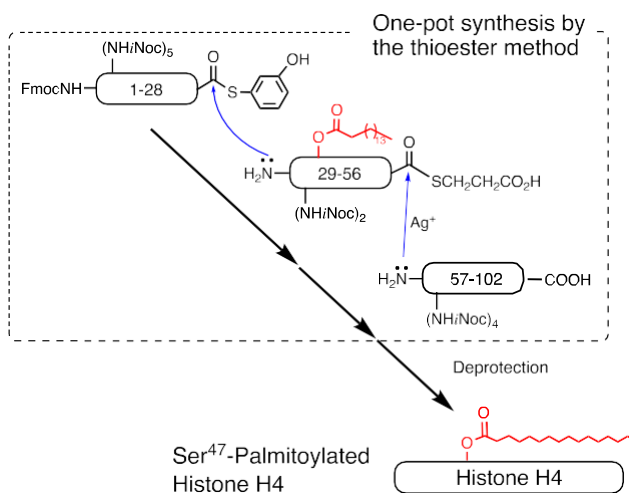
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Abstract

Palmitoylation is one of the post-translational modifications of proteins. Recently, palmitoyl modification was found in histone H4, one of the components of the nucleosome core. To analyze this unusual modification in the nuclear protein, we chemically synthesized Ser⁴⁷-palmitoylated histone H4. The entire sequence of H4 was divided into three segments and each was prepared by Fmoc-solid-phase peptide synthesis (SPPS). The palmitoyl group was introduced as a preformed palmitoyl Ser during SPPS or introduced at the end of SPPS by selective deprotection of the hydroxy group of Ser⁴⁷, followed by palmitoylation. After three segments were condensed in one-pot by the thioester method, the desired Ser⁴⁷-palmitoylated H4 was obtained.



Synthesis and *in vitro* studies of Gd-DTPA-Tris-3-AEA Complex As a new potential MRI contrast agent

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Abstract:

A new type of dendritic molecule Gd-DTPA-Tris-2-AEA, which work as a functionalized ligand coordinating with gadolinium (III) ion at the center of their frameworks with free amine moieties on the molecular surfaces, were readily synthesized with high yield. Its *in-vitro* studies evaluated the potentiality for MRI contrast agent and enhanced r_1 value was obtained in both water and albumin medium. The structures were established by ^1H , ^{13}C NMR, and mass spectral studies.

Key words: Dendriticligand; Gd- complex; MRI CAs; Relaxivity; T_1 and r_1 values

1. Introduction:

Contrast-enhanced magnetic resonance imaging (MRI) is a noninvasive diagnostic tool that not only provides high resolution anatomical images of soft tissue but also quantitatively assesses disease pathogenesis by measuring up-regulated biomarkers. However, currently used MRI contrast agents are mainly small molecule gadolinium chelates that lack sensitivity and often do not provide satisfactory image contrast enhancement in early disease stages. Contrast-enhanced magnetic resonance imaging (MRI) is a noninvasive diagnostic tool that not only provides high resolution anatomical images of soft tissue but also quantitatively assesses disease pathogenesis by measuring up-regulated biomarkers. However, currently used MRI contrast agents are mainly small molecule gadolinium chelates that lack sensitivity and often do not provide satisfactory image contrast enhancement in early disease stages. Magnetic resonance imaging (MRI) is a powerful, noninvasive, and widely applied diagnostic technique which allows to obtain images of the inside of the humanbody.^{1,2} Nowadays, more than one-third of the MRI scans are performed by administration of a contrast agent, usually a gadolinium complex.^{3,4} Gadolinium (III) ion is able, due to its favorable paramagnetic properties, to increase the relaxation rate of the surrounding water protons, making the region of interest brighter than the background. The contrast agents of first generation distribute in to the intravascular and interstitial space immediately after injection and in this context are called “non-specific agent” The medical need for tissue specific contrast agents has

Synthesis and Decoration of graphene oxide sheets with Luminescent di nuclear europium complexes

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A B S T R A C T

Graphene oxide sheets (GOSs) functionalized with Europium complex was prepared using a noncovalent approach. The adsorption of Europium complexes onto GOSs, as well as the individual nature of the hybrids, was confirmed. The GOS-Europium complex hybrids and their dispersion can emit bright red luminescence, which makes them useful in many practical fields, such as biological labeling and anti-counterfeiting.

Key words: Graphene oxide sheets (GOSs), Europium complex, Red luminescence, good thermal stability.

1. Intruduction

Emerging as atomically thin two-dimensional carbon materials, graphene sheets (GSs) have attracted tremendous attention in many potential applications, such as polymer composites, biosensors and drug delivery [1]. Recently, grapheme oxide sheets (GOSs), heavily oxygenated carbon monolayer's that contain numerous oxygen functional groups on their surfaces, have been extensively studied as promising precursors for the bulk production of GSs [2]. The functional groups on GOSs can facilitate not only their dispersion in a range of solvents but also their further functionalization [3,4]. Therefore, in addition to their reduction to GSs, GOSs are also useful platforms for aforementioned applications. Moreover, compared to zero-gap GSs, GOSs can be weakly fluorescent because of a defect-related optical gap, which may expand their application to the display and lighting fields, such as biological labeling and

Catalytic Hydrogenation of Sorbic Acid using Pyrazolyl Palladium(II) and Nickel(II) Complexes as Precatalysts

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ABSTRACT

We have prepared several pyrazolyl palladium and nickel complexes ([**(L1)**PdCl₂] (**1**), [**(L2)** PdCl₂] (**2**), [**(L3)** PdCl₂] (**3**), [**(L1)** NiBr₂] (**4**), [**(L2)** NiBr₂] (**5**) and [**(L3)** NiBr₂] (**6**)) by reacting 3,5-dimethyl-1H-pyrazole (**L1**), 3,5-di-*tert*-butyl-1H-pyrazole (**L2**) and 5-ferrocenyl-1H-pyrazole(**L3**) with [PdCl₂(NCMe)₂] or [NiBr₂(DME)] to afford mononuclear palladium and nickel complexes, respectively. These complexes were then investigated as pre-catalysts in the hydrogenation of 2,4-hexadienoic acid (sorbic acid). The active catalysts from these complexes demonstrate significant activities under mild experimental conditions. Additionally, the active catalysts show that the hydrogenation of sorbic acid proceeds in a sequential manner, where the less hindered C=C bond (4-hexenoic acid) is preferentially reduced over the more hindered C=C bond (2-hexenoic acid).

KEYWORDS

Pyrazolyl catalysts, sorbic acid, hydrogenation, selectivity.

1. Introduction

Hydrogenation of α,β -unsaturated compounds has been widely employed in the vitamins, fragrances, pharmaceuticals, petrochemicals, agrochemicals, and cosmetics industries.¹ One of the extensively used transition metal catalysts in these hydrogenation reactions is chlorotris(triphenylphosphine)rhodium(I), [RhCl(PPh₃)₃].^{2,3} The catalyst, RhCl(PPh₃)₃, catalyzes the chemo-specific hydrogenation of C=C bonds in the presence of other easily reduced groups, like nitro (NO₂) or carbonyl (CHO), as well as terminal alkenes even when the substrate has internal alkenes.^{2,3} Other transition metals complexes have been extensively studied as heterogeneous and homogeneous catalysts in the catalytic hydrogenation of olefins and α,β -unsaturated compounds. Among these metal complexes are ruthenium,^{4,5} rhodium,⁶ iridium,⁷ and platinum.⁸ However, nickel⁹ and palladium¹⁰ complexes have in recent times gained considerable attention as efficient catalysts in hydrogenation reactions. Shevlin *et al.* described the first homogeneous nickel-catalyzed asymmetric hydrogenation of α,β -unsaturated esters, using molecular hydrogen, that gave high yield and high enantioselective products.¹¹ Apart from the good reactivity and selectivity of the nickel catalysts, ligand manipulation makes them attractive for homogeneous catalysts. Nickel catalysts are cheap and cost-effective.

On the other hand, palladium catalysts are more expensive but exhibit superior catalytic and selectivity properties in the hydrogenation of unsaturated compounds.¹² For example, P[^]^P palladium pincer complexes are highly active catalysts for the chemo-selective transfer hydrogenation of α,β -unsaturated ketones.¹³ These highly reactive and selective palladium pincer complexes afforded saturated ketones from α -enones.¹³ Similarly, Bacci *et al.* reported hydrazinic-phosphine(P[^]N)palla-

dium(II) complexes as efficient catalysts for C=C bonds hydrogenation under mild experimental condition.¹⁴

However, because phosphines are sensitive to air and moisture,¹⁵ palladium complexes with nitrogen-donor ligands are emerging as an alternative to phosphorus-donor palladium complexes as hydrogenation catalysts. For example, {bis(aryl-imino)acenaphthene}-palladium(0) complexes are known to be efficient and highly chemo-selective in the hydrogenation of C=C bonds of α,β -unsaturated aldehydes.¹⁶ But despite numerous nitrogen-donor nickel(II) and palladium(II) applications in catalysis, little work has been reported on their catalytic properties in the hydrogenation of α,β -unsaturated compounds.

In this study, we report on pyrazolyl nickel(II) and palladium(II) complexes as catalysts for the hydrogenation of 2,4-hexanoic acid (sorbic acid), which is an α,β -unsaturated acid. This study forms part of a bigger project on partial hydrogenation of biofuels from triglycerides.

2. Experimental

2.1. General Information

Standard Schlenk and vacuum line techniques were used to handle all air and moisture sensitive compounds. All chemicals and gases were procured from the sources indicated for each one of them and include their purity: Gases – argon and hydrogen (>99 % purity) from Afrox (South Africa); solvents and reagents from Sigma Aldrich – Ethylformate (97 %), acetic anhydride (99 %), ferrocene (98 %), hydrazine monohydrate (98 %), hydrazine dihydrochloride (98 %), (ethyleneglycoldimethylether) nickel(II) bromide (98 %), formic acid (95 %) and 3,5-dimethyl-1H-pyrazole (**L1**) (99 %).

Literature procedures were used to prepare the following starting materials: 3,5-di-*tert*-butyl-1H-pyrazole (**L2**)¹⁷, 3-ferrocenyl-1H-pyrazole (**L3**)¹⁸ and [PdCl₂(NCMe)₂]¹⁹ as well as

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The Quality Control of Alcoholic Components of Disinfectants by a Simple Colour Test

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ABSTRACT

The identity and quality of liquid components for disinfectants, preferentially isopropyl alcohol and ethanol, can be determined with the naked eye using solvatochromic dyes and comparing their colour with a colour scale. Thus, any confusion with toxic methanol or other solvents can be excluded, as can also the application of raw materials in insufficient concentration or incorrect formulations. The production of a quick and easy to use simple low-cost test kit is described.

KEYWORDS

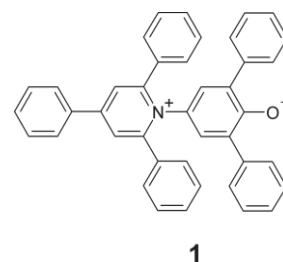
Disinfectants, alcohols, analytics, colour test, quality control.

1. Introduction

Disinfectants are one of the most efficient tools for the control of contact diseases and is becoming more important in pandemic spreads such as is currently the case with SARS-CoV-2. Disinfections of the hands with disinfectants may be achieved using comparably small amounts, requiring less water than detergents, such as soaps, and being generally more effective, is of central importance; however, disinfectants allow the application of only a very limited variety of components, because skin irritations are caused by frequent use. Thus the World Health Organisation (WHO) recommends isopropyl alcohol (IPA; CAS registry number RN 67-63-0) between 60 % (activity decreases rapidly below 50 %) and 90 % concentrations, where 75 % is used for the safe *Formulation 2*; some hydrogen peroxide is added as a booster and some glycerol for skin protection.¹ If there is no isopropyl alcohol available, *Formulation 1* containing ethanol (RN 64-17-5) in a higher concentration of 80 % is recommended as an alternative. Generally, the pharmaceutical industry provides certified isopropyl alcohol; however, the widespread supply may become problematic in pandemic situations. Therefore, it may become necessary to procure the components for disinfectant from various other technical sources, such as directly from suppliers in the chemical industry where local production of disinfectants would be helpful. Chemical analysis would be necessary in such cases, with the focus on confirming the safety of the chosen alcohol, determining the water content for sufficient activity, and verifying the alcohol content of the prepared formulation. A simple test, which could be carried out by less skilled or educated persons would be helpful, while a visual colour test without analytical equipment would be most effective.

2. Materials and Methods

The primary dye used in this study, namely **1** (phenolate betaine) ($E_7(30)$, RN 10081-39-7) developed by Dimroth and Reichardt,² is commercially available. The handling of **1** proved to be unproblematic and no adverse effects of **1**, such as toxicity, are known according to the *Chemical Abstracts* applied with the *SciFinder*[®]. Only very low concentrations, such as dyes in inks, are applied; however, **1** should be handled with care like other



only partially tested chemicals; only very low quantities are required for test kits, where the price of the dye used in the test kit is of minor importance. The dye can be synthesized according to the literature.^{2,3,4}

A stock solution of **1** is prepared in acetone with a maximal concentration according to the colouration in Fig. 1B; the colour is deeper in larger vessels because of the larger optical path lengths). Acetone is recommended because of its general availability, low toxicity and easy evaporation. 10 mL samples of the green stock solution were transferred into small sample glass vials of 20 mL total volume with a white, colourless screw cap (the latter does not interfere with the perception of colour). The filling height (level) was marked (Fig. 1B) and the acetone was allowed to evaporate in a fire-protected, ventilated environment with the exclusion of direct light (because of the limited lightfastness of **1**) until dry at room temperature, or heated to below the boiling point of acetone (56 °C). The caps of the dye-doped sample glass vials (Fig. 1C) were screwed on for sealing to obtain the test kit ready for use.

The alcohol for testing is filled into dye-doped sample glass vials up to the marked level (Fig. 1D) and the colour hue of the dissolved dye is compared with a colour scale (Tables 1 and 2).

The colour coordinates in the RGB room were directly taken

Table 1 Colour coordinates of the solution of **1** in various solvents.

Substance	Colour	Colour coordinates RGB		
		R	G	B
Isopropyl alcohol	Blue	37	72	136
Ethanol	Violet	112	76	122
Methanol	Red	149	103	114
Acetone	Green	27	89	84

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On the Mechanism of Uric Acid Oxidation with Lead Dioxide and with Alkaline Hydrogen Peroxide

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ABSTRACT

The metabolic pathways of uric acid have been studied in biological chemistry (enzymatic reactions). However, the course of some reported chemical reactions is unknown. In this communication, we provide the route of two independent oxidations of uric acid, with different reagents and reaction media. The electron flow is given, step by step, until the final product: allantoin. The intermediate reactions are fully commented.

Key words: Allantoin, Epoxidation, Nitrene, Push-pull effects, Ring closure and opening.

1. INTRODUCTION

The importance of uric acid is shown by the many papers devoted to the metabolic routes related to the formation and degradation of this compound. In the early papers, there are chemical reactions on uric acid oxidation.

Although the end products are known, the reaction course is unknown. In this communication, we provide the reaction mechanism of uric acid oxidation with lead dioxide in slightly acidic medium and also the oxidation with alkaline hydrogen peroxide.

This study is a follow-up of our papers on reaction mechanisms [1-5].

2. ANTECEDENTS

The mechanism of oxidation reactions is many times unknown. Although lead dioxide has been used as oxidizer in several transformations [6], the mechanism has not been given.

Thus, the oxidation of uric acid by means of lead (IV) oxide has a double interest due to the biological importance of the substrate and to know the exact role of the lead compound.

The experimental part was described by Mulder [7]. Some data about lead dioxide are given. It appears as brown hexagonal crystals, insoluble in water, and has hydrogen bond count 2. Its chemical structure is linear [8].

Lead dioxide is not a peroxide but it will act as a powerful oxidizing agent [9].

The other uric acid oxidation studied is by means of slightly alkaline hydrogen peroxide [10]. This communication has been commented [11].

Further reaction leads to cyanuric acid, 1,3,5-triazinane-2,4,6-trione [12].

The formation of sodium hydroperoxide is well known and Michael addition to α,β -unsaturated ketones with epoxide formation has been reported [13].

Although there is no enone in uric acid, there is reaction with this reagent. This point will be discussed in the next section.



Microwave-Assisted Organic Synthesis: A Green Chemistry Strategy

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ABSTRACT

Microwave heating, being very quick and specific, is widely used as an easy mode of heating in organic synthesis. Nowadays, the advantages of this technique have made it more widely used. The conventional methods of organic synthesis normally need a longer heating time, elaborate apparatus setup, which result in a higher cost, and the use of excessive reagents and solvents leads to environmental pollution. Microwave-assisted synthesis provides the benefits of higher yields, greater reaction rates and selectivity, at the same time generating new, improved, economically viable, and environment-friendly processes for the synthesis of a large number of organic molecules. This technique is considered an important approach toward green chemistry. Microwave synthesis also opens up new opportunities to the chemist in the form of new reactions that were not possible in conventional heating. This article focuses on the different applications of microwave-assisted synthesis, solid-phase synthesis, green chemistry, and nanotechnology and also discusses the basic mechanism involved in microwave heating.

Key words: Energy-efficient, Environment-friendly, Green chemistry, MAOS, Solvent-free.

1. INTRODUCTION

Microwave chemistry is the science of applying microwave radiation to enable chemical reactions. Earlier, the microwave was only used for domestic purposes for heating and cooking foods. The first microwave oven was introduced by Tappan in 1955 while the first application under organic synthesis was published in 1986. Since the year 2000, microwave-assisted synthesis has gained importance and can easily be used to carry out various syntheses in laboratories [1].

For centuries, conventional heating methods of using Bunsen burners, oil baths, and hot mantles have been used for carrying out chemical reactions. These methods are not only time consuming and tedious, but also energy inefficient and wasteful [2]. They also create a hot surface on the reaction vessel where the reagents decompose over time and creating toxic substances. These methods also require the use of solvents, which are often toxic, harmful to the environment and may require further steps involving their recovery. All these drawbacks of the conventional heating methods can be overcome by the use of alternate methods, use of microwaves being one such method [3,4]. Microwave-assisted synthesis has several advantages over the conventional methods. In this method of synthesis, high temperature is easily and quickly attained and cooling is also fast. Microwave heating does not heat the whole surface inside the appliance, as is the case with conventional heating that heat up the reaction mixture by conduction, but only uses the waves to heat the reaction mixture kept in it. This reduces the formation of unwanted side products, so the yield is enhanced and the synthesis is cleaner. Furthermore, the use of harmful organic solvents in large amounts is avoided, which is usually not possible in conventional synthesis methods. All these features make microwave-assisted synthesis an example of green chemistry, that is, it is energy efficient, atom efficient, faster, uses fewer solvents,

2. MECHANISM OF HEAT GENERATION BY MICROWAVES

The mechanism of heat generation in microwave-assisted synthesis is dipolar polarization [5]. When irradiated with microwaves, the molecules with a permanent dipole moment become aligned with the electric field component of the microwaves. This causes the molecules to oscillate and collide with each other. The oscillation of molecules produces friction between them, resulting in heat generation. Hence, to become microwave active, the reagent molecules should possess a dipole moment and should be polarizable. The greater the polarizability of the molecules more is the heating effect produced in the presence of microwaves.

Solvents also play an important role in this technique and each solvent absorbs energy differently. There are three types of solvents used, namely, low, medium, and high absorber of microwave radiation. While hydrocarbons are low absorbers, polar compounds such as alcohols are high absorbers and the medium one is water, acetone, acetic acid, etc. [7]

3. INSTRUMENTATION

Microwave-assisted synthesis is carried out in special microwave reactors that generally comprise five main components, namely, high voltage transformer, magnetron, waveguide, cooling fan, and cavity, as shown in Figure 1 [8].

and is cleaner [3]. It is also applicable to a large variety of organic reactions, making it highly versatile and useful [4]. The comparison of a conventional oven and microwave oven for synthesis is done in Table 1.



Graphene Nanocomposites are affected by fracture and fatigue

B Lavanya, S Loka Raghavendra *

Graphene, a single-atom-thick sheet of sp^2 -bonded carbon atoms, has generated much interest due to its high specific area and novel mechanical, electrical, and thermal properties.^[1–7] Recent advances^[8–10] in the production of bulk quantities of exfoliated graphene sheets from graphite have enabled the fabrication of graphene–polymer composites. Such composites show tremendous potential for mechanical-property enhancement due to their combination^[11–12] of high specific surface area, strong nanofiller–matrix adhesion and the outstanding mechanical properties of the sp^2 carbon bonding network in graphene. Graphene fillers have been successfully dispersed in poly(styrene), poly(acrylonitrile) and poly(methyl methacrylate) matrices and the responses of their Young's modulus, ultimate tensile strength, and glass-transition temperature have been characterized.^[11–12] However, to the best of our knowledge there is no report on the fracture toughness and fatigue properties of graphene–polymer composites. Fracture toughness describes the ability of a material containing a crack to resist fracture and it is a critically important material property for design applications. Fatigue involves dynamic propagation of cracks under cyclic loading and it is one of the primary causes of catastrophic failure in structural materials. Consequently, the material's resistance to fracture and fatigue crack propagation are of paramount importance to prevent failure.

Herein we report the fracture toughness, fracture energy, and fatigue properties of an epoxy polymer reinforced with various weight fractions of functionalized graphene sheets. Remarkably, only 0.125% weight of functionalized graphene sheets was observed to increase the fracture toughness of the pristine (unfilled) epoxy by $\approx 65\%$ and the fracture energy by $\approx 115\%$. To achieve comparable enhancement, carbon nanotube (CNT) and nanoparticle epoxy composites^[13–15] require one to two orders of magnitude larger weight fraction of nanofillers. Under fatigue conditions, incorporation of 0.125% weight of functionalized graphene sheets drastically reduced the rate of crack propagation in the epoxy ≈ 25 -fold. Fractography analysis

revealed that the extraordinary effectiveness of graphene to resist fracture and fatigue is related to deflection processes associated with the planar (two-dimensional) structure of graphene, which enables it to deflect cracks far more effectively than one-dimensional CNTs or low-aspect-ratio nanoparticles. Given the widespread use of epoxies in structural applications, these results are expected to translate into significant practical applications for such nanocomposite epoxies.

In order to synthesize bulk quantities of exfoliated graphene sheets and to effectively disperse these sheets in polymer composites we utilized a technique pioneered by Aksay and co-workers.^[8,9] This method generates bulk quantities of functionalized (i.e., partially oxygenated) graphene sheets (FGS) by the rapid thermal expansion ($>2000\text{ }^\circ\text{C min}^{-1}$) of completely oxidized graphite oxide. The oxygen functionalities on the graphene sheets facilitate their dispersion^[10,16] in polar solvents, which makes this process convenient for composite applications. The protocols used to oxidize graphite to graphite oxide and then generate FGS by the thermal exfoliation of graphite oxide are provided in the Experimental Section and the Supporting Information (we used the same protocols as described in References [8,9]). The procedures used to disperse FGS in a bisphenol-A based thermosetting epoxy^[17–19] are also described in the Experimental Section. Both compact tension samples for crack propagation study and dog-bone-shaped coupons (samples) for uniaxial tensile testing were fabricated and tested.

Figure 1a shows a scanning electron microscopy (SEM) image of a typical FGS flake synthesized by the above approach and deposited on a silicon wafer for imaging. The flake dimensions are $\approx 4.4\text{ }\mu\text{m} \times 2.4\text{ }\mu\text{m}$; note the wrinkled surface texture of the FGS, which could play an important role in enhancing mechanical interlocking and load transfer with the matrix.^[11,12] Figure 1b is a high-resolution transmission electron microscopy (HRTEM) image of the edge of a typical FGS flake, indicating that each flake is composed of ≈ 2 – 3 individual graphene sheets. The electron diffraction pattern (shown in the inset of Figure 1b) confirms the signature of few-layered graphene.^[11] Figure 1c shows an SEM image of a freeze-fractured nanocomposite sample with $\approx 5\%$ weight of FGS. The image clearly indicates epoxy-coated FGS flakes on the fracture surface of the sample. The inset in Figure 1c depicts a high-resolution SEM image, indicating the wavy edge structure of the FGS sheets that are protruding out of the fracture surface. At low weight fractions of FGS (below 0.5%), it was quite challenging to study the FGS dispersion by SEM analysis due to the planar sheet geometry of the FGS and the epoxy coating on the FGS, which allows only the exposed sheet edges to be discerned.

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Magnetostrictive characteristics of bonded $Tb_{0,3}Dy_{0,7}Fe_{1,9}$ composites

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Keywords: Smart Materials, $Tb_{0,3}Dy_{0,7}Fe_{1,9}$ /epoxy composites, Magnetostriction

Abstract. $Tb_{0,3}Dy_{0,7}Fe_{1,9}$ composites attract much attention due to their large magnetostriction, and small eddy current losses. In this work intelligent polymer matrix composite materials consisting of $Tb_{0,3}Dy_{0,7}Fe_{1,9}$ particles was obtained by mixing epoxy resin and $Tb_{0,3}Dy_{0,7}Fe_{1,9}$ powder with grains from 38 to 106 μm . The relationships among the manufacturing technology of these materials, their microstructure, as well as their magnetostriction were evaluated. Resulting composites can extend the possibilities of application the magnetostrictive materials simultaneously reduce the cost of $Tb_{0,3}Dy_{0,7}Fe_{1,9}$.

Introduction

Magnetostrictive composites are being investigated as active drive elements for several years [1-5] since it was noticed that disadvantages of monolithic $Tb_{0,3}Dy_{0,7}Fe_{1,9}$ could be overcome by combining $Tb_{0,3}Dy_{0,7}Fe_{1,9}$ particles with non-conductive matrix. The $Tb_{0,3}Dy_{0,7}Fe_{1,9}$ alloy exhibits giant magnetostriction (800÷1200 ppm) in a considerably low magnetic field (50÷200 kA/m) at room temperature but some negative attributes (in particularly losses associated with eddy currents at high frequencies, high price and brittleness) have limited its technological applications [6,7].

Investigation of composite materials obtained by consolidation of the $Tb_{0,3}Dy_{0,7}Fe_{1,9}$ particles using various methods and various kind of binder is carried out in many research centers in the world [4-5,7-9]. The aim of this work was to prepare the composite materials with epoxy matrix reinforced by the $Tb_{0,3}Dy_{0,7}Fe_{1,9}$ powder and investigation their response to applied magnetic field.

Experimental Procedure

Investigation were carried out on composite materials which were prepared by melting the $Tb_{0,3}Dy_{0,7}Fe_{1,9}$ alloy powders (Etrema Products Inc., USA) with a two-part epoxy resin. The components of the resin were mixed in equal parts by weight. The size of the $Tb_{0,3}Dy_{0,7}Fe_{1,9}$ particles were from 38 to 106 μm . In this work, specimens containing particle volume fractions of 10, 25 and 50% were made.

The particles and resin were homogenously mixed together and placed in rectangular aluminium mould of size 60x36x10 mm. The form was placed in a static magnetic field (120 μT measured in the center) made by two NdFeB permanent magnets (80x20x10 mm). These magnets produced magnetic field along the longitudinal direction of the mould and causes the particles to align with the magnetic flux lines, creating an anisotropic particle distribution (Fig. 1).

Micro-structure and thermal diffusion of $Gd_2Zr_2O_7$ powders

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Keywords: TBC, pyrochlore, zirconates, thermal diffusivity, low conductivity

Abstract. The selection of new TBC materials is restricted by few basic requirements such as: high melting point, no phase transformation between room and the operation temperatures, low thermal conductivity, chemical inertness to the combustion gases and environment, thermal expansion match with the metallic substrate, good adherence to the metallic substrate and low sintering rate of the porous microstructure. Among these properties, one of the most important is thermal diffusivity. The number of material that can be used as TBCs is limited and so far only a few materials have been found to basically satisfy these requirements. Recent research has shown that certain rare-earth zirconates, such as $Gd_2Zr_2O_7$, have even lower thermal conductivities than 7YSZ, and this has spurred an intensive research in discovering alternative TBC materials. The results of microstructure tests performed on the powders intended for thermally sprayed TBCs with APS method were presented in this article. The tests of phase and chemical composition of the analysed powder were performed. The carbon, sulphur and gas nitrogen contents were, among other things, determined during those tests. The x-ray powder diffraction phase identification in as received material was determined. The tested material showed the presence of $Gd_2Zr_2O_7$ compound as the predominant one and Gd_2O_3 and ZrO_2 oxides. The surface morphology analysis of the powder was carried out and its internal structure was characterized. The tested material shows porous structure typical for agglomerated powders. The second testing area applied to analysis of the powder thermal properties. The thermal diffusivity of the compressed samples with density similar to the solid material was determined with the laser flash (LF) method. The measurement results show that requirements for the materials used for new generation TBCs are met.

Introduction

From the beginning of construction of contemporary aircraft engines, in order to improve life and use properties of applied materials to a maximum, the systems of protective coatings are used. Contemporary constructions of engines, and development in technologies as well, lead to evolution of new protective coatings and to improvement of ones, which were sooner applied. The thermal barrier coatings TBC (*thermal barrier coating*) enable to lower temperature (fig.1) (at approx. 170°C) of operating elements, exposed to creeping, in a hot section of gas turbine (e. g. combustion chambers and directing and rotating blades) to a range, which enables to operate for a long time in conditions of high temperature influence and prolongs operation of them even three or four times, simultaneously reducing consumption of fuel [1].

Generally, the TBC applied in gas turbines is made up of two components: a bond coat created by the vacuum or low pressure plasma-sprayed MCrAlY (M = Ni, Co) and a top coat of yttria and partially stabilized zirconia produced by the atmospheric plasma spraying (APS) or electron beam-physical vapour deposition (EB-PVD) [3-5]. These superalloy/TBC systems can be applied in both aerospace and land-based gas turbine engines. In automotive use, the piston head for diesel engine is coated to enhance lifetime and performance as far as fuel demand reduction and power

A Study of Bharati Mukherjee's Women

M. Sridevi.

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Abstract

Bharati Mukherjee, an American writer of Indian origin, wrote mostly about the South Asian Diaspora in Canada and the USA. She wrote both fiction and non-fiction: while her fiction chronicles the weal and woe of South Asians in Canada and the USA, her non-fiction digs out the causes of their problems and sufferings. Therefore, her fiction is based on her research and has an air of authenticity in what she presents through her fictional characters. Moreover, her own experiences of living in both Canada and the USA also serve as a kind of background for her fiction. Mukherjee finds in her research that in Canada, South Asians fail to integrate with Canadian culture mostly because of Canada's discriminatory immigration policy, and in the USA, South Asians fail to acculturate because of their retrogressive attitude and expatriate mindset. Nevertheless, Mukherjee's women seem to be more progressive in attitude than her male characters unlike whom her women give up their retrogressive attitude and try to acculturate to the new setting. While her male characters live in America as South Asians, some of her women are busy making themselves Americans. Therefore, this paper makes an attempt to critically examine how Mukherjee's women, particularly her heroines, attempt to plunge into American melting pot culture.

Introduction

The problems of adapting to a new culture that South Asian immigrants face in the USA and Canada are a common theme in Bharati Mukherjee's fiction. This paper is a critical reading of two novels and some short stories of Mukherjee, in which she shows that South Asians migrate to North America and live there for decades, but unfortunately fail to be American. According to Mukherjee, South Asians fail to integrate with Canadian culture mostly because of Canada's discriminatory immigration policy, and in the USA, South Asians fail to acculturate to American life because of their retrogressive attitude and expatriate mindset. However, although this observation seems to be appropriate to Mukherjee's male characters, some of her women characters attempt to emerge as new persons ready to do what they are needed to do in America to be labeled as Americans. While the men live like expatriates carefully keeping them away from the American values of life, the women try to come out of expatriate mentality and become American by veering off the native culture. While the men are in what Mukherjee called "self-exile" in America, and are unable to remake themselves as Americans owing to their past memories and psychological attachment with their native land, the women shed their past and emerge as "self-assertive individuals, free from the bondage imposed by relationships—mostly of the past."¹ To comment on the divergent attitude of South Asian men and women to their settlement in America, Mukherjee says in an interview:

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'Female Voice' as Voiced in the Fictional World of Bharati Mukherjee with Special Reference to her *The Tiger's Daughter and wife*.

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ABSTRACT

*This is an attempt to project a woman's position in society and her place in it playing different roles as an obedient daughter, a devoted wife and a loving mother with a special focus on the female characters portrayed by Bharati Mukherjee in her fictional world with reference to **The Tiger's Daughter and Wife**. It shows how the various predicaments experienced by the females known as 'heroes' in feminine form, their culture shock and their struggle to cope with hostile circumstances stem out of the author's bitter experiences as an expatriate in Canada, making them appear to be fighters, adventurers, confident people occupying the central status in her fictional world.*

Key words: Female Voice.

A woman's position in society, her role and place in it has always been a core issue. Is she there just to play the role of an obedient daughter, a devoted wife and a loving mother? Does a woman not have an identity of her own and a purpose for living? The aim of different feminist groups has been the same i.e., to liberate women from male oppression and to promote women's rights. Radical feminists have, however, cautioned women against being slaves to their biological functions. A woman's status is largely based on the simple biological fact that she is the bearer of children whose care is her responsibility, thus her sphere is usually restricted to her familial roles. Simone De Beavouri in his **The Second Sex** states:

"One is not born, but rather becomes a woman. No biological, psychological or economic fate determines the figure that the human female present.

"Adam is portrayed as the master who gives names to all beasts and also to his wife whom he calls Eve" (p.148)

St. Paul also gives a secondary position to woman:

"A man ought not to cover his head, since he is the image and glory of God: but woman is the glory of man" (Bose, 12)

"an embodiment of sacrifices, silent sufferings humility, faith and knowledge" (Everett, 76)

Following the footsteps of those female writers, Bharati Mukherjee falls in line with their thinking so as to project feminine issues and problems in her writings.

in society; it is civilization as whole that products this creature, intermediate between male and much, which is described as feminine". (p.83)

In a patriarchal society, a female child is brought up under the strict supervision of her parents and is groomed as an object and thus prepared to be sold in marriage market. Marriage thus seems to be the only ambition of a girl's life and she as such is always somebody's daughter, someone's wife or some one's mother but never really has an identity of herself. No doubt, women are an integral part of human civilization but man has always treated them like beasts of burden and objects for pleasure. Man is seen as the master of everything on earth including women and he is glorified even in **The Bible** and his superiority is highly stressed here:

Women have slowly but surely raised their voices against inequality and oppression and female consciousness against male domination in all walks of life and feminist literature has, in fact, been a significant instrument in foregrounding the feminine values and issues. In feminist literature, women's experience becomes the central concern for it seeks to demythologize of humanity, and woman is the unnamed and the invisible. Hence, the need for women writers to write about their own literature for providing centrality to women in all ways thematically, structurally and stylistically. Women writers like Jane Austen, Charlotte Bronte, Dorothy Richardson, George Eliot, Virgin Woolf, Margaret Drabble, Kamalaya Markandaya, Anita Desai voiced some burning female issues in their respective works. In India, a woman has necessarily to be virtuous, chaste, submissive, homely, graceful and devoted to her family as she is considered to be:

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UNCONVERING JUVENILE PSYCHE: A COMPARITIVE STUDY OF R.K. NARAYAN'S "SWAMI" AND MARK TWAIN'S "TOM SAWYER"

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ABSTRACT

The main aim of this paper is to make a comparative study of two famous child heroes Tom Sawyer in the novel *The Adventures of Tom Sawyer* and Swaminathan in the novel *Swami and Friends*. The main aim of the researcher is to show that there is something universal in the experience of every little school boy by making a comparative study of these two boys. Many great writers have dealt with the theme of childhood. The world of children being a microcosm of the adult world both children and adults are mesmerised by books about childhood. R.K. Narayan and Mark Twain are two great writers who dealt with this theme in their novels *Swami and Friends* and *The Adventures of Tom Sawyer*. Both Narayan and Twain take us to the innocent and boisterous world of children. The two child heroes, Swami and Tom, have difference in their characteristics because they hail from different countries, cultures, and they lived in different times. Swami can be admired as an embodiment of Indian boyhood while Tom can be revered as the quintessence of American boyhood. But irrespective of their cultural difference both the boys shows some common characteristics. Their relationship with their friends, aversion towards their school, skirmishes with their teachers, the problems they face due to their interference with the adult world, rivalry with their peers, fear of examination and fun loving nature are not culture specific.

Key Words: Childhood, Adventures, Friendship, Universal Experience, Heroism.

AS© PUBLICATIONS

We would never have loved earth so
well if we had had no childhood in it

-George Eliot, *The Mill on the Floss*

adventurous world and antics and reminiscences
adults of their insouciant and innocent life of

INTRODUCTION

Many great writers have dealt with the theme of childhood. The books which portray the alluring world of juveniles mesmerised both children and adults for they portrays before children their



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The Theme of Education in the Novels of R.K. Narayan

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Abstract

R. K. Narayan is one of the most popular writers in the realm of Indian English Literature. He famously created the fictional town of *Malgudi* and populated it with a variety of people whose stories he narrated in his novels and short stories. He is a keen observer of life around him but does not take up an active role of preaching any ideology. He burdens neither his characters nor his readers with his views keeping a neutral authorial stance most of the times. And yet, he expresses his strong antipathy to the formal education system in his writing without any ambiguity. This is a recurrent theme to which he returns again and again. He voiced his concerns, regarding the impact of educational practices on children, in the Parliament when he was a member of Rajya Sabha. The present paper studies Narayan's preoccupation with the theme of education and his distaste for the oppressive English system of education. An attempt is also made to investigate his personal experiences by juxtaposing the autobiographical elements in his writing with his life.

Keywords: Education; Colonial; Curriculum; British Empire; Nation

R. K. Narayan has often been considered a 'Pure' artist; an author writing primarily for aesthetic purpose without any social, political or reformist agenda. One reason for such an approach is historical. Though he began writing in 1930s, which was a very volatile era in the political history of Indian nationalist struggle for freedom, his novels stay away from engaging in any political debate. The only exception being *Waiting for the Mahatama* (1955) but it was published after India's independence and the novel primarily focusses on the personal life of the protagonist albeit against a politically charged background. He usually writes in a self-absorbed, objective and even limited manner about the fictional town that he created. He offers a parallel to Jane Austen who wrote at the time of Napoleonic war without showing any direct involvement or influence and like her, he seems to be sitting on the fence unaffected by the events in his surroundings. "At a time when the country was going

The Picturization of the Female Voice as an Integral Part of the Fictional Forte of Bharati Mukherjee: An Appraisal

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ABSTRACT: *This is an attempt to project a woman's position in society and her place in it playing different roles as an obedient daughter, a devoted wife and a loving mother with a special focus on the female characters portrayed by Bharati Mukherjee in her fictional world with reference to **The Tiger's Daughter** and **Wife**. It shows how the various predicaments experienced by the females known as 'heroes' in feminine form, their culture shock and their struggle to cope with hostile circumstances stem out of the author's bitter experiences as an expatriate in Canada, making them appear to be fighters, adventurers, confident people occupying the central status in her fictional world.*

It is generally held that women play the role of an obedient daughter, a devoted wife and a loving mother. A woman did not have an identity of her own and a purpose for living her own life in her desirable way. To liberate women from male oppression and to promote women's rights and caution women against being as slaves based on biological functions of women, is the ultimate notion of various feminist groups. A woman's status is largely based on the simple biological fact that she is the bearer of children whose care is her responsibility, thus her sphere is usually restricted to her familial roles. Simone De Beauvoir in his **The Second Sex** states:

“One is not born, but rather becomes a woman. No biological, psychological or economic fate determines the figure that the human female presents in society; it is civilization as whole that produces this creature, intermediate between male and much, which is described as feminine”. (P 83)

In Indian society, a female child is brought up under the strict supervision of their patriarchal system and marriage seems to be the only ambition of a girl, she is groomed as an object in her life, neither has an identity of her own and prepared to be sold in marriage market. No doubt, women are an integral part of human civilization but man is seen as the master of everything on earth including women and has always treated women like beasts of burden and objects for pleasure. He is glorified even in **The Bible** and his superiority is highly stressed here:

“Adam is portrayed as the master who gives names to all beasts and also to his wife whom he calls Eve” (P 148)

St. Paul also gives a secondary position to woman:

“A man ought not to cover his head, since he is the image and glory of God: but woman is the glory of man” (Bose, 12)

Women have raised their voices against inequality, oppression and female consciousness against male domination. Feminist literature has been a significant instrument in making the women's experience become the central concern for it seeks to demythologize human ill-treatment, feminine values, and other related issues. In the field of Literature, Women writers are needed to write about their experiences, for providing the central priority to women in all such respects as thematically, structurally, and stylistically. In India, a woman has necessarily to be virtuous, chaste, submissive, homely, graceful and devoted to her family as she is considered to be:

“an embodiment of sacrifices, silent sufferings humility, faith and knowledge” (Everett, 76)

Women writers like Jane Austen, Charlotte Bronte, Dorothy Richardson, George Eliot, Virginia



ALIENATION AND ASSIMILATION OF A GENTILE IN ISAAC BASHEVIS
SINGER'S *THE SLAVE*

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ABSTRACT

Isaac Bashevis Singer was a Polish born Jewish American novelist, essayist, and short story writer who writes in Yiddish. He was basically brought up in religious ambience. He lost his mother and younger brother in the holocaust of Nazi. He had experienced and witnessed the brutality and wickedness of the Nazis against the Jews, homosexuals and transgender. In his novels, Singer emphasizes the suffering of his characters as a result of their doubt in the existence of God. Their internal conflict between faith and doubt leads to the dissolution of their families, ultimately leading them to realize that without faith in God, they are destined for failure. Eventually, they repent and return to God. This theme is not only relevant to the characters in Singer's novels, but also to the entire universe. He writes about the struggles and sufferings caused the alienation of the Jews, due to the displacement in the world of adoption where they lost their home of origin. His novel *The Slave* tells about a Jewish man, called Jacob who lived in a small village, Josefov in Poland, he was displaced from his village and enslaved by a gentile tribe. Jacob is a young man and highly knowledgeable in terms of his religious scriptures. Chelminsky massacre made him to be a slave. This novel depicts the endless struggles and misfortunes of the Jew, who leads an alienated life and strives to protect the life of a gentile woman, who assimilates the Jewish faith. His constant suffering made him to question the God. The true love of Wanda made her committed and assimilated the Judaism. The slave describes the alienation of a Jew and assimilation of a gentile.

Keywords: Alienation, Assimilation, Displacement, Slavery, Struggle, Degradation.

It is necessary to know the history of Jews were compelled to leave their home land, many of them tortured and exterminated nearly six millions of Jews were killed by the Nazi. It was the darkest moment in the entire human history, during the Second World War many millions of Jews fled to America and Europe for their survival. The displacement made them to lead miserable lives. Singer also one of the victims of displacement due to the holocaust, most of his characters encounters the alienation and suffers from cultural and religious barriers.

The novel *The Slave* (1962) was written in three parts Wanda, Sarah and The return after math of chelminsky massacre. The protagonist of the novel Jacob escapes from the massacre, later he was caught and sold to a tribe by Cossacks. Singer tried to find the root cause for the suffering of Jews; he used an allegorical technique to depict the suffering and struggle of his characters.

An Introduction to Fractals Geometry

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Abstract: Fractals were first formally defined by Benoit Mandelbrot in 1980's. A fractal is defined as a rough or fragmented geometric shape that can be subdivided in parts each being a reduced size copy of the whole. Fractals are self-similar across different scales. Mathematically, they are sets obtained through recursion that exhibit interesting dimensional properties. Fractal patterns with various degrees of self-similarity have been studied in images, structures and sounds and found in nature, technology and architecture. They are of particular importance in chaos theory as the graphs of most chaotic processes are fractals. Fractal dimension is used to measure the complexity of objects. The paper overviews the fractals, principles underlying their generation and fractal dimensions.

Keywords : self-similar, dimension, recursion

INTRODUCTION

One of the most intricate images in Mathematics is the Mandelbrot Set, which was discovered by Mandelbrot in 1980. The discovery of this image led to the development of fractal science. Fractal geometry can be considered different to classical geometry in that it does not deal in integer dimensions. More formally, in 1982, Mandelbrot stated that "A fractal is by definition a set for which the Hausdorff-Besicovitch dimension exceeds the topological dimension." Later, he simplified and expanded the definition to: "A fractal is a shape made of parts similar to the whole in some way." Still later, Mandelbrot settled on the use of term fractal dimension as a generic term applicable to all the variants.

Generally, theoretical fractals are infinitely self-similar, iterated and detailed mathematical constructs having fractal dimensions.

A figure is said to be self similar if magnified subsets look-like the whole and to each other. They may not look exactly the same to each other at all scales, but same type of structures must appear on all scales. All self-similar objects may not be fractals but all fractals are self-similar. Fractals have an infinite amount of detail. A smooth curve does not have the property of self-similar, for, on magnifying around any point on the curve, it will eventually look like a line. But this is never the case with a Fractal. There is always more detail as we magnify it. Being a relatively new subject of study, there is no widely accepted definition. One definition is: "A geometric figure or natural object is said to be fractal if

(a) its parts have the same form or structure as the whole, except that they are at a different scale and may be slightly deformed

(b) its form is extremely irregular or interrupted or fragmented, and remains so, whatever the scale of examination;

(c) It contains „distinct elements“ whose scales are varied and cover a large range.”

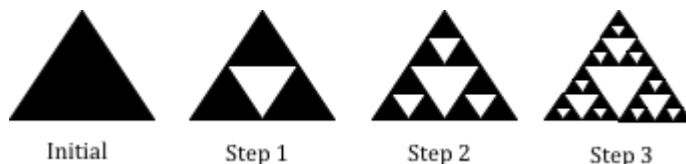
(B. Mandelbrot Les objects Fractals 1989)

MAKING A FRACTAL

Iterated Fractals: Sierpinski Gasket

The self-similar behaviour can be replicated through recursion: repeating a process over and over.

Example: Connect the mid-points of each side of a filled in equilateral triangle.



The process is repeated over and over, the shape that emerges is called the Sierpinski Gasket. Self-similarity is clearly visible as any piece of gasket looks identical to whole Sierpinski Gasket. In fact, it shows perfect self-similarity. It contains three copies of itself and each copy further contains three copies of itself.

Mathematical Analysis of Hymns for Meditation

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Abstract — In this work we study the mantra and Vedic chants used for meditation and convert them to time series with the frequency of 44100 Hertz. We then perform the mathematical and statistical analysis of these chants and compare these results with few of the popular known songs in Hindi, Kannada and Spanish/English. We also consider the Tirumala temple bell sound for our analysis and study. We conclude that the meditation songs are Lyapunov stable and in fact they are asymptotically stable. And hence are perfect for meditation.

Keywords — Correlation, Entropy, Lyapunov Spectrum, Power Spectrum, Time Series

I. INTRODUCTION

India is a very mysterious country. We find its mystery in its diversity, not just in the flora and fauna, but also in the tradition of the people and more importantly the influences on them and the cultural diversity. Yet some things have never changed. The Chanting of Vedic hymns and mantras are one such example. Today most of the yoga gurus and people use many of the Vedic chants as powerful form of meditation. Youtube has popularized them extensively. Thus many questions arise. Are these connected in any way as many of them are used for the similar purpose? Can we study their patterns?

With the invention of nonlinear time series analysis tools by Hegger Kantz and Shrieber [1] in late decades of the previous century, I felt that such a study is possible. Thanks to them that there is a freely available codes on internet as TISEAN 3.0.0 which executes these studies on any time series fed as data.

Here we first describe the Vedic chants and other songs which have been used for the study in the first section. In the next section about how the data have been extracted and what are the different studies and analysis done on the data. The third section discusses the analysis and interpretation and finally the fourth is the conclusion.

II. MATERIALS AND METHODS

1. THE DATA

For this study I considered the following mantras and downloaded them from the websites which provide them freely.

1. Maha Mryuthyunjaya Mantra chanted 108 times by Adi Yoga guru
2. Om Mantra chanting
3. Shivastuti for meditation freely available from a website
4. Maha Mryuthyunjaya Mantra fewer times available freely from a website.
5. Tirumala temple bell sounds
6. "Sonide nakhare" a Hindi film song.
7. "Ee sanje yakagide" a Kannada film song
8. "Bailamos" a Spanish song

One can argue that these songs or chants have to be understood first and then the music should suit in such a way that they can be useful for meditation. Hence I have chosen these from the websites which provide them for meditation. The temple bell for its sound resembling the Om mantra and other songs from films and pop music only for the sake of comparison. Also though Mathematically I will not be able to say anything regarding the meaning of the chants, the rendering and the chant when converted in the form of numbers would give out some patterns which is explained in this paper.

I first downloaded the mp3 files from the websites. Then converted the mp3 to .wav format using audacity. Audacity converts the file into left and right stereo audio files with the frequency of 44100 Hz. Then the audioread of OCTAVE was used to convert the .wav to data points.

Though the number of data points generated for these mantras were different from each other, the analysis is made in such a way that there is uniformity in them.

A Numerical Study on Pressure Drop Characteristics of Fluid Passing Through Two Modified Sudden Expansion Configurations

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Abstract: In this paper, new types of separation axioms in supratopological spaces, namely gpr^μ -separation axioms are introduced and discussed. Several characterizations and consequences of the properties given by these axioms are studied.

1. INTRODUCTION

In 1970, Levine [2] defined generalized closed sets in topological spaces and also introduced a class of topological spaces called $T_{1/2}$ spaces. The extended study in the field of generalized closed sets introduced several new separation axioms. In 1975, Maheswari and Prasad [3] defined the three new separation axioms called semi- T_2 , semi- T_1 and semi- T_0 using semi-open sets. After that many researchers introduced different types of separation axioms. In 1983, Mashhour et.al [4] derived supra topological spaces, investigated S -continuous maps and S^* - continuous maps. Extensive research in supra topological space made many topologists to introduce different types of open and closed mappings. These innovations further developed and in 2012, Mustafa and Qoqazeh [1] introduced the notions of supra- T_i for spaces $i = 0, 1, 2$. In 2012, Menon [6] introduced the notion of gpr^μ -open sets.

Moments of the Power Series Distributions

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Abstract: For the Power Series Distributions generated by an arbitrary entire function of finite order, applying methods of Karamata's Theory of Regular Variation, we obtain asymptotic behavior of its moments. As an illustration, we calculate the moments of distributions generated by the class of Mittag-Leffler functions of which the well-known Poisson Law is just a special case.

Keywords: Distribution moments, entire functions of finite order, regular variation, karamata.

1. INTRODUCTION

1.1. The classical discrete Poisson Law with parameter $\lambda > 0$ is given by

$$P_\lambda(X = n) = \frac{\lambda^n e^{-\lambda}}{n!}, \quad n = 0, 1, 2, \dots$$

Asymptotic behavior of its moments is well-known

$$E_\lambda X^k = \sum_n n^k P_\lambda(X = n) \sim \lambda^k = (E_\lambda X)^k \quad (\lambda \rightarrow \infty).$$

In this article we shall give a generalization of the above assertion and prove that the same asymptotic relation is valid for any discrete distribution generated by an entire function of finite order.

Namely, denote by A_ρ the class of transcendental entire functions with positive Taylor coefficients and of finite order ρ , $0 \leq \rho < \infty$.

(Note that an entire function is transcendental if it is not a polynomial i. e. if it has infinitely many non-zero Taylor coefficients).

Definition 1.1. For arbitrary $f(z) = \sum a_n z^n$, $f \in A_\rho$, define the law F_f with parameter $\lambda > 0$ by

$$P_\lambda(X = n) = a_n \lambda^n / f(\lambda), \quad n = 0, 1, 2, \dots$$

Then the law F_f is a Power Series Distribution generated by $f \in A_\rho$ (cf [1]).

Our aim here is to obtain asymptotic behavior of its k -th moment $E_\lambda X^k$ ($\lambda \rightarrow \infty$), where

$$E_\lambda X^k = \sum n^k P_\lambda(X = n) = \sum n^k a_n \lambda^n / f(\lambda), \quad k = 1, 2, \dots$$

Evidently,

$$E_\lambda X = \sum n a_n \lambda^n / f(\lambda) = \lambda f'(\lambda) / f(\lambda). \quad (0.1)$$

In general, consider the sequence of functions $f_k(\lambda)$ defined recursively by

$$f_k(\lambda) = \lambda f_{k-1}'(\lambda), \quad k = 1, 2, \dots; \quad f_0(\lambda) = f(\lambda).$$

Then $f_k(\lambda) = \sum n^k a_n \lambda^n$ and

$$E_\lambda X^k = f_k(\lambda) / f(\lambda), \quad k = 1, 2, \dots \quad (0.2)$$

1.2. We shall use in the sequel the concept of Karamata's regularly varying functions.

Definition 1.2. A positive measurable function $\ell(\cdot)$ is slowly varying if the asymptotic equivalence

$$\ell(tx) \sim \ell(x) \quad (x \rightarrow \infty),$$

holds for each $t > 0$.

Some examples of slowly varying functions are $\log^a x$; $\log^b(\log x)$; $\exp(\log^c x)$; $\exp(\log x / \log \log x)$, $a, b \in \mathbf{R}$, $0 < c < 1$.

Functions $g(\cdot)$ of the form $g(x) = x^\mu \ell(x)$ are regularly varying ($g \in R_\mu$) with index $\mu \in \mathbf{R}$ (cf [2], p. 18).

From those definitions follows

Proposition 1.1. A positive measurable function $g(\cdot)$ belongs to the class R_μ if the asymptotic relation

$$\frac{g(tx)}{g(x)} \rightarrow t^\mu \quad (x \rightarrow \infty), \quad (1.1)$$

holds for each $t > 0$.

Moreover, the relation (1.1) holds uniformly on each compact t -set in $(0, \infty)$ (cf [2], p. 6).

Theory of Regular Variation is very well-developed and has many applications in Analysis, Probability Theory, Number Theory etc (cf [2, 3]).

The so-called *Theorem on approximation by a regularly varying function* will play an important role in the sequel (cf [2], p. 81; [4]).

Proposition 1.2. Let h be a positive function with the property

$$\limsup_{x \rightarrow \infty} \frac{\log h(x)}{\log x} = \rho, \quad 0 \leq \rho < \infty;$$

then there exists $g \in R_\rho$ such that $g(x) \geq h(x)$ and

The Conditional Sequel To The Theory Of Information Function

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Abstract: Problem statement: A great deal of attention has been given to the theory of information. It has found its applications in science especially in the area of Biothecnology. Previous studies on the subject has been limited to either conditional or sequence problem solving. This study combines both conditional and sequence properties of the information function. By doing this, researchers can find

solutions to more problems that are applicable in real life. **Approach:** First, properties of the dynamical systems and the information function defined by Shannon has been provided, Then, the conditional sequence information function of a dynamical system together with its proof was presented. **Result:** This new function now exists now and ready for the use in many real life problems such as finding solutions to DNA sequence with conditional sickness. **Conclusion:** This new function created opens a new avenue to researches in solving more complex problems by using its developed properties.

Key words: Entropy, dynamical systems, information function, conditional sequence information function

INTRODUCTION

Currently many researchers are investigating bioinformation using very complex mathematical functions. Of particular interest to us is the information function defined by Shannon (1948). Both Khinchin (1957) and Shannon (1948) have investigated the properties of this information function. Brown (1976) and Gray and Davidson (1970) defined the entropy function of dynamical systems and investigated its properties. Tok (1986) defined the fuzzy information function and investigated its properties. Moreover, Newton (1970a; 1970b); Walters (1975; 2000) and Guzide (1990) (in Turkish) defined conditional sequence entropy and sequence entropy functions and investigated their properties.

In this study, we give the definition of a conditional sequence information function and prove that it exists.

First we give the some properties of dynamical systems necessary to our discussion and states the sequence information function and list its properties. The conditional sequence entropy defined by Zhang (1993). We then define the conditional sequence information function and finish with a proof of its existence.

Dynamical systems and information function: We will give very important background support and definition of dynamical system and information Function.

Definition 1: A measure-preserving dynamical system is defined as a probability space and a measure-preserving transformation on it. In more detail, it is a system (X, A, μ, T) with the following structure:

- X is a set
- A is a σ -algebra over X
- $\mu(A) \rightarrow [0,1]$ is a probability measure, so that $\mu(X) = 1$
- $T: X \rightarrow Y$ is a measurable transformation which preserves the measure μ

Definition 2: Consider two dynamical systems (X, A, μ, T) and (Y, B, ν, S) . Then a mapping $\phi: X \rightarrow Y$ is a homomorphism of dynamical systems if it satisfies the following three properties:

- The map ϕ is measurable
- For each $B \in B$, one has $\mu(\phi^{-1}B) = \nu(B)$
- For μ -almost all $x \in X$, one has $\phi(Tx) = S(\phi x)$

The system (Y, B, ν, S) is then called a factor of (X, A, μ, T) .

The map ϕ is an isomorphism of dynamical systems if, in addition, there exists another mapping $\psi: Y \rightarrow X$ that is also a homomorphism, which satisfies:

- For μ -almost all $x \in X$, one has $x = \psi(\phi x)$
- For ν -almost all $y \in Y$, one has $y = \phi(\psi y)$

Behavior of a Higher Order Difference Equation

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Abstract: In this work we study the asymptotic stability of the nonnegative equilibrium points of the difference equation $x_{n+1} = \frac{Ax_{n-1}}{B+C \prod_{i=l}^k x_{n-2i}}$, $n = 0, 1, \dots$ where A, B, C are nonnegative real numbers and

l, k , are nonnegative integers, $l \leq k$. We discuss the conditions under which there exist prime period two solutions and semicycles. Finally we investigate the oscillation and the existence of unbounded solutions.

Key words: Difference equation, periodic solution, globally asymptotically stable

INTRODUCTION

Difference equations have always played an important role in the construction and analysis of mathematical models of biology, ecology, physics, economic processes, etc^[1].

The study of nonlinear rational difference equations of higher order is of paramount importance, since we still know so little about such equations. Cinar^[2] examined the global asymptotic stability of all positive solutions of the rational difference equation

$$x_{n+1} = \frac{ax_{n-1}}{1+bx_n x_{n-1}}, n = 0, 1, \dots$$

Where a and b are nonnegative real numbers. Xiaofan yang *et al.*^[3] investigated the asymptotic behavior of solutions of the difference equations

$$x_{n+1} = \frac{ax_n + bx_{n-1}}{c+dx_n x_{n-1}}, n = 0, 1, \dots$$

Where $a \geq 0$ and b, c, d are nonnegative real numbers.

Gibbons *et al.*^[4] investigated the global asymptotic behavior of the difference equation

$$x_{n+1} = \frac{\alpha + \beta x_{n-1}}{\gamma + x_n}, n = 0, 1, \dots \quad (1.1)$$

where $\beta > 0$ and $\alpha, \gamma \geq 0$.

In this study, we study the global asymptotic stability of the difference equation

$$x_{n+1} = \frac{Ax_{n-1}}{B+C \prod_{i=l}^k x_{n-2i}}, n = 0, 1, \dots \quad (1.2)$$

where A, B, C are nonnegative real numbers and l, k are nonnegative integers, $l \leq k$.

The following particular cases can be obtained:

1. When $A = 0$, equation (1.2) reduces to the equation $x_{n+1} = 0, n = 0, 1, \dots$
2. When $B = 0$, equation (1.2) reduces to the equation $x_{n+1} = \frac{Ax_{n-1}}{C \prod_{i=l}^k x_{n-2i}}, n = 0, 1, \dots$, this equation can be reduced to the linear difference equation $y_{n+1} - y_{n-1} + y_{n-2l} + \dots + y_{n-2k} = \gamma, n = 0, 1, \dots$ by taking $y_n = x_n, \gamma = \ln \frac{A}{C}$
3. When $C = 0$, equation (1.2) reduces to the equation $x_{n+1} = \frac{A}{B} x_{n-1}, n = 0, 1, \dots$ which is a linear difference equation.
4. When $l = k = 0$, and $C = 1$ equation (1.2) yields equation (1.1) with $\alpha = 0$. For various values of l and k , we can get more equations.

Preliminaries: Consider the difference equation

$$x_{n+1} = f(x_n, x_{n-1}, \dots, x_{n-k}), n = 0, 1, \dots \quad (2.1)$$

Where $f : R^{k+1} \rightarrow R$

Definition 2.1^[5]: An equilibrium point for equation (2.1) is a point $\bar{x} \in R$ such that $\bar{x} = f(\bar{x}, \bar{x}, \dots, \bar{x})$.

Definition 2.2^[5]

1. An equilibrium point \bar{x} for equation (2.1) is called locally stable if for every $\varepsilon > 0$, $\exists \delta > 0$ such that every solution $\{x_n\}$ with initial conditions $x_{-k}, x_{-k+1}, \dots, x_0 \in]\bar{x} - \delta, \bar{x} + \delta[$ is such

Solving a system of integral equations by using some tripled fixed point theorems

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ABSTRACT A tripled fixed point theorems in ordered metric spaces is used in order to prove the existence and uniqueness of a solution for a class of integral equations. The conditions of the theorem are much weaker than those existing in literature and the theorem is useful for solving some general problems. An example to illustrate our theoretical results is also given.

1. INTRODUCTION

Fixed point theory in partial ordered metric spaces, that is, in metric spaces endowed with a partial ordering, has developed rapidly in recent years. The study of coupled fixed point theory has been considered in 2004 by Ran and Reurings [16] and in 2006 by Bhaskar and Lakshmikantham [10]. A rich literature on the existence of coupled fixed points of mixed monotone, monotone and non-monotone mappings, has been developed ever since publication of that paper (see [7], [8], [14]). Berinde and Borcut [6], introduced the concept of tripled fixed point and proved some related fixed point theorems. After that various results on the existence of tripled fixed points for various classes of mappings have been obtained, see [4], [11], [12], [13], [15]), for a selection of them.

In this paper we obtain the existence of a solution for a class of tripled integral equations in the framework of tripled fixed point theorem on partially ordered metric spaces.

2. PRELIMINARIES

In this section, we introduce notations, definitions and preliminary facts which are used throughout this paper.

Let (X, d) be a partially ordered set and d be a metric on X , with precondition that (X, d) is complete metric space. In addition, we define such a partial order in the product space $X \times X \times X$, for $(x, y, z), (u, v, w) \in X \times X \times X$,

$$(u, v, w) \leq (x, y, z) \iff x \geq u, y \leq v, z \geq w.$$

Definition 2.1. ([11]) Let (X, d) be a partially ordered set, $F : X \times X \times X \rightarrow X$ be a mapping. If $F(x, y, z)$ is monotone non-decreasing in x and z , and non-increasing in y , that is, for any $x, y, z \in X$

$$x_1, x_2 \in X, x_1 \leq x_2 \implies F(x_1, y, z) \leq F(x_2, y, z),$$

$$y_1, y_2 \in X, y_1 \leq y_2 \implies F(x, y_1, z) \geq F(x, y_2, z),$$

$$z_1, z_2 \in X, z_1 \leq z_2 \implies F(x, y, z_1) \leq F(x, y, z_2),$$

then we say that F has the *mixed-monotone property*.

Extended Hyperbolic Function and its Properties

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Abstract. Aim of this paper is to introduce extended hyperbolic function by using a modified extension of beta function [12] and to establish new properties like integral representation, Mellin transform and many more. Furthermore, we apply Prabhakar fractional integral operator, Caputo-Fabrizio operator and Atangana-Baleanu operator on it. Other than this, we present a graphical representation of the extended hyperbolic function with different values of α also a graphical comparison between Caputo-Fabrizio operator and Atangana-Baleanu operator of hyperbolic function for different values of r .

Keywords: Extended beta function; Extended Hyperbolic function; Prabhakar function; Mittag-Leffler function; Caputo-Fabrizio derivative; Atangana-Baleanu derivative.

1. Introduction

The Mittag Leffler function is a special function playing a key role in the solution of fractional order differ-integral equation. It is also used in various fields of science and engineering, eg. Random walk, Levy flights, fluid flow, etc. (see [7, 8, 9]). In one parameter, the classical Mittag-Leffler function is written as:

$$E_{\alpha}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)}, \quad (1)$$

here z is a complex variable, $R(\alpha) \geq 0$. If $\alpha = 1$, function is exponential and if $0 < \alpha < 1$, it exists between exponential and hypergeometric function $\frac{1}{1-z}$. The

A Study of the Green's Relations on n-Potent Semirings*

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Abstract. In this paper, we study the semirings which satisfy the identities $x^n \approx x$, $(2^n - 1)x \approx x$, $(x + y)^{n-1} \approx x^{n-1} + y^{n-1}$ and $(xy)^{n-1} \approx x^{n-1}y^{n-1}$. We give the characterizations of the binary relations $L \cdot \wedge D^+$, $L \cdot \wedge L^+$, $L \cdot \wedge R^+$ and $L^+ \wedge D \cdot$, and obtain the sufficient and necessary conditions which make these binary relations be congruences. Finally, we show that the classes of semirings which can be determined by the above congruences are indeed varieties of semirings.

Keywords: Green's relations; Congruences; Semirings; Varieties of semirings.

1. Introduction

By a semiring [13] we mean that an algebra $(S, +, \cdot)$ of type $(2, 2)$ such that

- (i) $(S, +)$ is a semigroup;
- (ii) (S, \cdot) is a semigroup;
- (iii) the distributive laws $x(y + z) \approx xy + xz$ and $(x + y)z \approx xz + yz$ hold in S .

The semigroup $(S, +)$ is called the additive reduct and (S, \cdot) the multiplicative reduct of the semiring $(S, +, \cdot)$. For the sake of simplicity, we use S to denote the system $(S, +, \cdot)$.

Ways to organize learning paths to discover solutions to competition problems

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ABSTRACT. In this article, we illustrate a method of organizing the process of discovering solutions to problems for mathematical contests. We describe the authors' experience in creating situations of learning individually, through cooperation and collaboration in pairs, and in small groups. The examples proposed for discussion can be considered mini-scientific works, which allow thorough research of the situation, but require detailed explanation and collaboration between students in order to refresh the supporting concepts and create generalizations.

1. INTRODUCTION

Discussions on the impact of excessive student guidance in the process of assimilating knowledge have been going on for many years. It is obvious that the dose of explanations and proofs differs from case to case. Often schools focus too much on knowledge transfer. Students usually remain passive, while the teacher strives to personally transmit the relevant material. The obsession with "passing on the material" allows for a smaller contribution from students. For this reason, we need a fundamental reorientation. The priority among teachers should not be to transfer knowledge to the students, but rather to allow students to access knowledge on their own. If students with an average level of knowledge are targeted in the teaching-learning process complete explanations are welcome. In the case of gifted student teams, the process of studying methods of solving special problems or solving complicated problems can be organized following a scheme of three steps: me \rightarrow pairs \rightarrow team. This scheme is designed in the following way: "me" \rightarrow "me and you" \rightarrow "all of us". The sequence allows for the probing of the solution or the execution of tests, particular cases. Naturally that these tests may be different for different students. In order to "shrink" the particular cases examined individually, we move on to the exploration of the problem situation in pairs. At this stage, the distribution of tasks is also accepted, if the exploration is laborious, so it is natural for students to cooperate to move faster in finding the solution. If working in pairs, the students find an elegant solution, its presentation to the whole team follows. If the pairs are far from a plausible solution, examination of the solution proposed by the authors of the problem and its presentation to the whole team follows. In this situation, students collaborate to develop the author's ideas and argue each reasoning based on their own knowledge.

We will illustrate this activity as an example of solving some problems proposed at the International Mathematical Olympiad.

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Key words and phrases. *enumerative combinatorics, solving problems strategies.*

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An algorithm for automorphisms of infinite dimensional Grassmann algebras

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ABSTRACT. Let G be the infinite dimensional Grassmann algebra. In this study, we determine a subgroup of the automorphism group $\text{Aut}(G)$ of the algebra G which is of an importance in the description of the group $\text{Aut}(G)$. We give an infinite generating set for this subgroup and suggest an algorithm which shows how to express each automorphism as compositions of generating elements.

1. INTRODUCTION

Let K be a field of characteristic zero and let A_m be the free unitary associative algebra of rank m generated by f_1, \dots, f_m . Then the m -generated Grassmann algebra G_m is defined as the factor algebra A_m/I_m such that I_m is the ideal of G_m generated by all elements of the form $f_i f_j + f_j f_i$, $1 \leq i, j \leq m$. We see that G_m is generated by $e_i = f_i + I_m$, $i = 1, \dots, m$. Clearly the Grassmann algebra G_m is of the canonical basis elements of the form

$$e_{i_1} \cdots e_{i_k}, \quad i_1 \leq \cdots \leq i_k, \quad k = 1, \dots, m$$

and 1. Note that $e_i e_j = -e_j e_i$ for all $i, j = 1, \dots, m$, since $e_i^2 = 0$ as a consequence of characteristic of K . The algebra G_m satisfies the identity

$$[[x, y], z] = (xy - yx)z - z(xy - yx) = 0 \tag{1.1}$$

for all $x, y, z \in G_m$. In particular one has $\text{ad}^2(x) = 0$ for $x \in G_m$.

The Grassmann algebra has become an important tool in many fields of mathematics as well as physics. One may see the book by Bourbaki [5] for a background. Working on the automorphism group of a given algebra has always become a remarkable approach in order to recognize and characterize the algebra. One of the works about the group of automorphisms of the Grassmann algebra is done by Berezin. Let U_m be the group of linear automorphisms and let B_m be the group of automorphisms of the form $T(e_p) = e_p + f_p(e_1, \dots, e_m)$, where f_p does not have a linear component. Berezin [4] determined the group of automorphisms of G_m as the semidirect product of the subgroups B_m and U_m when K is the field of complex numbers. Djoković [6] showed that when $\text{char} K \neq 2$, the group of automorphisms of G_m can be written as the semidirect product of the group of inner automorphisms of G_m and the subgroup of $\text{Aut}(G_m)$ which preserves the \mathbb{Z}_2 -grading of G_m . The description of the automorphism group $\text{Aut}(G_m)$ of the Grassmann algebra G_m can be explicitly found in the literature (see e.g. Laszlo [9]).

Theorem 1.1. *The group $\text{Aut}(G_m)$ of K -automorphisms of G_m is isomorphic to a semidirect product of those three subgroups.*

$$\text{Aut}(G_m) = \text{Inn}(G_m) \rtimes A_v \rtimes \text{Gl}_m(K)$$

An algorithm for automorphisms of infinite dimensional Grassmann algebras

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ABSTRACT. Let G be the infinite dimensional Grassmann algebra. In this study, we determine a subgroup of the automorphism group $\text{Aut}(G)$ of the algebra G which is of an importance in the description of the group $\text{Aut}(G)$. We give an infinite generating set for this subgroup and suggest an algorithm which shows how to express each automorphism as compositions of generating elements.

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$$\text{Aut}(G_m) = \text{Inn}(G_m) \rtimes A_v \rtimes \text{Gl}_m(K)$$

FAST ALGORITHMS OF DUALLY CHORDAL GRAPHS

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Abstract. We give a characterization of hereditary dually chordal graphs using weak decomposition. We also give a recognition algorithm for hereditary dually chordal graphs and we determine the combinatorial optimization numbers in efficient time.

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"Vasile Alecsandri" University of Bacău*

1. INTRODUCTION

The triangulated graphs (chordal) class has been noticed because of their properties. Among these properties we mention: perfection, recognition algorithms and ability to solve some combinatorial optimization problems (determining the stability number and minimum number of covering cliques) with linear complexity algorithms.

Interest for strongly chordal (M. Farber [5], see [3], [7], Strongly chordal graphs are defined in terms of a stronger ordering condition. A graph G is strongly chordal if and only if every induced subgraph of G has a simple vertex. A vertex v of the graph G is simple in G if the set $N[u] : u \in N[v]$ is linearly ordered by inclusion.) graphs arises in several ways.

Keywords and phrases: chordal graphs, dually chordal graphs, hereditary dually chordal graphs, weak decomposition, recognition algorithm.

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FUZZY UPPER AND LOWER M -CONTINUOUS MULTIFUNCTIONS

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Abstract. In this paper we introduce the notion of fuzzy upper and lower M -continuous multifunctions as generalizations of upper and lower M -continuous multifunctions [28], as fuzzy multifunctions between sets having certain minimal structures. We also prove that m -compact sets from a space with minimal structures have fuzzy m -compact images under surjective fuzzy upper M -continuous multifunctions, provided that some natural conditions are satisfied. Lastly we show that the notions of fuzzy upper and lower M -continuous multifunctions unify several forms of generalized continuity for fuzzy multifunctions from a topological space into a fuzzy topological space.

1. INTRODUCTION AND PRELIMINARIES

In the past few years, different types of fuzzy open-like sets, viz., fuzzy semiopen, fuzzy preopen, fuzzy ϑ -open, fuzzy δ -open, fuzzy δ -preopen, fuzzy α -open, fuzzy β -open have been introduced and studied by many researchers and using these concepts several types of fuzzy non-continuous functions are introduced and studied in [1], [4], [5], [14], [18], [22].

VERTICAL FOLIATION ASSOCIATED TO A CARTAN SPACE

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Abstract The cotangent bundle of a smooth manifold, as a particular submersion, carries a natural foliation called *vertical* defined by the kernel of the differential of the projection of the cotangent bundle on its base manifold. The vertical foliation is a Lagrangian one with respect to the natural symplectic structure of the cotangent bundle. It has new properties if the cotangent bundle has additional geometrical structures, for instance those induced by a non-degenerate homogeneous Hamiltonian.

A Cartan space is a manifold whose cotangent bundle is endowed with a smooth non-degenerate Hamiltonian K^2 which is positively homogeneous of degree 2 in momenta. Then the vertical foliation becomes a semi Riemannian foliation whose transversal distribution is completely determined by K and is orthogonal on the vertical distribution with respect to a semi Riemannian metric of Sasaki type. In this framework various linear connections will be associated to and some properties of the vertical foliation will be pointed out.

Reproducing Kernel for Periodic Boundary Conditions

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Abstract. In this paper, we introduced a reproducing kernel space which is a particular class of Hilbert space. We discuss various properties of the reproducing kernel. In particular, our aim is to construct kernel in reproducing kernel Hilbert space of the specific function space (Sobolev space) with the improved inner product and norm. Also, we derive the reproducing kernel for periodic boundary conditions.

Keywords: Inner product; Hilbert space; Reproducing kernel Hilbert space; Reproducing kernel; Periodic boundary conditions.

1. Introduction

Reproducing kernels were discovered during the initial stage of the twentieth century by Zarembo [20] in that effort the center of interest on harmonic function with boundary value. This was the earliest reproducing kernel with the reproducibility proved correlated with function family. Actually, in the early establishment develop of the reproducing kernel hypothesis, almost all the works were executed by Bergman [10, 11, 12, 13, 14], and most of the kernels discussed in the 1930's and 1940's are Bergman kernels. Bergman raise the conversation of the kernels with one or several variables to the harmonic functions, and utilized to solve Laplace equation. It can be stated that this is the establishment of a particular trend of reproducing kernel. Next development of the reproducing kernel theory was pushed by Mercer [19]. He invented the positive definite property of

Geometry in A-Metric Space

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Abstract. In this paper, we study the geometry of an A-metric space of Subba Rao [15], by introducing the concepts of metric betweenness and its properties t_1 , t_2 , B-linearity and D-linearity. It is proved that there do not exist equilateral triangles in any A-metric space (A, A, d) , where A is any representable autometrized algebra satisfying (R) and (S). It is also proved that any A-metric space is Ptolemaic.

Keywords: Autometrized algebra; A-metric space; Boolean metric space; B-Linearity; Contraction mapping; D-Linearity; G-metric space and lattice.

1. Introduction

In this paper, we study the geometry of an A-metric space of Subba Rao [15], where A satisfies the conditions:

$$(R): a * (a \wedge b) + (a \wedge b) = a.$$

$$(S): (a * (a \vee b)) \wedge (b * (a \vee b)) = 0, \text{ for all } a, b \text{ in } A.$$

Blumenthal [2] and Penning [6] studied the metric betweenness in a Boolean metric space and Swamy [17] studied the metric betweenness in l -groups. Subba

Thickness of oil films is affected by contact area

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Abstract—With the development of the tool machine industry, the precision and quality demand for processing is more exquisite, from the traditional industrial manufacturing equipment in the past, to the current development of high-speed, high-precision, high-efficiency intelligent automation tool machine equipment, in the face of today's globalization, customerization and environmental awareness trend.

Taking the vertical milling machine as an example, the feed system drives the machining in the direction of the tool machining to complete the cutting process. The rail contact surface of the feed system is grinding. It produces noise, bad vibration, processing rigidity is reduced, processing accuracy is reduced, friction almost thermal energy is generated, etc. Finally it reduces the service life of the servo motor. In this study, the contact between the slide rail and the slide seat was obtained by using the homemade device to obtain the influence of the contact area of the rail on the thickness of the lubricant. When the same contact area, the oil film thickness of the lower oil injection amount is small. The thickness of the oil film with higher oil injection amount is thicker. When the same oil injection volume, the thickness of the oil film of the larger contact area is small.

Index Terms—Lubrication, oil film, voltage measurement method.

I. INTRODUCTION

When machinery produces high-precision components, it needs its conditions for high precision, high speed, high efficiency, and the feed system is one of the important key systems of the tool machine. Among them, the ball screw and sliding guide as the main source of heat due to friction of the original. The effects of component heat include structural deformation and mechanism wear. In the end, the overall machining accuracy is greatly reduced.

Combined with the above factors, the advantages and disadvantages of the feed system will directly affect the overall accuracy and reliability of the tool machine, and the error factors affecting the feed system are shown in Fig. 1.

A. Oil Film Measurement Method

Mechanical component lubrication mechanism plays an important role in the joint mechanism system. In addition to the most basic lubrication supply, mechanical component cooling, but also affect the processing accuracy. Therefore, the determination of oil film thickness is very important.

Xie Qikai [1]. Used optical multi-beam interference theory to measure the thickness of the oil film, explore the

relationship between the thickness of the oil film and the resistance value, understand the relationship between the resistance value and the thickness of the oil film in dynamic situations, the faster the speed of the oil film thickness, the greater the resistance value, the larger the load, the smaller the thickness of the oil film, the smaller the resistance value. This experimental phenomenon is consistent with the Renault procedure, summarizing the above, the most affected factor is the thickness of the oil film, the oil film thickness increases its resistance value.

B. Feed System Lubrication Analysis

Lubricants provide reduced friction, resistance, cooling, cleaning, rust protection, sealing and earthquake resistance. There are many factors affecting lubricants, as illustrated in Fig. 2.

Joshia *et al.* [2], foreign scholars. Used rheometers and lubricants of different viscosity to do experiments, in which the steel ball sliding on the surface of the object to be measured. A smoother interface can be created, which reduces friction.

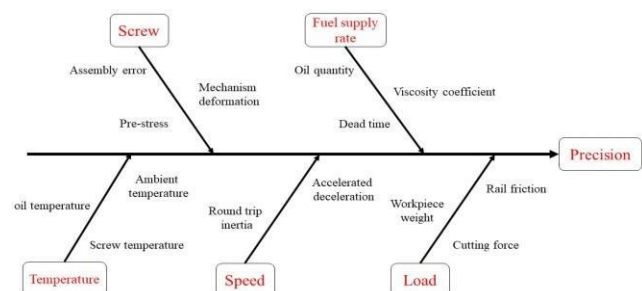


Fig. 1. Factors affecting the positioning accuracy of the feed system.

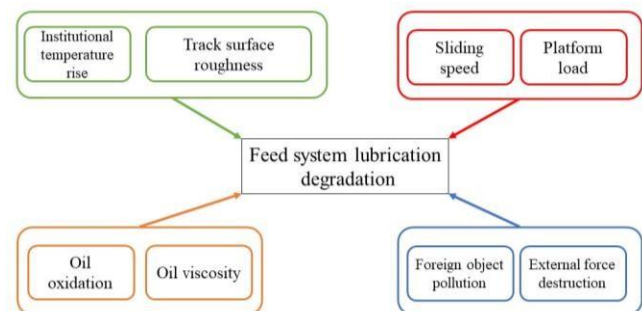


Fig. 2. Lubrication degradation factors of feeding system.

C. Feed System Friction Analysis

The motion mode of feed system drives the ball screw to transmit power to sliding track and sliding seat by servo motor, which forms reciprocating friction action. Therefore, lubricants play an important role in this area, providing benefits such as cooling, corrosion prevention and good sliding, as shown in Fig. 3.

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The validation limits for the SRT-MRT Lattice Boltzmann Method for Simulating Single-Phase Flows are limited.

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Abstract—The multi-relaxation time (MRT) Lattice Boltzmann method (LBM) was developed to overcome several constraints, which are inherent to the more famous single relaxation time (SRT) Bhatnagar–Gross–Krook (BGK) model. Constraints, such as fixed Prandtl number, fixed ratio between kinematic and bulk viscosity, and Reynolds number limitations undermine the SRT usefulness. Furthermore, the SRT method fails to accurately characterize high viscosity fluids' behavior near the domain's walls, an issue which can be circumvented with the MRT method. However, the MRT requires a careful selection of its relaxation parameters for achieving the desired outcome. The ad-hoc nature of this selection makes the method cumbersome, especially for three-dimensional (3D) domains. Additionally, it is known that the MRT solution requires about 10% - 15% more computational time than the SRT for the same domain size.

Four widely used single-phase flow conditions were explored by using the SRT and the MRT methods. It is shown that the SRT has good accuracy when used for simulating low viscosity fluid cases; however, the SRT exhibits a non-physical velocity jump at the domain surface boundaries when used for simulating high viscosity fluid flows. This issue can be resolved by augmenting the SRT domain's height, which in turn leads to an increase in the required computational time. The main advantages of the MRT are due to its capability in overcoming the velocity jump in most of the high viscosity fluid cases and in its ability to simulate flows with ultra-low viscosities, which was demonstrated in the characterization of the flow around S822 airfoil with Reynolds number $Re \approx 40,000$.

Index Terms—Lattice Boltzmann, multi-relaxation time LBM, BGK, parabolic flow, S822 airfoil, drag and lift.

I. INTRODUCTION

The MRT LBM was introduced by D'Humières [1] to overcome defects inherent to the Lattice gases, which suffered from important statistical noise due to averaging Boolean variables for calculating the macroscopic variables. At the time, when several researchers simulated the motion of particles by their occupation number rather than their Boolean occurrence and used a relaxation process towards equilibrium prescribed by the kinetic theory, D'Humières suggested the addition of new degrees of freedom for the choice of equilibrium distribution.

Since its inception, the MRT LBM presented an interesting simulation platform, which attracted the attention of several researchers, who tried to analyze, further develop and use it for simulation cases, which were inaccessible to the SRT LBM users. Lallemand and Lue [2] obtained a generalized hydrodynamics (wave vector dependence of the transport coefficient) by solving the dispersion equation of the linearized lattice Boltzmann equation either analytically or numerically. The authors applied the concept for selecting the adjustable parameters to optimize dispersion, dissipation, anisotropy and the Galilean invariance of their model. The generalized hydrodynamics was used to study the stability of two-dimensional shear flow with shock, in which the simulation results matched their theoretical analysis. D'Humières *et al.* [3], extended the MRT method to D3Q15 and D3Q19 three-dimensional domain, to simulate lid-driven cavity flow for Reynolds numbers up to $Re = 2000$. J.-S. Wu, Y.-L. Shao [4] simulated two-dimensional near-incompressible steady lid-driven cavity flows with Reynolds number between 100 and 7500 by using MRT and BGK models. The results were compared with Navier-Stokes simulation results for the same flow domain and flow conditions. The authors reported that the MRT was able to improve the solution convergence, to decrease the spatial oscillations near sharp edges as well as it was successful in simulating high Reynolds number cases. The improvements were due to the different relaxation rates used for different physical modes, which were embedded in the MRT scheme. Rui *et al.* [5] proposed an incompressible MRT LBM, with the equilibria in momentum space were derived from a previous BGK model for incompressible flow proposed by Guo *et al.* [6]. The Model was successfully applied to steady state Poiseuille flow, cavity driven flow and double shear flow in 2D domains. Jafari S. and Rahnama M. [7] used the generalized lattice Boltzmann equation for the computation of turbulent channel flow and compared successfully their results for mean velocity distribution, turbulent statistics and vortical structures with the large eddy simulation with shear-improved Smagorinsky model for the subgrid-scale turbulence effects. The model showed good numerical stability and ease in parallelization.

E. Aslan *et al.* [8] studied the classical case of the two-dimensional lid cavity for incompressible steady laminar flow using the SRT and the MRT methods. For high Reynolds numbers ranging between 200 and 2000, the results were compared with the finite-volume predictions of the incompressible Navier-Stokes equations. The MRT showed more stable results than the SRT for high Reynolds numbers. The authors compared the convergence speed between MRT and SRT within the stability range, and they

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Graphene nanocomposites can be synthesised with great efficiency

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ABSTRACT: Graphene consists of a monolayer of sp^2 bonded carbon atoms and has attracted considerable interest over recent years due to its extreme mechanical, electrical, and thermal properties. Graphene nanocomposites have naturally begun to be studied to capitalize upon these properties. A range of complex chemical and physical processing methods have been devised that achieve isolated graphene sheets that attempt to prevent aggregation. Here we demonstrate that the simple casting of a polymer solution containing dispersed graphene oxide, followed by thermal reduction, can produce well-isolated monolayer reduced graphene oxide. The presence of single layer reduced-graphene oxide is quantitatively demonstrated through transmission electron microscopy and selected area electron diffraction studies and the reduction is verified by thermogravimetric, X-ray photoelectron spectroscopy, infrared spectrum, and electrical conductivity studies. These findings provide a simple, environmentally benign and commercially viable process to produce reduced-graphene oxide reinforced polymers without complex manufacturing, dispersion or reduction processes

KEYWORDS: Graphene oxide, nanocomposite, dielectrics, electrical conductivity, TEM, thermal reduction

The inclusion of nanoscale particles into a matrix material can lead to orders of magnitude enhancement in the mechanical, electrical, optical, and thermal properties relative to the neat polymer. These significant improvements can be achieved with a relatively low loading of the nanofiller due to the high surface area to volume ratio. Graphene has drawn significant interest in recent years for polymer nanocomposites due its high specific surface area ($2600 \text{ m}^2/\text{g}$) and enormous mechanical, electrical, and thermal properties.¹⁻⁴ The modulus and fracture strength of single layer graphene membranes have shown values of $\sim 1 \text{ TPa}$ and $\sim 130 \text{ GPa}$, respectively, with 25% strain at failure.² The thermal conductivity has been estimated to be $4840\text{--}5300 \text{ W/mK}$ through analysis of the shift in the Raman G peak with increasing incident laser power.³ Graphene has also been shown to have ballistic electron transport with electron mobility as high as $15\,000 \text{ cm}^2/(\text{V sec})$.⁴ The results of these studies have clearly demonstrated the potential for graphene to result in materials and devices with extraordinary properties.

Various processing methods have been investigated for producing graphene-reinforced nanocomposites; however the majority rely on graphene oxide as the starting material due to

thus significant research has been performed to investigate methods to produce polymers with reduced graphene oxide (RGO) sheets.⁸

The majority of the research in the field has focused on GO^{9-11} or performed reduction of the GO prior to its dispersion into the polymer, which yields nanocomposites with multilayer platelets rather than single layer sheets.¹²⁻¹⁸ Three primary methods are used for the synthesis of reduced

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challenges associated with producing large scale quantities of isolated pristine graphene sheets. Recent results have shown the direct exfoliation in highly polar organic solvents such as dimethylformamide (DMF)⁵ and N-methylpyrrolidone (NMP)⁶ by sonication or in chlorosulfonic acid⁷ through simple dissolution, but these methods are not currently suited for polymers since the colloidal suspensions cannot support high graphene concentrations and the stability of the mixture strongly depends on the surface energy of the solvent.⁶ The highly oxidized nature of GO interrupts the electrical properties of the material and

SYNTHESIS OF AMINO-DERIVATIVE FROM THYMOQUINONE EXTRACTED FROM NIGELLA SATIVA AND ITS SPECTRAL CHARACTERISATION

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Abstract

Thymoquinone (TQ) is a bioactive constituent of (*Nigella sativa*) black seed oil. TQ shows potential pharmacological properties against numerous diseases. It exhibits wonderful antioxidant, anti-inflammatory, anticancer, and other important biological activities. Thymoquinone (TQ), also known as 2-isopropyl-5-methyl-1,4-benzoquinone effectively extracted HPLC and compared to the standard. It is a solid bright yellow compound having scaly crystals with a melting point of 49–50 °C and gives a characteristic intense smell of pepper. It gives an in detail studied of spectrum and the synthesis of amino derivative form TQ. Its purification, characterization by FTMS, IR, ¹HNMR, ¹³CNMR and synthesis of its amino derivative (ATQ) is reported along with characterization by LCMS, IR, ¹HNMR and ¹³CNMR. Finally, the present status of adjuvant potency of TQ and its characterisations are summarized.

Keywords: Nigella sativa, Thymoquinone, antioxidant, anti-inflammatory, anticancer

Isolation of Thymoquinone :

Thymoquinone (TQ), also known as 2-isopropyl-5-methyl-1,4-benzoquinone, obtained from seeds of *Nigella sativa* ¹¹⁻¹³ is an important constituent of oil. Through high performance liquid chromatography (HPLC), Ghosheh and co-workers developed the method for the analysis of the oil of *Nigella sativa* seeds. The constituents from the oil were separated by using C18 mini columns and quantification of these recovered constituents by HPLC was completed on a reversed-phase μ Bondapak C18 analytical column⁴. Isocratic mobile phase of water:methanol:2-propanol (50:45:5% v:v) at flow rate of 2 ml/min and 254 nm radiation was used for detection of TQ.

Isolation of TQ from seeds of *Nigella sativa* by subjecting 25 g of finely powdered seeds to Soxhlet extractor with hexane and solvent was separated under vacuum followed by stream of nitrogen⁵. The extract was encumbered on silica gel column and eluted with diethyl ether, hexane, 15% diethyl ether in hexane and methanol 500 mL each and analyzed on HPLC after evaporation and reconstitution in methanol. HPLC analysis showed 659 mg/g in 15% diethyl ether in hexane fraction, and 367 mg/g of thymoquinone in hexane fraction⁶. Supercritical fluid carbon dioxide extraction (SCFE-CO₂) of *Nigella sativa* oil at 150 bar and 40°C for 120 min produced 4.09 mg of thymoquinone per ml of CO₂ extract as reported by Solati.

HPLC Extraction of TQ from *Nigella sativa*

Extraction of TQ from commercially available *Nigella sativa* oil was performed by sonication as this is reported by Velho-Pereira and colleagues. *Nigella sativa* oil was obtained for the

IoT based Smart Irrigation System using Soil Moisture Sensor and ESP8266 NodeMCU¹A.Arshya Fathima, ²Dr.K.Tanveer Alam, ³Dr. T.Syeda Jeelani Basri, ⁴Syed Faiazuddin¹Lecturer in Physics, St. Joseph Degree College, Kurnool, (AP), India²Assistant Professor, Department of Electronics and communication, Rayalaseema University, Kurnool, (AP), India³Associate Professor, Department of Chemistry, G Pullaiah Engineering College and Technology(A), Kurnool, AP, India⁴Lecturer in Computer Science, Silver Jubilee Government Degree College, Kurnool, (AP), India**Abstract:**

We are going to construct a smart agricultural monitoring system which can collect crucial agricultural data and send it to an IoT platform called Ubdots Clouds in real time where the data can be logged and analyzed. IoT based Smart agriculture system is an developing technology, where its data from small to large scale and its surrounding are collected using smart electronic sensors. It also helps minimize depletion by using solenoid valves which are automatic controlled by IoT technology. IoT is a shared network of objects or things which can interact with each other provided the Internet connection. Using IoT we can directly send the collected data to a central server in real time. This complete system works only when this embedded device interacts with smartphone Ubdots cloud application. When programming the device, we can include id and password in it. This id and password should match with id and password of smart phone wifi id and password. Then only system can work and information transmission is possible in between embedded device and Ubdots cloud. Since we have automated the date collection, the data integrity is assured and since the data processing is done using computers, experts may get advanced analytical software tools to draw most accurate predictions. The collected data are analyzed by experts and local farmers to draw short term and long term conclusion on weather pattern, soil fertility, current quality of crops, amount of water that will be required for next week to a month etc.

Keywords: Node MCU, IoT, Ubdots Clouds, Relay section, Soil moisture sensor, Submersible pump

I. Introduction:

IoT plays an important role in agriculture industry which can feed 10 billion people on the Earth by 2050. We can take smart farming a step further by automating several parts of farming, for example smart irrigation and water management. We can apply predictive algorithms on microcontrollers or SoC to calculate the amount of water that will be required today for a particular agriculture field. As a part of the system development, few sensors applied such as: a soil moisture sensor to detect the water level in soil; These sensors are connected to a Wi-Fi

Oxidation Mechanism And Kinetic Effect of EthyleneDiamine Tetra Acetic Acid (EDTA) By Bromoamine-T in pH Medium

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Abstract

Kinetics and mechanism studies of the oxidation of ethylene di amine tetra acetic acid (EDTA) by bromamine-T (BAT) in acetic buffer of pH 5 have been investigated. The reaction showed first order in [BAT] and fractional order in[EDTA] and [H⁺]. Addition of reaction product (toluene sulphonamide) or varying the ionic strength of medium has no effect on the rate. A mechanism involving electrophilic attack by positive halogen of BAT at neutral nitrogen of EDTA was proposed.

Keywords: Kinetics, Mechanism, Oxidation, bromamine, ethylene diamine tetra acetic acid.

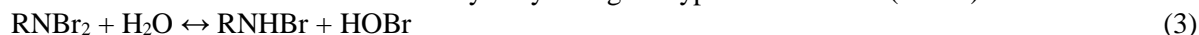
INTRODUCTION

N-bromo toluene sulphonamide (Bromamine-T, BAT) was introduced as analytical reagent for estimation of various reactants in aqueous media¹, and an active oxidant for the oxidation of amino acids².

Bromamine-T is analogous to chloramines-T³⁻⁴ and Bromamine-B⁵⁻⁶ CH₃C₆H₅SO₂NHBr(RNHB⁺)⁷, and behaves like a strong electrolyte in aqueous solution. The anion CH₃C₆H₅SO₂NBr⁻, (RNBr⁻) picks up a proton



The dichloramine-T and the free acid hydrolyse to give hypobromous acid (HOBr)



The reactive species HOBr ionizes as



K_a = 2.0 x 10⁻⁹ at 250C

The present article reports our observation on the kinetics of oxidation of ethylene diamine tetra acetic acid by BAT in acetate buffer of pH 5, little is known about the kinetic and mechanism of its oxidation by various oxidants, the oxidant so far tried for the investigation was Ce(IV)⁸⁻⁹, chloramines-T¹⁰, iron III¹¹ and sulfuric acid¹².

EXPERIMENTAL

A recrystallised BAT compound¹³⁻¹⁴ was used. Solution of BAT was freshly prepared, because decomposition occurs on standing or exposure to light, and for this purpose a brown volumetric flask was used. All UV kinetic measurements were performed using a Py-Unicam PV 8700UV / Vis. Spectrophotometer.

Characterization, Molecular Modeling And Antibacterial Activity Study Metal complexes Of Schiff base derived from 3-Bromo, 5-Chloro Salicyldehyde With Alanine

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Abstract- Biologically active tridentate Schiff base ligand derived from 3-bromo-5-chloro salicyldehyde with alanine (DL-Alanine) and their Fe(II), Co(II), Ni(II) and Cu(II) complexes have been synthesized and characterized by physical and spectroscopic techniques. The vibrational spectrum suggests that the Schiff base ligand coordinated to the metal ions in a tridentate manner with ONO donor sites of the nitrogen atom of the imine group, oxygen atom of carboxylate group and with phenolic oxygen to give an octahedral geometry. TOF-Mass spectrum explains the successive degradation of the molecular species and justified ML₂ complex. Electronic spectra and magnetic properties of the complexes are consistent with the proposed octahedral geometry. The structure optimization by MM2 calculation supports an octahedral geometry of the complexes. The preliminary *in vitro* antibacterial activity of all the complexes at two different concentrations was screened against four bacterial pathogens namely, *Streptococcus*, *Salmonella typhi*, *Staphylococcus aureus* and *Escherichia coli* showed moderate activity and slightly higher compared to the ligand.

Index Terms - Antibacterial activity, Metal complexes, Molecular modeling, Schiff base, Spectral studies.

1. INTRODUCTION

Schiff bases derived from an amino and carbonyl compound are important class of ligands that coordinate to metal ions via azomethine nitrogen played a significant role in the development of coordination and bioinorganic chemistry and are considered remarkable responsible for antibacterial, antitumor, antifungal, anticancer, diuretic and herbicidal activities [1]. It has been widely used as dyes and pigments, catalysts, polymer stabilizers [2],

luminescence chemo sensors [3] and intermediates in organic synthesis [4]. Schiff base can also be used as corrosion inhibitors for different metal-electrolyte systems, since they adsorb and form a corrosion-mitigating surface film through their electron-rich centers, including the imine moiety, this moiety can offer strong bonding with metallic ions because of its π -acceptor properties [5]. Moreover, several studies addressed the tribiological activities of Schiff bases and their role as biolubricant additives [6]. Additionally, the use of Schiff bases as catalysts in fixation of CO₂ to mitigate its accumulation in the atmosphere has been widely studied [7].

The improved biological properties of metal complexes over their precursor ligands, chelation leads to formation of a more stable metal organic framework, since chelation improves the lipophilicity of the compounds [8]. The choice of metal connectors and the bridging ligands permits the utilization of these materials in areas, heterogeneous and biomimetic catalysis; sensor technologies; luminescence; drug delivery and proton conductivity [9]. Bioinorganic chemistry also focus upon, the function of inorganic substances in living systems, including the transport mechanism, speciation and mineralization of inorganic materials and also the use of pharmacotherapy and diagnosis. These substances can be metal ions complexed ions, coordination complexes or inorganic molecules [10]. The chelating property of Schiff bases plays a significant role in its antioxidant activity and this could be helpful in the development of compounds with anticancer activity in transition metal complexes [11].

Schiff base ligands containing nitrogen and oxygen donor atoms are considered structural model of

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Available online 1 April 2020

Abstract

Spray pyrolysis of di-*n*-butyltin(IV) diacetate (DBTDA) has led to the deposition of [200]-oriented SnO₂ film on a glass substrate. In order to clarify growth mechanism of the preferential orientation the sprayed SnO₂ thin film has been investigated by using the atomic force microscopy and the X-ray photoelectron spectroscopy. The results have suggested that the sprayed solution forms the SnO₂ small particles on the glass substrate and they spread overall relatively soon. At the very early stage each particle grows with almost the same rate and only its density increases with no change in a surface roughness.

Keywords: SnO₂ thin film; Spray pyrolysis; Preferential orientation; Nucleation; Film growth; AFM; XPS

1. Introduction

Tin(IV) oxide (SnO₂) is an n-type semiconductor material with wide band gap energy, high donor concentration and large mobility [1]. The material is transparent in the visible and reflective in the infrared regions. Thus, the SnO₂ thin films have been utilized as transparent electrodes in sophisticated electronic devices [2–4]. The material also has an advantage in availability of constituent atoms different from ITO (indium tin oxide).

We have reported a deposition of highly oriented SnO₂ thin films on a glass substrate from the organotin compounds by using a spray pyrolysis technique. The results indicated that the (200)- and (110)-oriented thin films were prepared from (C₄H₉)₂Sn(OOCCH₃)₂ (DBTDA) [5] and (C₄H₉)₄Sn (TBT) [6], respectively. Two chemical species, O-Sn-O and Sn, relevant to deposition of the oriented thin films were produced in majority through the pyrolysis of DBTDA and TBT, respectively [7], with which the oriented growth can be attributed to a matching between the atomic configuration and each crystalline plane [8].

Spray pyrolysis, one of the well-known chemical techniques applied to form a variety of thin films such as noble metals, metal oxides and chalcogenide compounds, results in good productivity from a simple apparatus. The spray pyrolysis is a process in which a thin film is deposited by spraying a solution on a heated substrate where the constituents react to form a chemical compound. The chemical reactants are selected so that products except the desired compounds are volatile at the temperature of deposition. We call this technique an SPD (spray pyrolysis deposition) method. One successful application of the technique is in the large-scale formation of CdS thin films for solar cells [9].

In the present study, we have observed initial growth stages of the SnO₂ thin film sprayed on a glass substrate by using the atomic force microscopy (AFM), and measured photoelectron signals from both the film and the substrate by using the X-ray photoelectron spectroscopy (XPS) to clarify the initial growth process of the [200]-oriented SnO₂ thin film.

2. Experimental

2.1. Formation of SnO₂ thin film

Di-*n*-butyltin(IV) diacetate (DBTDA) (N 95% purity) was used as a starting compound. It, with no further purification,

Nanosized glass frits as an adhesive promoter for ink-jet printed conductive patterns on glass substrates annealed at high temperatures. **

By B.Suneetha, B.NagaLatha, G.Pullaiyah College of Engineering & Technology, Kurnool, Govt Medical College, Kadapa

Ink-jet printed metal nanoparticle films have been shown to anneal at high temperatures (above 500 °C) to highly conductive metal films on glass or ceramic substrates, but they suffer from cracking and inadequate substrate adhesion. Here, we report printable conductive materials, with added nanosized glass frit that can be annealed at 500 °C to form a crack-free dense microstructure that adheres well to glass substrates. This overcomes the previous challenges while still retaining the desired high film conductivity. Controlling the particle characteristics and dispersion behavior plays an important role in successfully incorporating the glass frit into the conductive inks.

1. Introduction

In recent years, increasing attention has been given to the development of convenient and low-cost processing techniques for the fabrication of conductive features such as electrodes, conductive lines, and interconnects for use in modern electronic, electro-optic, and photovoltaic applications. Although photolithography and electrochemical deposition have been widely adopted in the microfabrication of conductive features, they are time-consuming, complicated, and expensive.^[1,2] Therefore, there is a need for direct digital printing techniques that are simpler and more economical. One of the most promising alternatives is ink-jet printing technology, which is suitable for direct write of patterns and which can deliver precise quantities of materials.^[3–9]

Most previous work on the fabrication of conductive patterns using ink-jet printing technology has focused on solution-processable conductive materials that can ensure high thin-film conductivity ($>10^5 \text{ S cm}^{-1}$) at low annealing temperatures ($<200 \text{ °C}$) suitable for low-cost plastic electronics. Candidate conductive materials include doped conjugated

polymers such as polyanilines,^[10] polypyrroles,^[11] and PEDOT.^[12] However, they are characterized by low electrical conductivity (typically 10^2 S cm^{-1}) and poor electrical and thermal stability. Metal nanoparticles, on the other hand, have depressed melting points – owing to surface effects – and hence can be annealed to conductive films at temperatures com- patible

with plastic electronics ($<200 \text{ °C}$). Nanoparticles of noble metals such as gold^[13–15] and silver,^[16,17] which possess high electrical conductivity (on the order of 10^5 S cm^{-1}) and operational stability, have been used for the direct writing of conductive elements in printed electronics.

However, a number of challenges remain, despite successful applications of this technique. Thin films of these materials tend to crack during annealing due to the large intrinsic volume reduction that accompanies complete sintering of the nanoparticles, resulting in weak substrate adhesion and poor cohesion within the metal films. These problems are aggravated if the conductive features are annealed at very high temperatures ($>400 \text{ °C}$). There are several technologically important applications involving glass or ceramic substrates that demand high-temperature annealing, such as plasma panel displays (PDP), solar cells, ceramic MEMS, microelectronic packaging, and sensors. Polymeric materials and resins present in most commercial conductive inks usually no longer serve as binders after high-temperature heat treatment. Cracking and poor substrate adhesion of the conductive films should be prevented in order to achieve optimal performance and reliability in printed conductors.

In the present work, we developed silver nanoparticle-based ink-jet-printable ink that is suitable for high-temperature annealing. Our approach was to incorporate a nanosized glass frit as an adhesion promoter within the ink (Fig. 1). The glass frit was required to be sufficiently small so as not to clog the nozzle and needed to have an appropriate glass transition temperature (T_g) to melt during annealing, so as to improve