Contents lists available at ScienceDirect

Materials Today: Proceedings

journal homepage: www.elsevier.com/locate/matpr

Synthesis, biological evaluation and molecular docking studies of heterocycle encompassed benzoxazole derivatives as antimicrobial agents

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ARTICLE INFO

Article history:
Available online xxxx

Keywords:
Benzoxazole
Cyano acrylate
Antimicrobial activity
MIC
Molecular docking

ABSTRACT

Novel heterocycles containing benzoxazole nucleus have been synthesized from ethoxy cyano acrylate. All the synthesized molecules were subjected to structural elucidation using spectrometric and spectroscopic characterization using analytical proton NMR (^{1}H), carbon NMR (^{13}C), Fourier transform Infrared spectroscopy (FT-IR) and Liquid chromatography Mass spectrometry. *In silico docking* studies were carried out to investigate the structural insights into the binding mode to evaluate antimicrobial potency. The docking results against the X-ray crystallographic structure of Staphylococcus aureus UDP-N-acetylenolpyruvylglucosamine reductase (MurB) (PDB ID: 1HSK) protein have shown minimum binding energy of −6.1, −7.6, −7.1, −7.8, and −8.2 for 1A, 2A, 3A, 4A, and 4B molecules respectively. Among which, **4A** and **4B** molecules have evolved as potential antimicrobial agents from initial screening of the molecules against fungi, gram-positive, and gram-negative bacteria using the agar well diffusion method and minimum inhibition concentration technique.

Selection and peer-review under responsibility of the scientific committee of the Web International Conference on Accelerating Innovations in Material Science – 2020.

1. Introduction

A large number of Heterocyclic molecules being used as drugs in the field of medicinal chemistry [1-3]. Benzoxazole is one of the widely investigated heterocyclic molecules as an antimicrobial [4,5] and antioxidant [6] agent. Some of the derivatives of benzoxazole are also screened for anti-diabetic and anti-inflammatory studies. literature has revealed that substituted benzoxazoles and related heterocycles are biologically active with lower toxicities [7,8] and also shows *in-vitro* enzyme inhibitory activity [9]. To improve memory and learning, some phenyl substituted benzoxazole derivatives found as interesting acetylcholinesterase inhibitor along with the capacity to inhibit the oxidation process [10]. Benzoxazole derivatives are also studied as anti-breast cancer agents for the new generation [11]. According to the literature survey the heterocycles containing pyrazole moiety shows excellent antimicrobial as well as anti-cancer activity [12-17]. Some of the heterocyclic encompassed benzoxazole molecules were synthesized and reported as biological potent molecules [6,18-20]. Considering all the above therapeutic uses of benzoxazole molecules and the effective antimicrobial nature of functionalities like aminopyrazole [21] and halogens [22-24], it was planned to synthesize halogen containing heterocycle encompassed benzoxazole molecules by ethoxy cyano acrylate, as depicted in Scheme 1.

The synthesized molecules were screened for *in silico* antimicrobial studies against target Staphylococcus aureus UDP-N-acetylenolpyruvylglucosamine reductase. *In silico* studies plays major role in predicting the best conformation considering lowest binding energy and the number of hydrogen bonds. Based on docking studies, all the molecules were subjected to *in-vitro* antimicrobial investigation.

2. Experimental

2.1. Chemistry

Trimethyl silane (TMS) was used as reference standard for ^{1}H and ^{13}C NMR spectral analysis with ▫ values as ppm. Bruker

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https://doi.org/10.1016/j.matpr.2021.05.671
2214-7853/© 2021 Elsevier Ltd. All rights reserved.
Selection and peer-review under responsibility of the scientific committee of the Web International Conference on Accelerating Innovations in Material Science – 2020.

Please cite this article as: M. Rodrigues, B.S. Sharath, B. Bennehalli et al., Synthesis, biological evaluation and molecular docking studies of heterocycle encompassed benzoxazole derivatives as antimicrobial agents, Materials Today: Proceedings, https://doi.org/10.1016/j.matpr.2021.05.671

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Materials Today: Proceedings
Available online 23 March 2021
In Press, Corrected Proof

Tribological properties of areca sheath fiber composites

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https://doi.org/10.1016/j.matpr.2021.02.689

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Abstract

Polymer composites with different fiber fractions 0, 12, 24, 36 and 48 wt% of short areca sheath fibers were prepared and the relative effect on its physical, mechanical and tribological characteristics were examined. From the investigation it is found that the theoretical or the measured density decreases with increase in the fiber concentration. On the other hand, void fraction increases with the increase in the fiber concentration. An optimum values of investigated mechanical properties such as the hardness (72.56 HRB), Young's modulus (1.98 GPa), and the Impact strength (4.724 J) have been observed with the increase in fibre fraction. Furthermore, the flexural strength, flexural modulus and the tensile strength get decreased with the increase in the fibre fraction. The abrasion test is conducted to study the tribological behavior of the specimens implementing Taguchi orthogonal array (L_{25}) and the variance analyzing techniques. The tribological study has shown that 36 wt% specimen experiences minimal wear rate at a higher sliding velocity of 1.2 m/s. The wear rate of all the composites is fairly minimal at higher sliding velocities and during the application of lesser normal load. The coefficient of friction (COF) increases up to a distinct value relating to sliding velocity and normal load. Further rise in the sliding velocity or normal load will result in the drop of COF.

Keywords

Polymer; Areca sheath fiber; Void fraction; Fiber fraction; Abrasive wear; Taguchi analysis

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IOP Conf. Series: Materials Science and Engineering 1065 (2021) 012020 doi:10.1088/1757-899X/1065/1/012020

Physical, chemical and surface morphological characterization of single areca sheath fiber

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Abstract: The technological advance in various streams necessitated the increased demand for lesser weight and minimal cost materials. The concerns to ensure environmental sustainability, those newer materials were expected to be decomposable. In the current study, chemical, physical and mechanical and morphological aspects of areca sheath/frond fiber are investigated. It is observed that, the cellulose, hemicelluloses and lignin wt. % are 65.02, 8.26 and 18.62 respectively. The XRD study confirms the percent crystallinity of 81.33% and the crystallinity index of 0.77. The fiber further exhibited the tensile strength of 59.62±2.20 MPa. The TGA study reveals the higher degradation rate at 322.2 °C and the residual mass at 500 °C is 33.23%. The morphological study is done through scanning electron microscopy (SEM). The other properties such as density (0.9 g/cm^3), the fiber length, diameter, and moisture uptake are also reported. From the very promising results, the fiber can be used as a reinforcement agent and the composites may find potential applications in automobile panels, interiors, structural light weight bearing sheets, etc.

1. Introduction:

The propensity to save the environment can be witnessed with great amount of eco-friendly approaches by the human beings. The vivid research activities in the field of natural fiber composites during the recent past few years can be attributed to it [1-3]. The inclination towards the natural fibers as a reinforcement in the polymer composites is because of its intrinsic qualities viz., reduced weight,

Materials Today: Proceedings 44 (2021) 4972–4975

Contents lists available at ScienceDirect

Materials Today: Proceedings

journal homepage: www.elsevier.com/locate/matpr

Effect of fiber fraction on the physical and mechanical properties of short areca sheath fiber reinforced polymer composite

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ARTICLE INFO

Article history:
Received 7 December 2020
Received in revised form 14 December 2020
Accepted 21 December 2020
Available online 13 February 2021

Keywords:
Polymer
Areca sheath fiber
Void fraction
Fiber fraction
Mechanical properties
Physical properties

ABSTRACT

The fiber fraction in a composite will have a significant influence on its behavioural aspects and is reported in the current study. With different fiber fractions (0, 12, 24, 36 and 48 wt%) of the areca sheath fiber reinforcing agent, composite specimens were prepared and its physical and mechanical properties were examined. The measured density of the neat epoxy to the higher fiber fraction composite specimen (48 wt%) varies from 1.147 to 0.9524 g/cm^3, from which it is evident that the density decreases with increase in the fiber concentration. On the other hand, void fraction for a neat epoxy is 0.26% which increases with the increase in the fiber concentration and is 6.14% for the 48 wt% fiber loaded specimen. An optimum values of investigated mechanical properties such as the hardness (72.56 HRB), Young's modulus (1.98 GPa), and the Impact strength (4.724 J) have been observed with the increase in fibre fraction. The flexural strength for the neat epoxy is 46.28 MPa starts decreasing with the inclusion of fibers and reaches 12.05 MPa at a higher fraction of 48 wt%. The similar declining behaviour may be observed for the flexural modulus of 0.26 GPa and tensile strength of 14.02 MPa at high fiber fraction.

Selection and peer-review under responsibility of the scientific committee of the International Conference on Advances in Materials Processing & Manufacturing Applications.

1. Introduction

In the current years, many conventional materials being used in automobiles, structural applications, etc., have been replaced by the very promising novel materials and fiber reinforced composites have a major contribution in this regard. The fibers used in such composites are of natural and synthetic types. Natural fibers have a very interesting history as these were being used in the manufacture of ropes, mats, cushions, baskets, etc. Now the same fibers have made headway in the manufacturing of fiber reinforced composites too [1]. The natural fibers like sisal, hemp, banana, flax, cotton, etc., due to their abundant availability, very low cost, less weight, less damage to the processing equipment, good relative mechanical properties and biodegradability, has attracted the considerable attention of manufacturers [2–5]. The cons of these fibers have to be addressed properly to make the best use of its good qualities. As the fibers contain cellulose, hemicelluloses, lignin, pectin and other waxy substances, it is having an affinity to absorb moisture from the surroundings. Moisture absorption will cause the fibers in weak binding with the polymer matrix. Another challenge is the coupling between the fiber and the polymer. This issue can be addressed with the surface modification techniques which improves the interfacial strength between them. Among the different surface modification methods, few are under the customary practice and proved to be the better ones, viz., alkaline treatment, silane treatment, and the acetylation. The untreated as well as the treated fibers have been tested under different experimental conditions for their compatibility with the matrix materials by various authors and the fibers like sisal [6], jute [7], abaca [8], soybean [9], oil palm [10], hemp [11], flax [12], bamboo [13], henequen [14] etc., are well recognized and have been used as reinforcement in designing polymer composites. Areca sheath natural fibers also finding a niche in the dilating field of natural fiber reinforced composite materials and the study on its promising features are ongoing.

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https://doi.org/10.1016/j.matpr.2020.12.892
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Selection and peer-review under responsibility of the scientific committee of the International Conference on Advances in Materials Processing & Manufacturing Applications.

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Materials Today: Proceedings 45 (2021) 4763–4767

Contents lists available at ScienceDirect

Materials Today: Proceedings

journal homepage: www.elsevier.com/locate/matpr

Tribological studies of epoxy composites using surface modified areca sheath fibres

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ARTICLE INFO

Article history:
Available online 19 February 2021

Keywords:
Areca sheath epoxy composite
Surface modification
FESEM analysis
Tribological study
Wear testing

ABSTRACT

Natural fibre composites has its application in automobile industries and in structural applications. The major drawback is the failure of the machineries because of wear under friction. Current work is on tribological behavior of areca fibre-epoxy composites. Surface modification of the fibre was done using 1% alkali, 0.5% $KMnO_4$, 4% $(C_6H_5CO)_2O_2$ and 1% $C_{17}H_{35}COOH$. FTIR and FESEM analysis confirmed surface modification of fibres after chemical treatment. Wear testing was studied at different sliding speed of 1.88, 3.77 and 5.65 m/s under 10, 20 and 30 N of load. Studies proved that: least wear rate were observed in composites with fibres, which were treated with 1% $C_{17}H_{35}COOH$. As the sliding speed and applied load increased, wear rate exhibited by composites increased. The FESEM micrograph for samples after tribological study is reported.

Second International Conference on Aspects of Materials Science and Engineering (ICAMSE 2021).

1. Introduction

In the current world; focus being on environment and sustainability, the synthetic fibre composites are gradually replaced by natural fibre composites because of their disadvantages like greater density, high cost, non-renewable source of origin and its non-biodegradability. Scientists are targeting more on bio-based products as a substitute for synthetic fibre composites made up of glass fibre, carbon, aramid [1]. The green composites basically include composites developed out ofnatural fibres like abaca, jute, kenaf, sisal, hemp, coir, palm, pineapple, ramie which has lesser fibre density making them fit for production of composites with lesser weight, suitable mechanical property and those which are eco-friendly in nature maintaining eco-balance [2]. As discussed by Omrani et al in year 2017, the natural fibre composites have wide applications in fields like construction materials, packaging materials, sports equipment, aero-space, aviation and so forth with major focus being in the field of automobile industries in producing variety of applications like dash board in vehicles, door panels, seat back and other [3–5]. Low cost and low weight of the natural fibres in comparison with glass and carbon fibres; brings the attention of the researchers to substitute synthetic fibre composites (SFC) with natural fibre composites (NFC) so as to reduce the fuel consumption, reduce the cost of automobiles generated and to benefit the global economy.

The major failure in different industries is with respect to the failure of machine parts because of tribological loading condition which caused rapid loss in finances. The drawback associated with incorporating NFCs in automobiles or any application, is its sensitivity towards the wear under friction. The tribological representation of fibres, plays a major role along with its mechanical characterization during composite analysis [6]. This will result in the production of composites with greater wear resistance. The wear rate is greatly influenced by fibre composition, fibre alignment, resin used for composite fabrication, the load applied, sliding distance, sliding speed, temperature [7,8]. Few of the work have been carried out considering the combinations of different natural fibres and resin and to study their tribological behaviour under different circumstances. Ashok Kumar et al in year 2016, investigated on wear testing of eco-friendly composites which can be used for brake materials in automobile application. Basalt fibre reinforced phenolic composites showed best result in comparison with flax fibre composite and flax/basalt hybrid composite. Different loads were applied between 9 N and 50 N at different sliding velocities from 0.104 to 0.523 m/s for 30 min of time duration. Basalt fibre reinforced phenolic composites showed best wear resistance which could be used as substitute for asbestos in brake pad application [9]. C W Chin et al. in year 2009 explored the potential of

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https://doi.org/10.1016/j.matpr.2021.01.495
2214-7853/© 2021 Elsevier Ltd. All rights reserved.
Second International Conference on Aspects of Materials Science and Engineering (ICAMSE 2021).

PRINCIPAL
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Materials Today: Proceedings 44 (2021) 4143–4149

Contents lists available at ScienceDirect

Materials Today: Proceedings

journal homepage: www.elsevier.com/locate/matpr

Potential of using areca fibres in composite fabrication

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ARTICLE INFO

Article history:
Received 3 October 2020
Received in revised form 12 October 2020
Accepted 16 October 2020
Available online 24 November 2020

Keywords:
Areca epoxy composites
IR analysis
SEM analysis: tensile testing
Flexural testing
Comparative study

ABSTRACT

Natural fibre composite fabrication has become an emerging field these days where the combination of different natural fibers and resins has been made and their properties are studied. This study is with respect to the potential of areca husk and sheath fibre reinforced epoxy composite at different fibre loadings. The surface modifications of the fibre with 1% alkali treatment improved the mechanical properties of husk and sheath fibre composites. The IR studies revealed the surface modification of the fibres after alkali treatment. Husk fibre showed optimum mechanical properties at 50% fibre loading and the sheath fibre showed optimum mechanical properties at 55% fibre loading. The tensile strength of husk and sheath composite is 14.85 N/mm^2 and 25.93 N/mm^2 respectively and the flexural strength is recorded as 1.37 N/mm^2 and 1.75 N/mm^2 respectively. In comparison with the strength of husk and sheath fibre composites, there is drastic increase in the mechanical property of sheath composites. Tensile strength for sheath fibres increased by 80.31% at optimum fibre loading which is 55% and the flexural strength increased by 14.5% respectively. Thus, the study reveals that in comparison with areca husk and sheath fibre composites, the sheath fibre composites has the greater potential and proves to be promising material in composite fabrication.

Selection and peer-review under responsibility of the scientific committee of the International Conference on Advances in Materials Processing & Manufacturing Applications.

1. Introduction

The major task of Scientists, in the current scenario is to develop a product which is eco-friendly and is of some benefit to the society. Because of the emerging problems occurring in the world with respect to global warming and environment sustainability, the focus is more on developing green products which does not create any harm to the nature maintaining eco-balance [1]. As a need of an hour, investigation with respect to bio-based products is on demand which can replace the mad-made synthetic fibre composites because of its demerits like non-biodegradability, high cost and the impact that is produced by these synthetic fibres like glass, carbon, kevlar on the surroundings because of its hazardous nature. The investigation is done considering different natural fibres like jute, hemp, sisal, coir, abaca analysing their physical properties to inculcate these in composite fabrication in combination with different resins [2]. The density of the fibres and resins used for composite fabrication also plays a major role in deciding the mechanical properties of the final product developed. As the density of the fibre decreases, the aspect ratio will increase which leads to tremendous increase in the properties of the composite manufactured. The researchers have contributed to a greater extent where these fibre composites have replaced the synthetic fibre composites and showed its application in various fields like marine industries, packaging industries, in constructing sport equipment and the major eye is in the field of automobile industries where the aim is to develop light weight vehicles so that the consumption of the fuel is reduced and the economy of the country would be benefited [3]. The investigation with respect to different fibres like jute, coir, hemp, flax, kenaf are plenty, but research with respect to areca fibres are scanty in literature.

As quoted by Dhanalakshmi et al, Karnataka contributes around 50% of the total areca productions in Country [4]. Hence, there is need to explore the use of areca fibres in composite fabrication. As of now, it is been seen that the husk and the sheath fibres are used for the production of cups and plates in certain regions. If these fibres are effectively studied, they can be incorporated into composite fabrication and can be utilised in various applications like dashboard of automobiles, packaging materials and construction industries. Research is carried out using areca husk fibre composites by various researchers where it is proved as a promising

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https://doi.org/10.1016/j.matpr.2020.10.461
2214-7853/
Selection and peer-review under responsibility of the scientific committee of the International Conference on Advances in Materials Processing & Manufacturing Applications.

ISSN: 0973-3469, Vol.18, No.(1) 2021, Pg. 48-55

Material Science Research India

www.materialsciencejournal.org

Surface Modification of Areca Fibre by Benzoyl Peroxide and Mechanical Behaviour of Areca-Epoxy Composites

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Abstract

Natural fibre composites are playing great role in current life scenario where the focus is more on replacing synthetic fibre composites with natural fibre composites. In this current study, investigation was done on tensile and flexural behaviour of benzoyl peroxide treated areca sheath fibre epoxy composites. The surface modification of the fibre was confirmed by FTIR analysis. Treatment concentration was the major criteria which effects mechanical properties of the composites. At 4% concentration tensile strength and flexural strength was found to be maximum which was reported as 37.05 N/mm^2 and 235.5 N/mm^2 respectively which gradually decreased with increasing concentration of benzoyl peroxide. SEM analysis proved that at lesser concentration, the bonding between fibre and resin was effective which reduced as the concentration of benzoyl peroxide increased. This results in ineffective stress transfer between reinforcing material and the matrix which was the reason for failure of composites manufactured at higher treatment concentration.

Article History
Received: 31 December 2020
Accepted: 03 March 2021

Keywords
Areca Sheath Fibre;
Benzoyl Peroxide;
Ftir Studies;
Fibre Epoxy Composite;
Flexural Strength;
Sem Analysis;
Tensile Strength.

Introduction

Fibre reinforced polymer composites play a major role in wide variety of applications like aircraft, sport equipment, marine applications, automobile industries because of its higher mechanical properties and hence they serve as a promising material in the field of composite.[1, 2] But with respect to environmental concern, synthetic fibre composites creates a negative vibe because of its adverse properties like non-renewability, high cost and its hazardous nature. As a result of this, researchers began to think about natural fibre composites because of its advantages like easy availability, less density, renewability and eco-friendly nature,[3, 4] The major drawback associated with natural fibre composite is its hydrophilic nature and its inability to interconnect with hydrophobic resin. Many researchers have investigated chemically

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Doi: http://dx.doi.org/10.13005/msri/180106

Contents lists available at ScienceDirect

Materials Today: Proceedings

journal homepage: www.elsevier.com/locate/matpr

Effect of surface treatment on wetting behavior of copper

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ARTICLE INFO

Article history:
Received 7 December 2019
Accepted 20 January 2020
Available online xxxx

Keywords:
Copper substrate
Electrochemical etching
Electro-deposition
Surface roughness
Contact angle
Superhydrophobic surfaces

ABSTRACT

Super-hydrophobic surfaces are very useful in cleaning activities. Surfaces with water contact angles above 150° are regarded as superhydrophobic surfaces. In the present study an attempt has been made to achieve superhydrophobicity on copper substrate by electrochemical etching and electro-deposition of Co–Ni alloy and Co–Ni-Graphene composite. A contact angle of about 105° was obtained on Cu surface with electro-deposited Co–Ni alloy and on electro-deposited Co–Ni–G alloy contact angle was found to be 106°. The contact angle was significantly higher at about 142° with electro etched surface. Corrosion test was carried out with electrochemically etched Cu. Electrochemical etching time was varied from 30 to 240 min. The electro-etched Cu substrate etched for 60 min. showed better corrosion resistance with a corrosion rate of 0.197 mm/year. The surface topography of both etched and electrodeposited samples was studied by atomic force microscopy (AFM) and the results were correlated with the wettability data.

Selection and peer-review under responsibility of the scientific committee of the International Conference on Laser Deposition: Nanostructures, Hetero-structures and 2D layers.

1. Introduction

Wetting is one of the most important properties of liquids to spread over a solid substrate. Wetting of a solid by liquid is of great technological importance. Some applications require a good wetting between liquid and substrate surface such as soldering and printing whereas some others demand poor wetting (repellence) such as painted surface and solar panels. Contact angle is a measure of the degree of wetting or wettability of a surface by a liquid [1].

Wettability is an important characteristic of solid surfaces, and is usually measured by the contact angle between water and the surface. If the contact angle is less than 90°, the surface is hydrophilic; if it is greater than 90°, the surface is hydrophobic and if it is greater than 150°, the surface is superhydrophobic [2]. A super-hydrophobic surface is the one that repels water to such an extent that contact angles obtained are extremely high; they are generally defined as surfaces with water contact angles above 150° but it has also been less commonly adopted as 140° [3]. The microscopic geometric structure of the surface is one parameter which determines wettability; Free energy is another parameter-higher the free energy, higher is the wettability, and vice-versa. In general, a solid surface becomes hydrophobic when treated to give micro- or nano-roughness structures and low surface energy. Many kinds of surface treatment techniques, including optical micro-lithography, dry and wet etching, surface coating and precision diamond dicing processes were reported [4–7]. To reduce the production costs and increase the processing speeds, laser machining processes techniques such as laser ablation, laser milling, and laser deposition have been employed [8–10]. These techniques have been effectively used to manufacture components with enhanced hydrophobic properties.

There is little research is carried out on the developing a simple technique of fabricating super-hydrophobic surfaces on various substrates. Realization of super-hydrophobic surfaces via simple coating methods to design a solid surface with appropriate surface roughness and low surface energy are rarely attempted [11].

Different topography can be achieved by creating rough surface either by etching or by coating the surface. Wenzel regime

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https://doi.org/10.1016/j.matpr.2020.01.379
2214-7853/© 2020 Elsevier Ltd. All rights reserved.
Selection and peer-review under responsibility of the scientific committee of the International Conference on Laser Deposition: Nanostructures, Hetero-structures and 2D layers.

Please cite this article as: S. Kalgudi, G. P. Pavithra, K. N. Prabhu et al., Effect of surface treatment on wetting behavior of copper, Materials Today: Proceedings, https://doi.org/10.1016/j.matpr.2020.01.379

Tensile and Flexural Behaviour of Areca Husk Fibre Reinforced Epoxy Composite

Sakshi S. Kamath, D. N. Punith, S. Preetham, S. N. Gautham, Janardhan, K. Lalith Yashwanth, and Basavaraju Bennehalli

Abstract Nowadays, because of the issues related to the environment, it is becoming mandatory for the usage of eco-friendly products for betterment of the people. Hence, here is an attempt made where the harmful synthetic fibre composites used for marine, automobile, constructive applications can be replaced by eco-friendly, biodegradable natural areca fibre composites. Physical properties of areca husk fibre were studied, and it revealed that maximum fibres have length range from 40 to 50 mm with the diameter ranging from 0.200 to 0.299 mm. These untreated and 1% NaOH treated fibres were used for composite fabrication at different fibre loadings like 45, 50, 55, 60, and 65%. It was found that 50% is the optimum fibre percentage. Tensile strength and flexural strength for untreated fibre composite at 50% fibre loading were found to be 7.40 N/mm^2 and 4.01 N/mm^2, respectively, and 54.91 N/mm^2 and 6.81 N/mm^2, respectively, for alkali-treated fibre composites.

Keywords Areca husk fibre · Mercerization · Linear density diameter method · Tensile testing · Flexural testing

1 Introduction

Increasing environmental awareness and decrease in fossil fuels are influencing researchers to use biodegradable natural material in composite manufacture as the substitute for synthetic fibres. The non-biodegradability, environmental impact and high cost of the synthetic fibres used as the reinforcing material in the composite manufacture is questioning the mankind about its usage and hence finding an alternative for using natural fibres as the substitute for composite fabrication [1]. The advantages

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C. Prakash et al. (eds.), *Advances in Metrology and Measurement of Engineering Surfaces* , Lecture Notes in Mechanical Engineering,
https://doi.org/10.1007/978-981-15-5151-2_4

Journal of
MECHANICAL and ENERGY
ENGINEERING

ISSN: 2544-0780 | e-ISSN: 2544-1671
Vol. 4(44) | No. 4 | December 2020 | pp. 335-340
DOI: 10.30464/jmee.2020.4.4.335

EGG SHELL AS A FILLER IN COMPOSITE MATERIALS – A REVIEW

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(Received 19 November 2020, Accepted 11 December 2020)

Abstract: Current focus is on polymer and metal matrix composites for their increased mechanical properties. The strength of the composites is further enhanced by incorporating different types of additives which includes fillers, flame retardants, silanes, coupling agents and so on. One such additives is egg shell powder which influences the strength of composites and thus, gains the attention of researchers for its incorporation in composite fabrication. The work is in progress with respect to utilizing waste egg shell in composite fabrication, which not only finds solution for the waste disposal, but also enhances the strength of composites manufactured. This work is the compilation of work done by different researchers with egg shell in composites, so that the need of its utilization in the manufacture of composites will be stronger.

Keywords: natural fibre composites, chicken egg shell powder, mechanical property, water absorption property

1. INTRODUCTION

Composite materials are made up of one or more reinforcements (discontinuous phase) like fibres embedded in a matrix (continuous phase), resin. The composites are of three types which include metal matrix, ceramic matrix and polymer matrix composite. Polymer composites can be achieved with a wide variety of fibre reinforcements either synthetic in origin e.g. carbon fibre, glass fibres, aramid or natural fibres like flax, hemp, coir, abaca and sometimes hybrids too wherein both synthetic and natural fibres are used together [1]. Synthetic fibres to their credit have, good elasticity can handle heavy loads and are long lasting and are readily available than their natural counterparts. Though synthetic fibres are easy to produce and are available in plenty but come with a disadvantage that they are non-biodegradable and hence are not eco-friendly and leave a trail of carbon footprint right from their production and until disposal [2]. On the contrary, natural fibres are available in plenty either cultivated for the same or available as by-products of agricultural industry and their properties are comparable to synthetic fibres. Thus, natural fibre polymer composites (NFPC) are possible alternatives to the synthetic fibre composites and are fast replacing synthetic fibres in composite materials [3]. To any type of composites, additives are added, so as to bring about certain positive changes. Among many additives, fillers are the class of additives which when added fill the voids in the composites and because of this makes the end product much stronger. Red mud powder [4], coconut shell powder [5], tamarind extract powders [6] and egg shell powders are the popular natural fillers added.

The most commonly used inorganic filler nowadays in composite fabrication is calcium carbonate being water repellent. The easiest source available for $CaCO_3$ is chicken egg shell which is produced in plenty every year as a waste material. In US, Environmental Protection Agency (EPA) has placed eggshell waste at 15th place as a waste produced every year and the European Commission regulations treats egg shell as the most hazardous waste [7]. The major source of egg shell waste is poultries, food manufacturing industries, homes, 14

Polysaccharides as Novel Materials for Tissue Engineering Applications

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Abstract

Tissue engineering is emerging as a significant and potential area of medical therapy wherein tissue, and organ failure is suitably addressed by implanting polymeric scaffolds that could imitate the organ and nurture into the required functionality. Including many natural and synthetic polymers, polysaccharides are considering as an essential class of biomaterials for the fabrication of tissue engineering scaffolds. The polysaccharides being similar to the biological macromolecules can be readily accepted and degraded through metabolic processes within the biological environment of the human body. They are biocompatible, biodegradable, low cost and have similar nature to that of the natural extracellular matrix. However, low mechanical strength is one of the challenging features that need to be taken care of while selecting the polysaccharide for tissue regeneration. Thus, this chapter addresses different types of polysaccharide-based scaffolds, including chitosan, cellulose, alginate, dextran, starch, pectins, pullulan, gellan xanthan, agar, and glycosaminoglycans. These polysaccharides are commonly used in tissue engineering applications. A brief account of the basic principle of tissue engineering, selection criteria of biomaterials and different fabrication techniques of the scaffolds were discussed in the beginning, and this was followed by the elaboration of the applications of different polysaccharides-based scaffolds for tissue engineering. While concluding, the emphasis was also given to describe the current challenges and future perspectives of the scaffolds derived from different polysaccharides. To compile this chapter and to provide adequate information to the readers, we have explored all the possible materials accessible in the literature.

Keywords: Tissue engineering, scaffolds, polysaccharides, biomaterials and biodegradable

14.1 Introduction

The term "Tissue Engineering" was introduced in medicine in the year 1987 and is the most exciting, emerging and broadly interdisciplinary field of science. The prime goal of tissue engineering is to restore or improve the biological tissues and their functions by applying

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Inamuddin, Mohd Imran Ahamed, Rajender Boddula and Tariq Altalhi (eds.) Polysaccharides: Properties and Applications, (301–324) © 2021 Scrivener Publishing LLC