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Tensile Properties of Polyhydroxyalkanoates/Calcium Phosphate through Simulation Analysis

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Abstract: Tensile testing was done through simulation analysis by using Solidworks Simulation. Material used in this research is Polyhydroxyalkanoate (PHA) and Calcium Phosphate (CaP). The type of PHA used in this study is Polyhydroxybytyrate (PHB). Reinforced composites are popular for use in many industrial applications, because of their inherent high specific strength and stiffness. The aim of this study is to determine the tensile properties of composite with different number of ply of PHA/CaP through simulation analysis and also to investigate the effects of different volume of samples based on ASTM standard on the tensile properties of composite. The ASTM standard is limited to ASTM D3039. ASTM D3039 specimens are rectangular in shape with a constant cross-section. The standard dimensions are length of 250mm, width of 25mm and thickness of 1 mm. Parameters that were used in this journal are the number of CaP ply in PHB composite and volume of composite CaP/PHB. The tensile properties of material have been identified through simulation testing through Solidwork software. The result shows that the higher number of CaP ply in PHB composite the lower the result of stress, displacement, and strain which will result in more strength. From the first set, 4/20 CaP ply in PHB composite has the lowest stress which was 5.280 MPa , displacement which was $9.658 \times 10^{-3} mm$ and strain which was 3.834×10^{-5} . This proved that reinforcement of CaP help in enhance the physical properties of the final composite. The higher the volume of CaP/PHB composite the, lower the result of stress, displacement and strain which will result in more resistance of composite. From the second set, CaP/PHB volume of $10000mm^3$ has the lowest stress which was 3.297 MPa , displacement which was $6.121 \times 10^{-3} mm$ and strain which was 2.493×10^{-5} . This research prove that reinforcement CaP enhance the strength of final composite PHB.

Keywords: Simulation, Polyhydroxyalkanoates, ASTM

1. Introduction

Tensile properties indicate how the material will react to forces that are applied in tension. Composites reinforced with fibers of synthetic or natural materials are gaining more importance as demands in the market. The composite for this research is Polyhydroxyalkanoate and the reinforcement for the composite is Calcium Phosphate. Microorganisms produced polyesters which is Polyhydroxyalkanoates (PHA) under unbalance growth conditions. This material is high demand as biomaterials for medical devices and tissue engineering as they are biodegradable and thermoprocessable [7]. Polyhydroxyalkanoates are emerging as a class of biodegradable polymers for applications in tissue engineering. Members of the Polyhydroxyalkanoates family grow a wide variety of materials, from hard and brittle materials to soft and strong. Calcium Phosphate materials have received a lot of research attention due to their chemical similarity to bones and teeth. Calcium phosphate bioceramic forms are broadly being developed in biomedical applications as their highlight biocompatibility, bioactivity and osteoconduction characteristics [5].

FEM has been implemented rigorously for solving a wide variety of problems in applied science and engineering and it has been rapidly developed over the years. FEM software has become an important tool for testing specimens for numerical analysis until today. FEM software issued for improving result quality through simulations and process analysis techniques to improve processes. The finite element method (FEM) is the dominant main technique in structural mechanics [2].

CAD is important and used in many applications including automotive, architectural design and aerospace industries. Most of industry that involves with design such as mechanical, architecture or engineering fields are vital to work with CAD software [3]. Solidworks is a CAD/CAE/CAM/PDM desktop system, and the first 3D mechanical CAD software in Windows developed by the SolidWorks Company. It provides product-level automated design tools [4]. Solidworks is a tool that assists design engineers to exploit their imagination and insert creativity to their designs. It is a 3D mechanical CAD (computer-aided design) program that is used to maximize the production of your design and engineering resources [1].

1.1 Problem Statement

Polyhydroxyalkanoate is positively impact global climate situations by reducing nondegradable plastics used. Besides, PHA is also used widely in medical purposes as sutures, drug delivery and scaffolds material for tissue engineering. However, Polyhydroxyalkanoates has a few disadvantages that need to be modified. Polyhydroxyalkanoate has a poor mechanical properties, limited functionalities and incapability with conventional thermal properties. In order to increase the tensile properties of PHA, reinforcement is added. Reinforcement will help in obtain better properties of product.

1.2 Purpose of Study

The purpose of this research is to design, develop and simulate test specimens enabling accurate details in optimum parameters. This project is based on static simulation analysis in mechanical properties of Polyhydroxybutyrate polymer matrix that reinforced with Calcium Phosphate. Furthermore, the purpose of this research is to investigate the tensile properties through Solidworks simulation analysis. Moreover, to discover the effects of various volumes of samples based on ASTM D3039 on the tensile properties through simulation analysis.

2. Materials and Methods

The materials and methods section, otherwise known as methodology, describes all the necessary information that is required to obtain the results of the study.

2.1 Materials

Material used for this study is a polymer composite which are Polyhydroxybutyrate (PHB) and Calcium phosphate (CaP). As discussed, this study will involved the use of Solidworks software. In developing the specimen in Solidworks software and produce a tensile properties of material used, parameters need to be correct. Table below shows parameters used for this research.

No	Number of CaP ply in PHB composite
1	1/20
2	2/20
3	3/20
4	4/20

Table 2.2 :Volume of CaP/PHB samples

No	Volume of CaP/PHB samples
1	6250 <i>mm</i> ³
2	$7500 mm^{3}$
3	8750 <i>mm</i> ³
4	$10000 mm^{3}$

2.2 Methods

The simulation method is used in this study. This method will benefit in many aspects compared to experimental. Some of the advantages are running simulations will reduce in wastage as the materials are not tested using machine. Simulations method will also prevent accidents in lab. Researchers do not have to deal with actual machines and specimen. Researchers also can be ready with prediction of experimental result, if the simulation has been done earlier. Equipments used in this simulation are Solidworks software. The specimen is designed in Solidwork software. Then, the tensile test is prepared and run by using Solidworks simulation.

This process will start by drawing specimen in Solidworks. Then, samples dimensions are inserted based on ASTM. Next, composite is defined by inserting type of material, number of ply and angle of ply. Then, fixtures and force is added. Moreover, the study will be mesh and run. The output will be the result of tensile properties. The process will repeat the step to test other sample. Figure 3.1 below is a flowchart of solution concept for this study.

Numerical result will be generated as the output for the analysis. One of the advantages of FEA is the process of computational simulation remove the need to conduct physical experiment which reduces manufacturing and operating cost. This also can eliminate risk of wasting material or any danger which can show up while doing physical testing. FEA also has its disadvantages which the testing assumption is based on perfect material without defect. This includes the inability to take operating in real life as consideration. [6]

3. Results and Discussion

The properties and characterization of samples could be determined from data gathered. Some testing has been conducted to analyze the characteristics and mechanical properties of PHB/CaP composite. The mechanical properties as result of PHB/CaP were analyze through the simulation of tensile testing. All the samples were prepared through the Solidworks software stated in Chapter 3. This

research was done on four different samples of 2 sets. The first set differs by the number of Ca/P ply in PHB composite. The parameters are 1/20, 2/20, 3/20, 4/20. The second set differs by the volume of samples. The parameters were $6250mm^3$, $7500mm^3$, $8750mm^3$, $10000mm^3$.

3.1 Results

The first set is the simulation of testing CaP/PHB samples differs by the number of CaP ply in PHB composite. Figure 1 shows the graph of number if CaP ply in PHB composite versus stress, strain and displacement. The testing includes applying fixture to one side and tensile force at the other side. The force used in this testing is 100N. The result shows from minimum to maximum value in stress, displacement and strain properties of sample. The maximum stress result from sample 1/20, 2/20, 3/20 and 4/20 are 6.663 *MPa*, 6.605 *MPa*, 5.664 *MPa* and 5.280 *MPa* respectively. From the stress result, it can be observe that the maximum stress decreased as the number of Ca/P ply in PHB increased. The lowest stress is 5.280 *MPa* which for sample 4/20 CaP ply in PHB composite. This sample has the highest number of CaP ply in PHB compared to other sample.

Based on the result obtained, it was shown that the more number of CaP ply in PHB will result in more strength in the sample. This can be proved from the hypothesis stated. The higher the number of CaP ply in PHB will result in lower stress, shorter displacement and lower strain.



Figure 3.1: Graph of Number of CaP ply in PHB Composite versus Stress, Strain and Displacement

The second set is the simulation of testing CaP/PHB samples differs by the volume of CaP/PHB composite. Figure 2shows the graph of volume of CaP/PHB composite versus stress, strain and displacement. The testing includes applying fixture to one side and tensile force at the other side same as the first set. The numbers of CaP ply in PHB composite used for all the sample in this set is four. The force used in this testing is also 100N. The result shows from minimum to maximum value in stress, displacement and strain properties of sample. The maximum stress result from sample $6250mm^3$, $7500mm^3$, $8750mm^3$ and $10000mm^3$ are 5.280 MPa, 4.405 MPa, 3.764 MPa and 3.297 MPa respectively. From the stress result, it can be observe that the maximum stress increased as the volume of CaP/PHB decreased. The highest stress is 5.280 MPa which for volume $6250mm^3$ CaP/PHB composite.

Based on the result of simulation, it was also shown that the higher volume of CaP/PHB will result in more strength and higher resistance in the sample. This can be proved from the hypothesis stated based on the result. The higher the volume of CaP/PHB will result in lower stress, shorter displacement and lower strain.



Figure 3.1: Graph of Volume of CaP/PHB Composite versus Stress, Strain and Displacement

Reinforcement CaP helps enhance the strength and stiffness of final composite of PHB. Polymer without the reinforcement would offer relatively poor mechanical properties. Based on the result, this research proved that reinforced composite has more strength which can withstand more stress and external force. Also, the percentage of reinforcement also affects the strength of composite. From this result, 4/20 CaP ply is the highest number of ply used and has the highest strength and toughness compared to other parameter used which are 1/20, 2.20 and 3/20. Moreover, the volume of the composite also affects the strength of composite. From the result, $10000mm^3$ is the highest volume of PHB/CaP composite and has the highest strength compared to other lower volume parameters.

The expected result of this research is to obtain details in optimum parameters of Polyhydroxyalkanoate/Calcium Phosphate (PHA/CaP) composite that obtained high mechanical properties through Solidwork simulation. Based on the result, the optimum parameters were proved. However, the details of tensile properties are limited as there are no result of yield strength, tensile strength and other properties. This occurs because of the limitation of material properties. There are no specific data for CaP/PHB composite but there only are general data of CaP and PHB individually.

4. Conclusion

Findings and analysis throughout this research were done in order to achieve the objectives Based on the result, it can be concluded that the objectives of this research were successfully achieved. The findings and analysis of the research found that the highest number of CaP ply in PHB resulted in lowest stress which indicates more strength to the sample. Also, the research found that the highest volume of CaP/PHB composite also resulted in lower stress which indicates more resistance of the material. The physical properties of material have been identified from previous journals. Samples are drawn in Solidwork Modelling software according to the dimensions. It was indeed shown here that for set 1, 4/20 CaP ply in PHB composite was the best ply number which produce good strength properties of CaP/PHB composite among another sample. For set 2, the volume of 10000mm³ of CaP/PHB composite was the best volume among other sample which produces more resistance properties of CaP/PHB. This research proved that reinforcement of CaP helps enhance the strength and stiffness of final composite of PHB. This research expected outcome is to obtain best parameter for PHB/CaP reinforcement and the optimum parameters were obtained. Based on the result, this research proved that reinforced composite has more strength which can withstand more stress and external force.

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