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MICROMECHANICAL MODELING OF BASALT FIBER AND GLASS FIBER REINFORCED PA66 MATRIX COMPOSITE MATERIALS

Ferdi YILDIRIM [*]

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Abstract: In this study, mechanical properties of basalt fiber (BF) and glass fiber (GF) reinforced polyamide66 (PA66) matrix composite materials were investigated using the mean field homeogenization (MFH) method. BF and GF reinforced PA66 matrix composite materials with 5, 10, 20, 40 wt% additives were modeled using MFH based Digimat-mean field (Digimat-MF) software. With Digimat-MF software, micromechanical modeling of composite materials was performed and maximum tensile strength and elastic modulus were calculated. In addition, representetive volume element (RVE) modeling of composite materials was performed using Digimat-finite element (Digimat-FE) software. Then, micro-scale damage analysis (stress and strain regions) were evaluated on RVE models of composite materials. According to the results obtained, the mechanical properties of BF reinforced PA66 (BF/PA66) and GF reinforced PA66 (GF/PA66) composite materials were compared. The results showed that BF/PA66 composite materials exhibited superior mechanical properties compared to GF/PA66 composite materials at all additive ratios.

Keywords: Digimat, Polymer composite, Mechanical properties

Bazalt Fiber Ve Cam Fiber Takviyeli PA66 Matrisli Kompozit Malzemelerin Mikromekanik Modellenmesi

Öz: Bu çalışmada ortalama alan homojenizasyonu (mean field homeogenization, MFH) yöntemi kullanılarak bazalt fiber (BF) ve cam fiber (GF) takviyeli poliamid66 (PA66) matriksli kompozit malzemelerin mekanik özellikleri incelenmiştir. Ağırlıkça % 5, 10, 20, 40 katkı oranındaki BF ve GF takviyeli PA66 matriksli kompozit malzemeler MFH esaslı Digimat-ortalama alan (Digimat-mean field, Digimat-MF) yazılımı kullanılarak modellenmiştir. Digimat-MF yazılımı sayesinde kompozit malzemelerin mikromekanik modellemesi gerçekleştirilerek maksimum çekme dayanımı ve elastik modülleri hesaplanmıştır. Bununla birlikte kompozit malzemelerin temsili hacim unsuru (representetive volume element, RVE) modellemesi Digimat-sonlu eleman (Digimat-finite element, Digimat-FE) yazılımı kullanılarak gerçekleştirilmiştir. Daha sonra kompozit malzemelerin RVE modelleri üzerinde mikro boyutta meydana gelen hasar analizleri (gerilme ve uzama alanları) değerlendirilmiştir. Elde edilen sonuçlara göre BF takviyeli PA66 (BF/PA66) ve GF takviyeli PA66 (GF/PA66) kompozit malzemelerin mekanik özellikleri karşılaştırılmıştır. Sonuçlar değerlendirildiğinde BF/PA66 kompozit malzemelerin tüm katkı oranlarında GF/PA66 kompozit malzemelere kıyasla daha üstün mekanik özellikler sergilediği görülmüştür.

Anahtar Kelimeler: Digimat, Polimer kompozit, Mekanik özellikler

[*] Department of Mechanical and Metal Technologies, Ortaköy Vocational School, Aksaray University, 68400, Ortaköy, Aksaray

Corresponding Author: Ferdi Yıldırım (ferdiyildirim@aksaray.edu.tr)

1. INTRODUCTION

Polymer materials such as polyamide (PA), polyethylene (PE), polypropylene (PP), polystyrene (PS) and epoxy are increasingly used in industrial applications due to their low weight and low cost (Cheewawuttipong et al., 2013; Zhou et al., 2007). PA66 polymer materials are preferred in systems such as bearings and gear wheels where metal type engineering parts are used, thanks to their advantages such as low weight, dimensional stability and vibration absorption (Çuvalci et al., 2014; Samyna et al., 2007; Samyn and Tuzolana, 2007). In order for polymer materials to be used as an industrial product, it is of great importance to improve their mechanical, thermo-mechanical, thermal and electrical properties. Therefore, it is possible to improve these properties of polymer materials with fillers. In many engineering areas such as space, aerospace and defense industries, polymer matrix composite materials are often preferred over other traditional materials such as metals and ceramics due to their superior properties (Mansor et al., 2013; Kumar et al., 2012). Polymer matrix composite materials have attracted increasing attention of researchers due to the significant advantages of low weight to high strength ratio. In the production of polymer matrix composite materials, particle shaped (spherical) and fiber shaped reinforcements are generally preferred. Fiber reinforced polymer matrix composite materials exhibit superior properties such as high strength and high impact resistance (Mishra et al., 2022; Sun et al., 2019).

Short fiber reinforced polymer matrix composites are widely used in specific industries today. Thanks to their significant advantages such as good mechanical properties, easy raw material procurement and production process, low production cost and the ability to produce complex shaped parts, such composite materials find applications in different fields including electrical components, automotive parts, chemical industry, medical applications and healthcare sector (Isaincu et al., 2021; Mortazavian and Fatemi, 2015; Mortazavian and Fatemi, 2017; Tseng et al., 2020; Dean et al., 2019; Li et al., 2018). In the composite manufacturing industry, glass fiber, aramid and carbon fiber are mostly preferred as reinforcing materials. The use of such synthetic materials is an environmental problem as they cause global warming (Farsani et al., 2024; Leman, 2020). The use of natural fiber materials instead of synthetic fiber reinforcements can contribute to the prevention of these environmental problems (Derusova et al., 2018; Behnia et al., 2016; Sarasini et al., 2020; Bing et al., 2020). Natural basalt fibers obtained from volcanic igneous rocks are promising for industrial applications as they have higher strength and high heat resistance compared to glass and carbon fibers (Hao and Yu, 2010; Kumar et al., 2015). Another important properties of basalt fibers is their superior impact and chemical resistance compared to carbon fibers, as well as their non-toxic properties in high temperature processes (Anandamurthy et al., 2017). Modeling and prediction of the mechanical properties of short fiber reinforced composite materials is an important requirement for material design for optimum efficiency. Many methods have been applied for fiber modeling and prediction together with an accurate material characterization (Isaincu et al., 2021; Mortazavian and Fatemi, 2015; Mortazavian and Fatemi, 2017; Tseng et al., 2020; Dean et al., 2019; Li et al., 2018).

In the literature, there are computer modeling techniques that can predict the mechanical properties of composite materials according to the production parameters. The cost and time loss of experimental processes have increased the interest in these techniques. The compatibility of experimental and simulation data obtained as a result of the studies has accelerated the studies in this areas in recent years. Among the computer modeling techniques of composite structures, multi-scale modeling technique has been successfully applied by some researchers in the design and analysis of different composite materials (Arora and Pathak, 2020; Liu et al., 2015; Micota et al., 2021; Yıldırım et al., 2022).

In the previous years, Eshelby model was used by most researchers to obtain the effective properties of composite materials with linear elastic behavior. In later years, various homeogenization methods have been proposed to predict the effective properties of composite materials exhibiting nonlinear behavior such as elastoplastic properties (Withers, 1989;

Hutchinson, 1976; Lebensohn and Tomé, 1993; Hill, 1965; Berveiller and Zaoui, 1978). It is very difficult to predict the effective properties of composite materials with complex shape and high volume fraction by analytical models. Homeogenization methods give the most accurate results in predicting the effective properties of such composite materials (Gaurav and Himanshu, 2019). Among the homogenization techniques, the mean field homogenization method stands out in terms of computational efficiency (Ogierman and Kokot, 2013). The MFH method basically provides approximate solutions for the prediction of volume averages of stresses and strains both at the macro level and at each micro phase (DIGIMAT, 2012; Ogierman and Kokot, 2013).

In simulation studies, modeling the reinforcement phase (such as aspect ratio, matrix-filler interface, dispersion and agglomeration of the reinforcement material) in the matrix structure is the most important step in order to predict the mechanical properties of composite materials with a good approximation (Siot et al., 2019). An MFH method is used to obtain the optimum mechanical properties of a matrix material containing fillers at the nano/micro scale. Digimat-MF software, an MFH tool is efficiently used to predict the nonlinear behavior of composite materials. Digimat composite modeling software allows the modeling of a wide range of composite structures such as metal, polymer, ceramic matrix. Thanks to Digimat software, the response of the composite structure can be accurately predicted by examining the effect of the filler, which is one of the components of the composite structure. For example, the interface region between the matrix and the particle, particle size effect, particle agglomeration and particle distribution can be modeled by taking into account the parameters that greatly affect the effective properties of the composite structure (DIGIMAT, 2009).

Digimat-MF a composite modeling tool based on mean field homogenization within Digimat software is frequently preferred for modeling composite structures (Gaurav and Himanshu, 2019; Siot et al., 2019; Hussein and Kim, 2018; Shin et al., 2017; Moon et al., 2018; Elmarakbi et al., 2017; Ogierman and Kokot, 2014). Digimat-MF provides accurate and efficient predictions of composite structures at the macroscopic scale based on nonlinear semi-analytic homogenization theory. Digimat-MF is a micromechanical material modeling software that provides a wide range of composite structure modeling possibilities where the material behavior of the components in the composite structure, microstructure morphology and the loading applied to the composite material can be determined. In addition, Digimat-MF can predict the mechanical, thermal, thermomechanical and electrical behavior of the composite structure using Mori-Tanaka or Interpolative Double Inclusion models. On the other hand, spherical particles, platelet-shaped particles, flake-shaped particles and fibers in the composite structure can be modeled as desired and accurate results can be obtained (MSC Software Company, 2009; ABAQUS, 2008; Adam et al., 2009; Selmi et al., 2007).

The aim of this study is to predict the mechanical properties of BF/PA66 and GF/PA66 composite materials based on a micromechanics based modeling approach. In addition, the damage states (stress and strain regions) in the composite structure components (matrix and fibers) are analyzed at the micro scale. For this purpose, Digimat-MF (Figure 1) and Digimat-FE (Figure 2) modeling tools in Digimat software were used to predict the mechanical properties of these composite materials with high accuracy. According to the analysis results, the mechanical properties of two different composite materials were compared.

There are almost no studies in the literature on modeling and predicting the mechanical properties of BF/PA66 and GF/PA66 polymer composites using Digimat software. The importance of this study is to estimate the mechanical properties and determine the optimum composite strength (elastic modulus and tensile strength) by making the desired fiber modifications (fiber reinforcement ratio and fiber type in the matrix) of BF/PA66 and GF/PA66 composite materials, thanks to the Digimat software. On the other hand, thanks to the use of natural BF reinforcement material instead of inorganic GF in the PA66 matrix, an environmentally friendly composite model with optimum mechanical properties was obtained.

2. MICROMECHANICAL MODELING

The micromechanical modeling approach refers to the analysis of the state of the components of materials (such as fibers and matrix) at the microscopic level. Through micromechanical modeling of composite materials the macroscopic behavior of the composite can be predicted based on its component behavior at the microscopic level (Abhilash et al., 2020).

Digimat software was preferred for modeling a composite material and predicting the mechanical properties based on the homogenization method of the component properties of the composite material. Digimat platform is preferred in different engineering and research applications due to its ability to model complex composite materials and analyze their properties accurately. Digimat homogenizes the components of the composite structure into a single material property at the microstructure level based on their individual material properties. Then, Digimat offers the opportunity to perform structural analysis at macro level by interfacing with finite element analysis programs (Micota et al., 2021).

2.1. Digimat-MF

Micromechanical modeling of BF/PA66 and GF/PA66 composite materials was performed in the Digimat-MF homeogenization module based on the first order Mori-Tanaka homogenization technique (Figure 1). Thanks to this modeling approach the mechanical properties of 5, 10, 20, 40 wt% BF/PA66 and GF/PA66 composite materials were obtained.

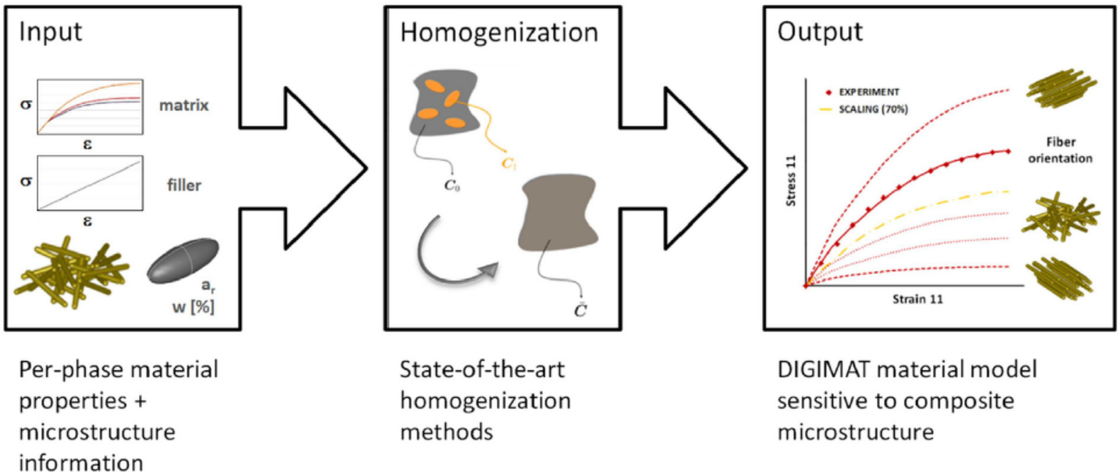


Figure 1:
Digimat-MF modeling approach (DIGIMAT, 2012)

In the composite material modeling phase with Digimat-MF software the material properties given in Table 1 were taken as basis. PA66 matrix material is defined as isotropic hardening, exponential laws and elastoplastic to accurately predict its behavior in the plastic region (*DIGIMAT, 2012*). BF and GF material behavior is modeled as isotropic and elastic.

Table 1. PA66, BF and GF material properties (DIGIMAT, 2009; Mishra et al., 2022; Micota et al., 2021; Micota et al., 2021)

Phase	PA66	BF	GF
Density (g/cm3)	1.140	2.65	2.58
Poisson's ratio	0.37	0.3	0.22
Young's modulus (MPa)	3000	89000	72000
Yield stress (MPa)	20	-	
Hardening modulus (MPa)	22	-	
Hardening exponent	108	-	
Fiber shape	-	Cylinder	Cylinder
Fiber aspect ratio	-	25	25

2.2. Digimat-FE

Digimat-FE is a finite element based RVE generating homogenization tool within Digimat software (Figure 2). Digimat-FE allows to optimize the behavior of composite materials with different reinforcements and complex geometries by modeling them with finite element method (Abhilash et al., 2020; Sumit et al., 2020; URL-1, 2024). Finite element modeling of the RVE was performed in three dimensions (3D). RVE dimensions are given in Figure 3.

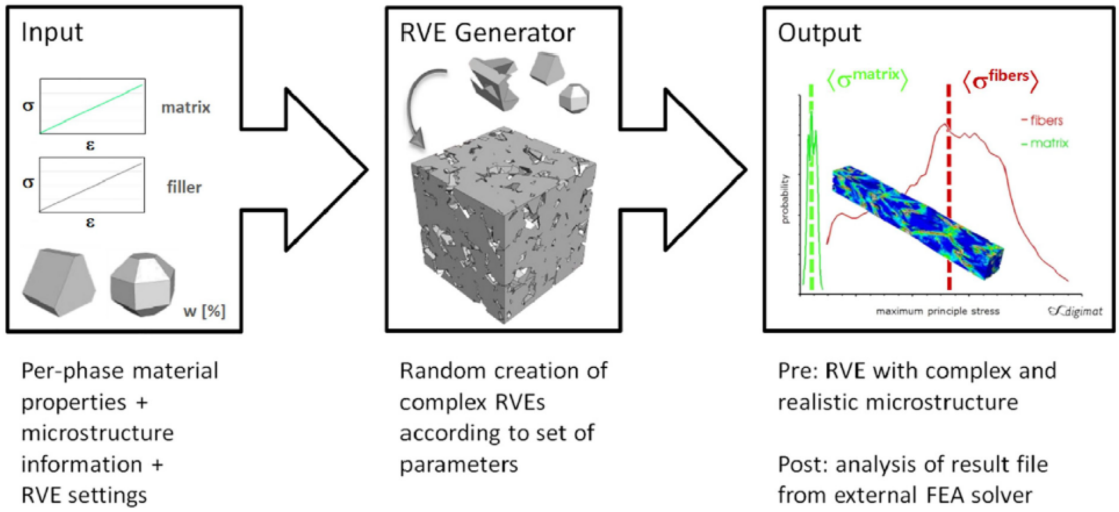


Figure 2:
Digimat-FE modeling approach (DIGIMAT, 2012)

Matrix and fiber properties were defined based on Table 1. Fiber reinforcement rates of 5, 10, 20, 40 wt% were selected (Figure 5). Fiber orientation was defined randomly. RVE dimensions were defined as 500 µm x 500 µm x 500 µm and fiber dimensions as L250 µm x D10 µm. The fiber type was cylindrical and the aspect ratio was kept constant at 25. It is very difficult to define a tetrahedral mesh model as the complexity of the RVE structure increases with the increase in the weight % of the fibers. Therefore, automatic voxel mesh definition was applied to 3D RVE models (Figure 3). Based on the coordinate system, the number of voxels in x, y and z directions was 50. The voxel mesh type facilitates the finite element solution. Automatic "Periodic" unidirectional boundary conditions were defined to the RVE models using the Digimat FE internal solver (Figure 4). The fibers are considered to be perfectly bonded to the matrix material (Abhilash et al., 2020).

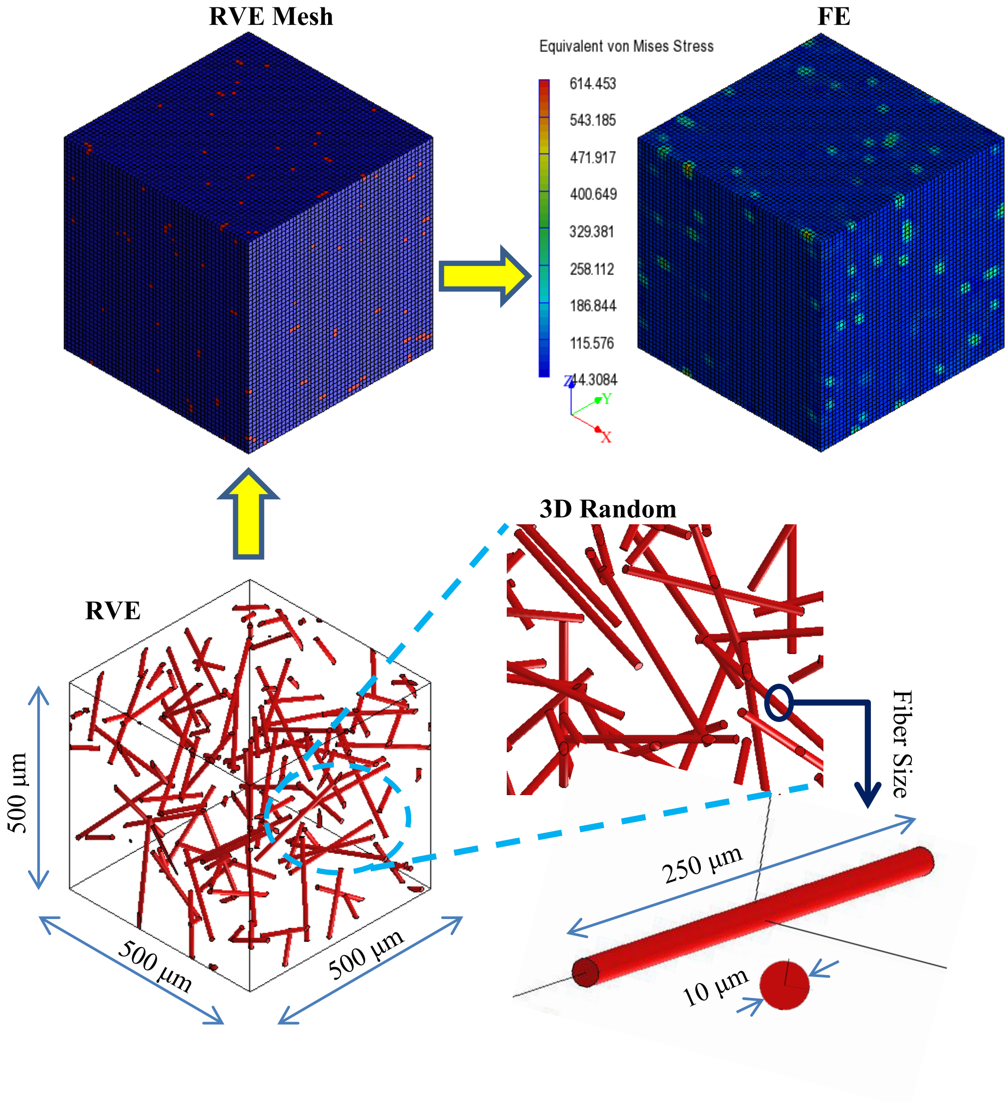


Figure 3:
RVE model of BF/PA66 and GF/PA66 composite structures with Digimat-FE

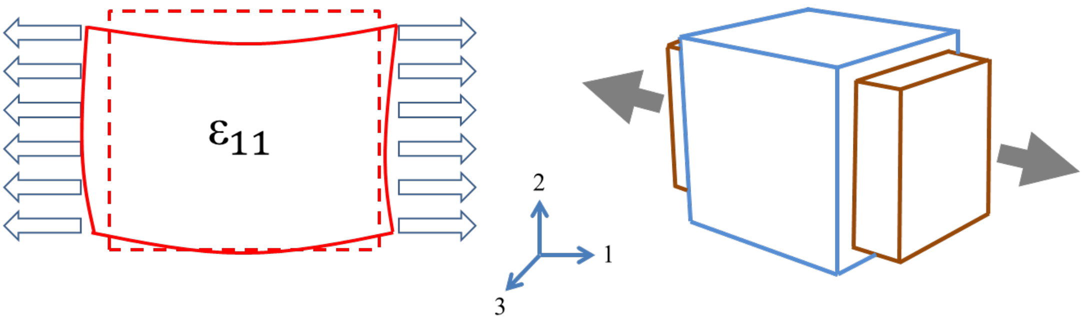


Figure 4:
RVE periodic boundary conditions (DIGIMAT, 2012)

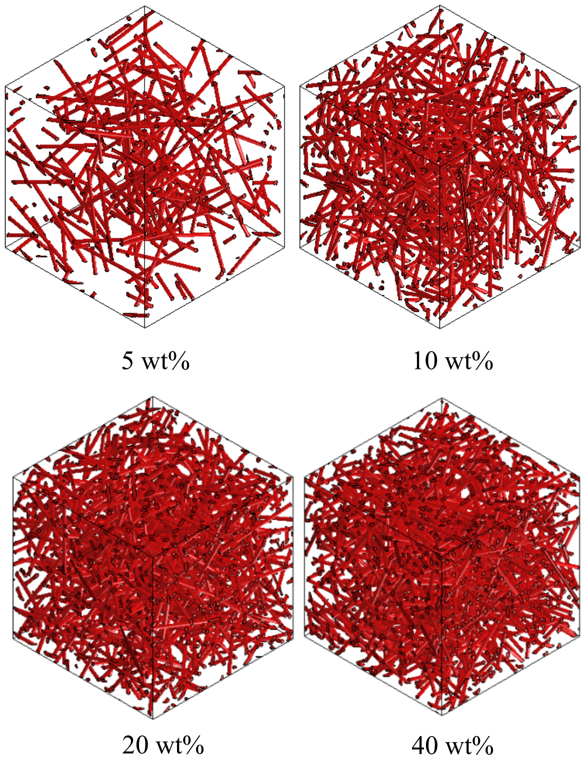


Figure 5:
RVE models of BF/PA66 and GF/PA66 composite structures according to wt% ratios

3. RESULTS AND DISCUSSION

3.1. Digimat-MF

With Digimat-MF software the mechanical properties of PA66 polymer material were investigated by adding BF and GF at 5, 10, 20, 40 wt% reinforcement ratios. Stress-strain graphs of BF/PA66 and GF/PA66 composite materials are given in Figure 6 and Figure 7, respectively. In addition, the maximum tensile strength and elastic modulus of the composite materials were calculated (Table 2 and Table 3). The maximum tensile strength values of BF/PA66 and GF/PA66 composites increased linearly with increasing fiber weight ratio (Figure 8). Similarly, the elastic modulus values of BF/PA66 and GF/PA66 composites increased linearly with increasing fiber weight ratio (Figure 9). Considering the experimental studies in the literature, GF and BF reinforcement on PA66 polymer caused an increase in both the tensile strength and elastic modulus of the composite structure (Lee at al., 2019; Lingesh et al., 2022; Meszaros and Szakacs, 2016; Mouhmida et al., 2006; Zhou and Mallick, 2005). Therefore, the results obtained in this study appear to be compatible with the literature. BF/PA66 composite material exhibited higher tensile strength and elastic modulus compared to GF/PA66 composite material at all reinforcement ratios. This is thought to be due to the fact that BF material exhibits superior mechanical properties (such as young modulus, poisson ratio) compared to GF material. The two most important phenomena affecting the tensile strength of composite materials in terms of mechanical properties are interface adhesion between the reinforcement material and the matrix material and particle agglomeration. The fact that the matrix material and the reinforcement material have close surface energies causes good wetting and a homogeneous distribution instead of agglomeration. Good wetting of the matrix material and the reinforcement material and a homogeneous distribution increase the overall strength of composite materials (Yang et al., 2019; Yang et al., 2021; Wang et al., 2018). Therefore, the reason for the linear increases in the maximum tensile strength of the composite structures is that the fibers are assumed to be perfectly bonded to the matrix material and are modeled assuming that no agglomeration occurs. The linear increase in the elastic modulus of composite structures with increasing reinforcement ratio is expected. Therefore, in this study, the reason for the linear increases in the maximum tensile strength of composite structures is that the fibers are assumed to be perfectly bonded to the matrix element and they are modeled considering a homogeneous distribution without any agglomeration. The increase in the elastic modulus of composite structures is thought to be due to increased fiber volume ratio and better interfacial strength (Liang, 2012; Wang et al., 2014). On the other hand, it is thought that the increase in the mechanical properties of composite structures is due to the fact that fiber type materials have a more rigid structure with a high aspect ratio (Mastura et al., 2022).

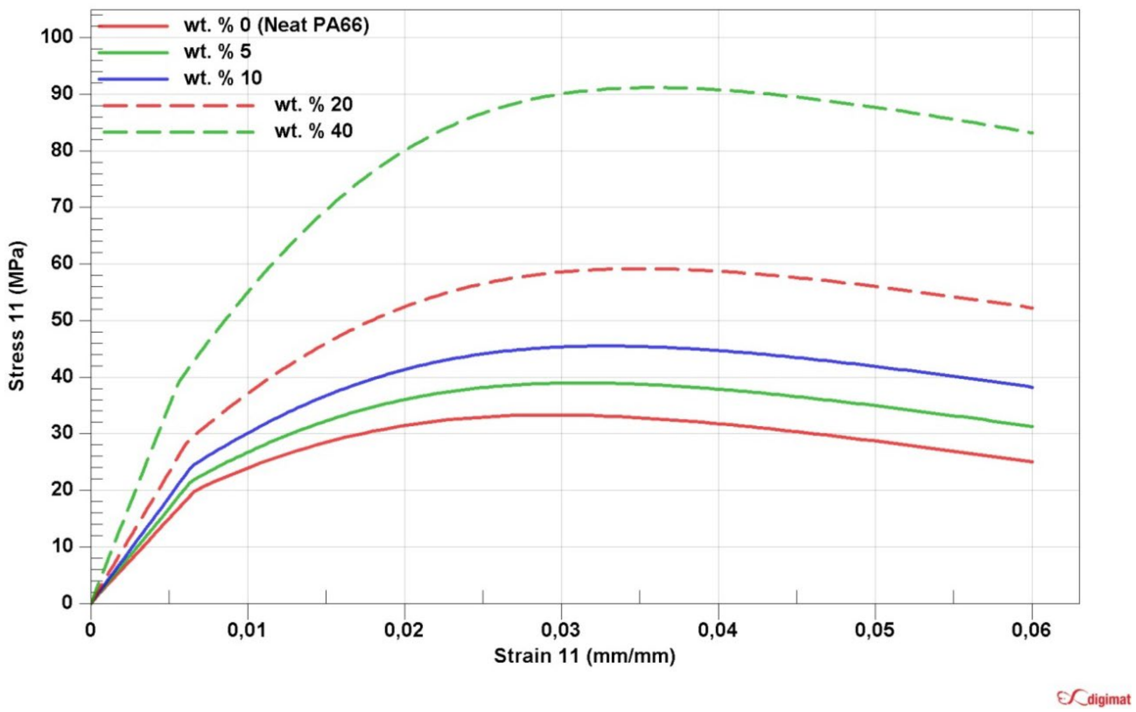


Figure 6:
Stress-strain curve of BF/PA66 composite structures

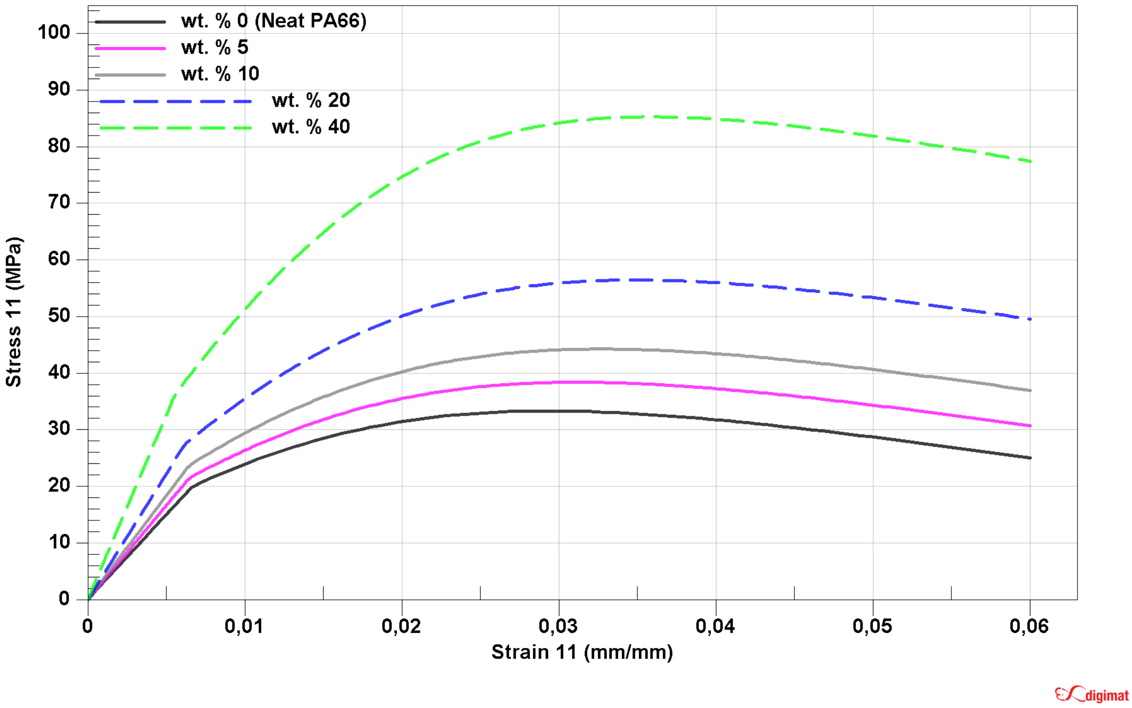


Figure 7:
Stress-strain curve of GF/PA66 composite structures

Table 2. Mechanical properties of BF/PA66 composites obtained with Digimat-MF

wt%	Max. Tensile Strength (MPa)	Elastic Modulus (MPa)
0 (Neat PA66)	33.70	3000
5	39.07	3366.5
10	45.74	3763.3
20	59.36	4653.6
40	91.87	7005.4

Table 3. Mechanical properties of GF/PA66 composites obtained with Digimat-MF

wt%	Max. Tensile Strength (MPa)	Elastic Modulus (MPa)
0 (Neat PA66)	33.70	3000
5	38.47	3324
10	44.49	3673.4
20	56.59	4455.1
40	85.47	6530.6

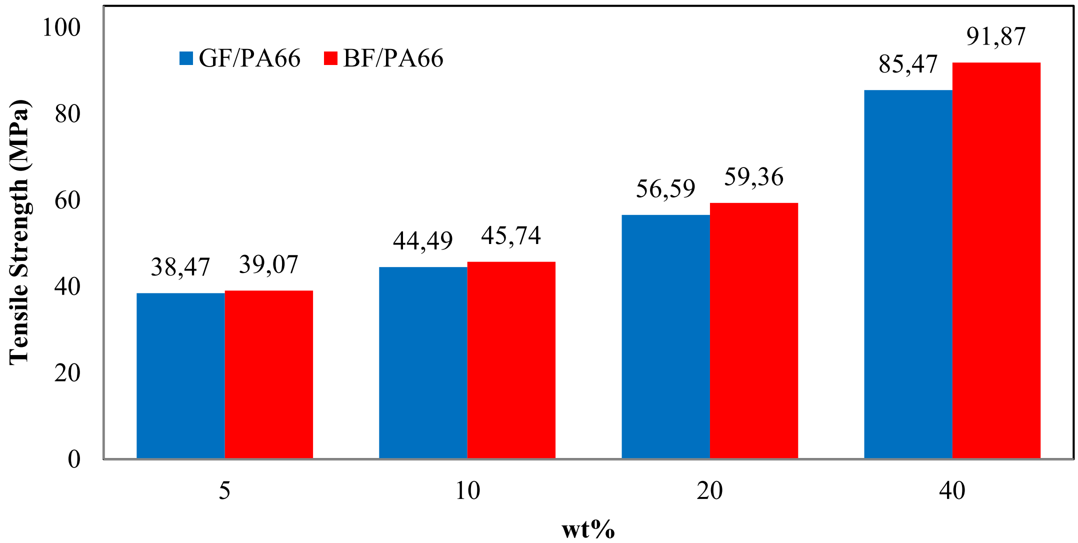


Figure 8:
Maximum tensile strengths of BF/PA66 and GF/PA66 composites

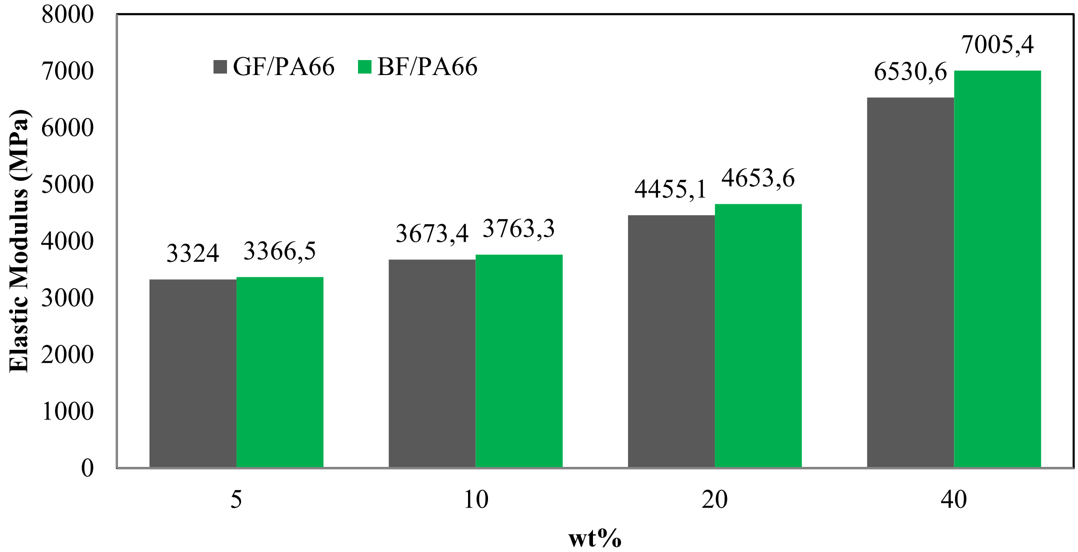
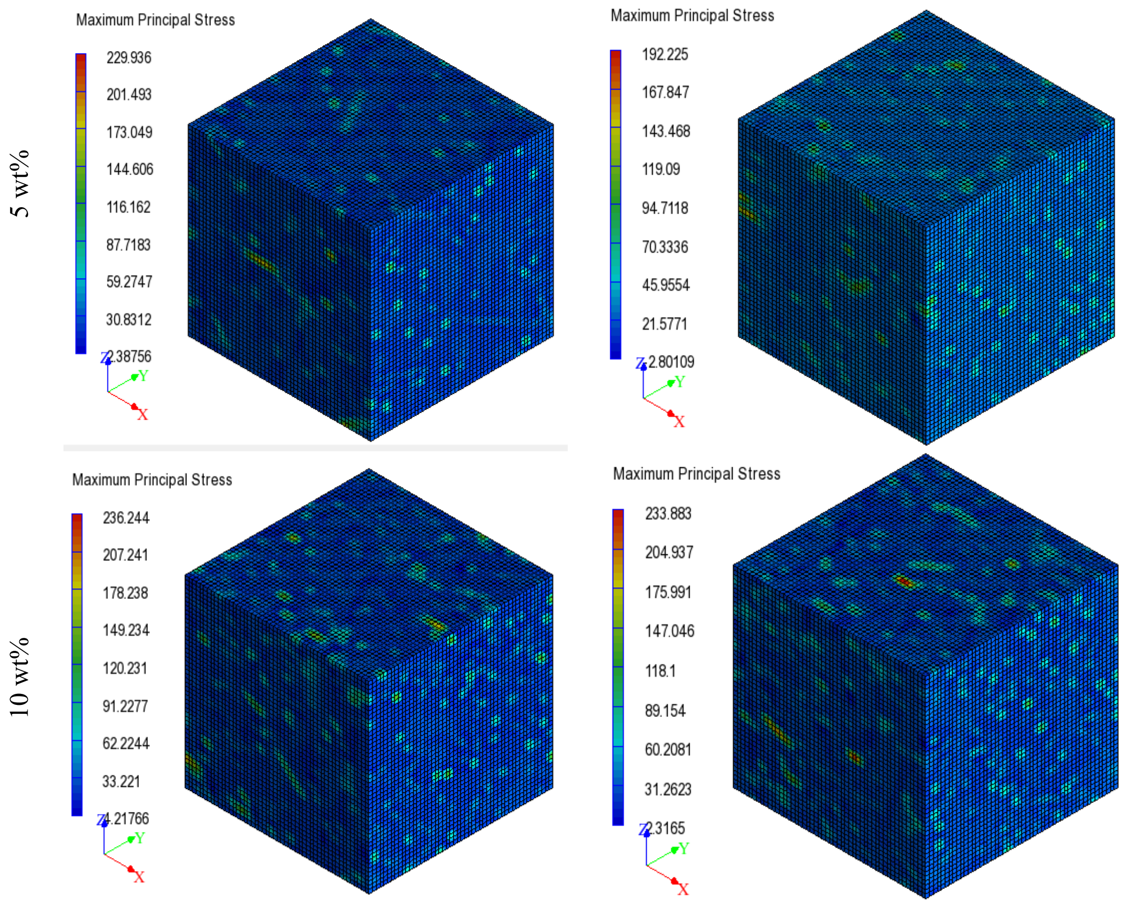


Figure 9:
Elastic modulus of BF/PA66 and GF/PA66 composites

3.2. Digimat-FE

Using Digimat-FE, RVE modeling of BF/PA66 and GF/PA66 composites was performed and the response of the composite structure was analyzed. The effects of basalt and glass fibers on the composite structure in response to the load applied to the composite structure were investigated. In this way, the changes in the stress and strain regions at the micro scale occurring in the composite structure were evaluated.

The stress fields occurring in the randomly distributed RVE models of BF/PA66 and GF/PA66 composite materials are shown in Figure 10 and the strain fields are shown in Figure 11. Looking at Figure 10, it is seen that the stress concentrations in both BF/PA66 composite structures and GF/PA66 composite structures increase with increasing reinforcement ratio. However, when looking at Figure 11, it is seen that, contrary to the stress concentrations of BF/PA66 composite structures, the elongation amounts decrease with increasing reinforcement ratio, and the elongation amounts of GF/PA66 composite structures increase with increasing reinforcement ratio. It is seen that the stress concentrations occurring in BF/PA66 and GF/PA66 composite materials occur in certain parts of the structure and in the fibers. Stress concentrations occurring in the fiber reinforcement material are evidence that the load acting on the composite structure is transferred from the matrix material to the fibers. In this way, the load acting on the composite structure is carried by the fibers, which are more rigid than the matrix material, causing the strength of the composite structure to increase (Harris, 2004; Zhenkun et al., 2010).



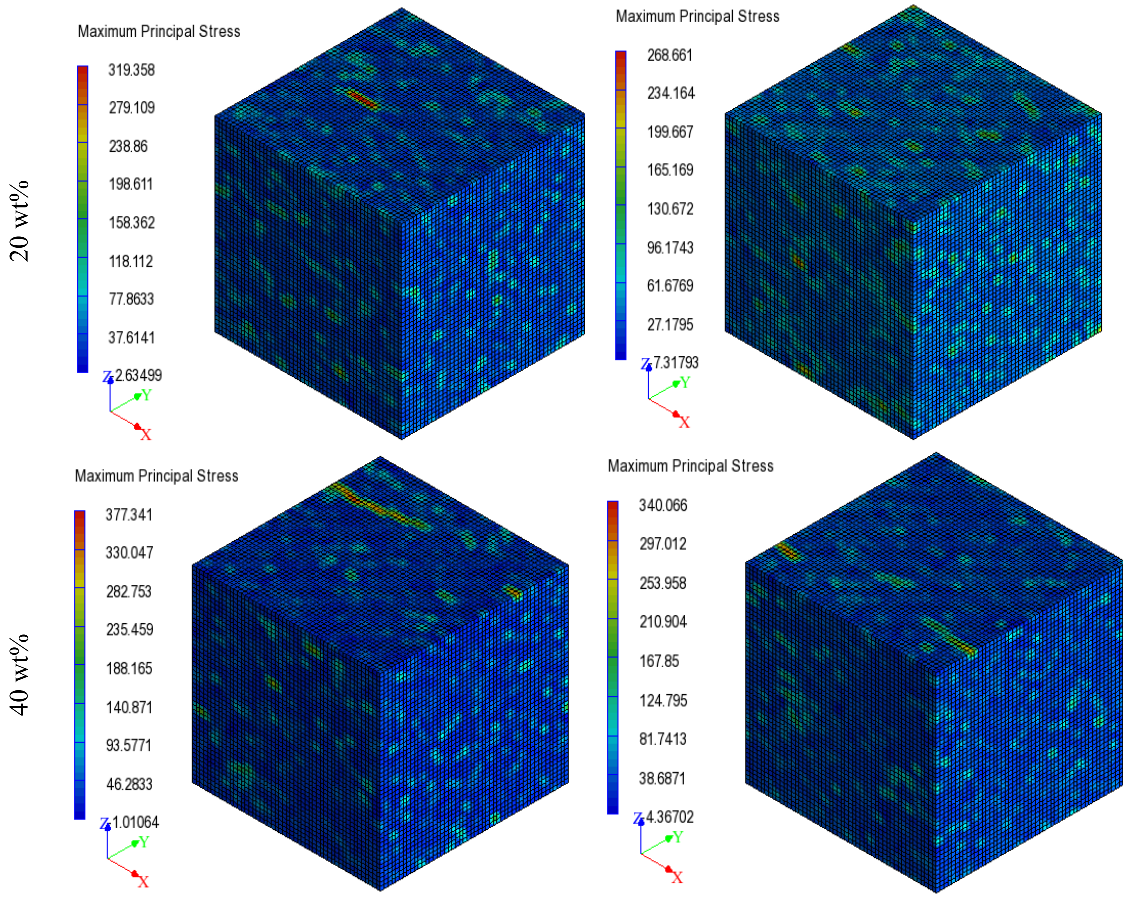
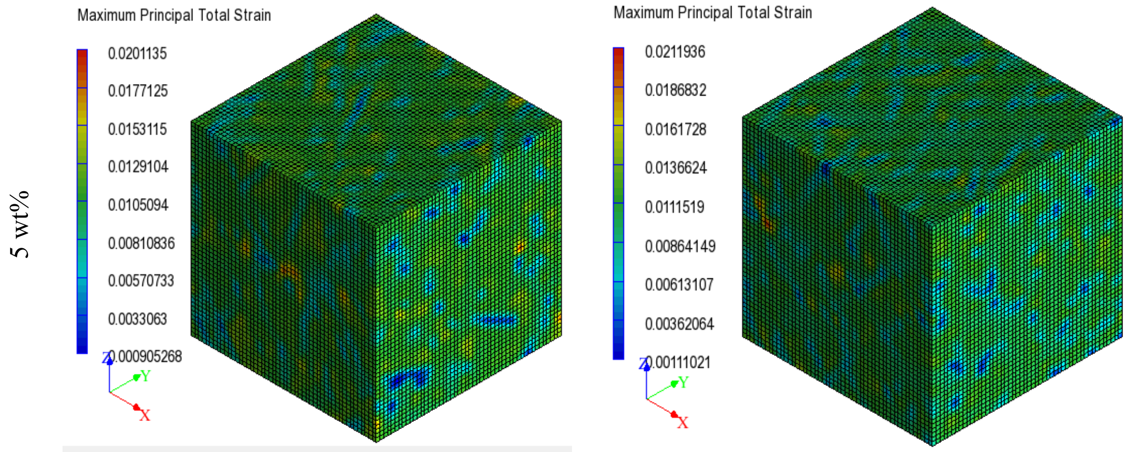


Figure 10:
Stress areas of BF/PA66 (left) and GF/PA66 (right) composites



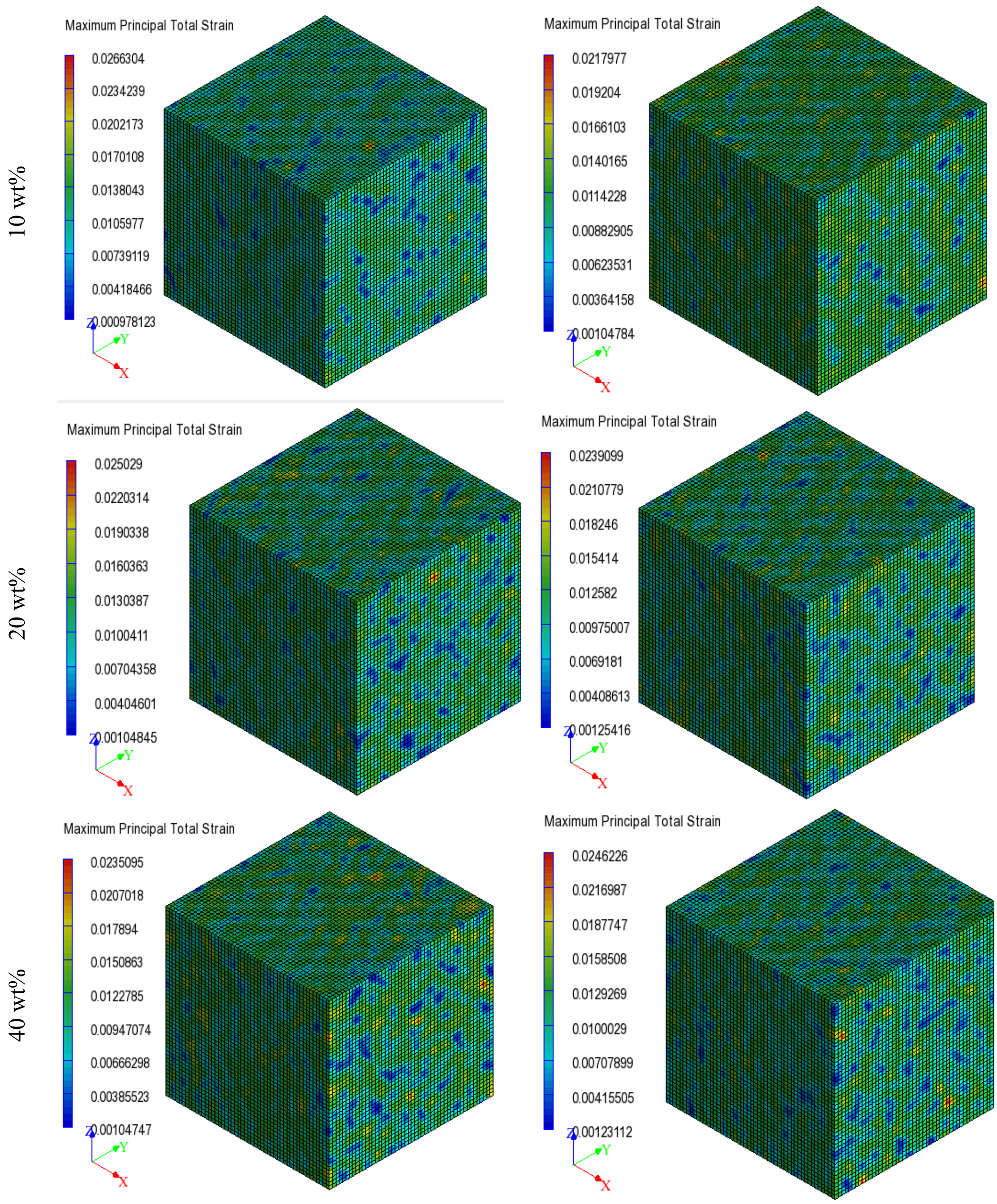


Figure 11:
Strain fields of BF/PA66 (left) and GF/PA66 (right) composites

4. CONCLUSION

In this study, the mechanical properties of BF/PA66 and GF/PA66 composite materials with 5, 10, 20, 40 wt% reinforcement were investigated using Digimat software. The modeling of BF/PA66 and GF/PA66 composites was carried out in Digimat-MF and Digimat-FE software based on MFH. Maximum tensile strengths and elastic modulus of BF/PA66 and GF/PA66 composite materials were calculated with these software. According to the results obtained, different effects of basalt fiber and glass fiber on PA66 matrix composite structure were investigated. In addition, the stress and strain regions occurring at the micro scale in BF/PA66 and GF/PA66 composite materials were analyzed and evaluated. The results obtained as a result of this study are given below;

1- When the mechanical properties of BF/PA66 composite material are evaluated; While the tensile strength of neat PA66 material is 33.70 MPa, the tensile strength of BF/PA66 composite material with 40 wt% reinforcement ratio is 91.87 MPa. While the elastic modulus of neat PA66 material was 3000 MPa, the elastic modulus of BF/PA66 composite material with 40 wt% reinforcement ratio was obtained as 7005.4 Mpa. It was observed that the addition of basalt fiber in PA66 material increased both the tensile strength and elastic modulus of BF/PA66 composite material.
2- When the mechanical properties of GF/PA66 composite material were evaluated; tensile strength of GF/PA66 composite material with 40 wt% reinforcement ratio was obtained as 85.47 MPa. The elastic modulus of GF/PA66 composite material with 40 wt% reinforcement ratio was obtained as 6530.6 MPa. It was observed that the addition of glass fiber in PA66 material increased both the tensile strength and elastic modulus of GF/PA66 composite material.
3- When the mechanical properties of BF/PA66 and GF/PA66 composites were compared; BF/PA66 composite material exhibited higher tensile strength and elastic modulus than GF/PA66 composite material at all reinforcement ratios.

As a general conclusion; the use of natural fibers such as basalt fiber instead of synthetic glass fiber will make a positive contribution in terms of preventing environmental damage. At the same time, the preference of basalt fibers instead of glass fibers in composite material production will provide a high improvement in the mechanical properties of composite structures. On the other hand, time and cost parameters brought by experimental processes are the most important issues in terms of workload in the composite production sector. Digimat composite modeling tools will ensure that factors such as time and cost are minimized in the most efficient way in terms of predicting the mechanical properties of composite materials and damage analysis.

In this study, the Digimat-MF modeling approach used for micromechanical modeling of composite materials offered practical and accurate solutions. Although this modeling approach is not limited to polymer matrix composite structures, it can also be applied to ceramic and metal matrix composites. In future studies, it is planned to analyze micromechanical modeling of polymer matrix hybrid composite materials with the Digimat-MF modeling approach.

CONFLICT OF INTEREST

The author declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

AUTHOR CONTRIBUTION

Author Ferdi Yıldırım contributed to all stages of the study, including conceptualization, research, methodology, writing-original draft, visualization, sources and formal analysis.

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