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Prediction of the Elastic Properties of Ultra High Molecular Weight Polyethylene Reinforced Polypropylene Composites Using a Numerical Homogenisation Approach

Jong-Hwan Yun [1], Yu-Jae Jeon [2] and Min-Soo Kang [3,*]

[1] Mobility Materials-Parts-Equipment Center, Kongju National University, Gongju-si 32588, Republic of Korea
[2] Department of Medical Rehabilitation Science, Yeoju Institute of Technology, Yeoju 12652, Republic of Korea
[3] Division of Smart Automotive Engineering, Sun Moon University, Asan-si 31460, Republic of Korea
* Correspondence: kang10101@sunmoon.ac.kr

Abstract: The elastic properties of polypropylene (PP) and ultra-high molecular weight polyethylene (UHMWPE) textile composites were predicted using finite element analysis (FEA). A three-dimensional (3D) model of composites was generated by introducing a cloth made from UHMWPE fibers into a PP matrix. Regarding the weaving type, the reinforcement was fabricated by replicating plain and twill-woven materials. Additionally, the elastic properties of the composites were compared and evaluated by varying the volume fraction of UHMWPE in the composites from 45% to 75%. The elastic modulus of the composites containing textiles prepared using the plain weaving method was greater than that of the composites containing textiles prepared using the twill weaving method. Along the axial direction, the shear modulus calculation results for the plain-woven reinforcement textiles were distinct. However, the shear moduli in both directions were similar in the twill-woven reinforcement materials. Moreover, the future development of composites should quantify the simulation by measuring the tensile strength and shear strength of real materials.

Keywords: polypropylene; ultra-high molecular weight polyethylene; plain-woven; twill-woven; composites; volume fraction

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1. Introduction

Composites are mixtures of different materials that possess unique properties that cannot be achieved by the constituent materials. In contrast to single-substance materials, the microstructure of composites is neither consistent nor continuous but multiphase. Recently, a demand for weight reduction in many material components has emerged, and thus, the development of polymer-based composites is ongoing. Lightweight, high-strength composites have been developed and implemented based on the fiber reinforcement mechanism. Carbon and glass fibers are commonly used as reinforcements. Owing to its high tensile strength, light weight, and low thermal expansion rate, carbon fiber is extensively used in the aerospace, civil engineering, military, automobile, sports, and various other industries. Furthermore, research and development have been conducted to apply woven fiber-reinforced composites to automotive components, such as B-pillars, battery trays, and trunk floors, which require complicated forms and stability [1]. Despite the advantages, carbon fibers are significantly more expensive than fiberglass or plastic, which are comparable materials. Furthermore, although carbon fibers are highly robust under pulling or bending pressures, they are weak under compression or impact forces. Glass fibers are often used because they are light, strong, and possess the same thermal expansion coefficient as concrete. However, they are less elastic than steel and readily lose mechanical properties at high temperatures. Therefore, several alternatives to these fiber reinforcements have been developed. Ultra-high molecular weight polyethylene (UHMWPE), also known as high-strength high-modulus polyethylene, is one of the world's high-performance materials at present. Owing to its wide range of good characteristics, such as corrosion resistance, wear resistance, and low density, UHMWPE is currently used in military protective materials, military machinery components, aerospace equipment, and other military industries. Among the high-performance fibers, UHMWPE fiber is second only to polyethylene (PE) and polypropylene (PP) fibers in terms of density, and it is the ideal ballistic fiber material with the lowest density. Thus, it is feasible to improve the bulletproof performance of a material while decreasing its weight to achieve the lightweight effect [2–5]. Moreover, it may be possible to produce lightweight, high-strength, and high-rigidity components for various sectors by fabricating composites with UHMWPE. Recently, intensive research has been conducted on the development of composites with high strength using UHMWPE fibers [6–10]. Moreover, several matrix materials for composites have been explored. Among them, PP is the most prevalent. PP is composed of carbon and hydrogen and is a general-purpose resin. PP is a versatile polymer with excellent processing capabilities that can be transformed into films, extrusions, and injection-molded pieces [11]. Furthermore, PP has a high manufacturing volume among all plastics and is a lightweight substance with a specific gravity of 0.9. Consequently, research has been conducted to fabricate composites by combining PP with UHMWPE with the aim of developing high-strength materials [12–19].

The focus of these studies has been on the development of high-strength UHMWPE/PP composites using UHMWPE fibers or discontinuous fillers. However, there is a drawback to fabricating composites by layering and mixing these fiber-based composites in multiple orientations. It is thought that simple composites can be fabricated by weaving UHMWPE yarns into composite reinforcement materials in the form of textiles to enhance the convenience of the process. However, developing composite fillers with these textiles is highly complicated. Therefore, the elastic properties of composites generated by computational simulation will be predicted, and the results will be used as a fundamental database to develop composites based on UHMWPE textiles. The finite element analysis (FEA) method is a powerful tool for predicting the mechanical and physical properties of fibers and composites using numerical simulation. The primary objective is to obtain accurate models of the geometry of woven textiles while describing their mechanical and physical behavior. Compared with experimental studies, numerical approaches have several benefits. Experiments are time-consuming and should only be conducted when there are several variables or when exploring existing textiles. However, the use of three-dimensional (3D) models enables efficient analysis and prediction by facilitating the design of all types of fabric architectures [20–23]. Woven composites are characterized by complex geometries and possess large variations in fiber volume fraction and mechanical behavior because of the type of weaving and interaction between fiber bundles. Therefore, the application and analysis of the structures of parts of woven composites are complicated. To solve the aforementioned problems, various studies have been conducted to model the microstructures of fiber bundles by setting the representative volume element (RVE), which is the unit structure of woven fibers, and to predict RVE characteristics. Thus, the need for a material property prediction method has emerged. Recent research has defined the curvature of woven fibers according to weaving patterns, including plain-woven, twill-woven, and theoretically calculated the fiber volume fraction and fundamental parameters of woven composites [24–27]. Based on these analytical techniques, research has been conducted to predict the physical properties of diverse materials and the behavior of composite materials [28–31]. If research on these fabrics continues, they could replace complex fiber-reinforced composites. Current fiber reinforcement mechanisms are uniaxial and require the simultaneous lamination of fiber-reinforced composites at different angles, which results in a complex and time-consuming process. To overcome these drawbacks, there is a need to develop biaxially isotropic composites.

To compensate for the shortcomings of existing fiber-based composites, the development of woven isotropic composites will expand the range of applications of polymer composites. For further research on UHMWPE/PP woven composites, it is necessary to analyze their elastic properties using finite element analysis methods. In this study, theoretical simulations are used to estimate the elastic properties of composites with the aim of developing high-strength PP-based, UHMWPE-reinforced composites. By replicating plain and twill-woven textiles using UHMWPE fibers, textiles are manufactured, and composite 3D models are generated. Additionally, composites composed of textiles woven with UHMWPE fibers are incorporated into a PP matrix, secured with PP, and analyzed. Furthermore, the volume fractions of PP and UHMWPE in the composites are modified and compared. FEA is performed to analyze the properties of the composites containing textiles with different volume fractions of UHMWPE ranging from 45% to 75%.

2. Materials and Methods

The FEA prediction of fiber structure is largely dependent on the textile 3D models. Conditions such as the twisted structure of the fiber, the material model, and the associated contact boundary conditions should all be considered. Furthermore, modeling is complicated by the nonuniform structure of the 3D textiles and the spatially variable material properties caused by the fiber architectures. Realistic textile geometries should be considered to effectively predict the performance of 3D woven textiles and composites. There are two types of finite element textile models that represent textile microstructures, namely the macroscale continuum and discrete approaches. Furthermore, textiles can be modeled as homogeneous materials at the macroscopic level [32–34]. A discrete mesoscopic analysis can be performed based on the yarn structure. The microscale approach can be used to model the representative methods of fibers in the yarn structures in textiles [35–37]. Micro- and meso-scopic simulations enable deformation analysis during the preforming process and fiber structure construction during the resin injection step. Thus, in this study, an FEA model was generated using micro-modeling to analyze the elastic properties of composites. Figure 1 shows the basic 3D model and tensor notation used in this study. Tensors are illustrated according to the direction of stress to analyze the composites composed of UHMWPE textiles. Here, E represents the elastic modulus, while 1, 2, and 3 represent the x, y, and z axes, respectively. Furthermore, G represents the shear stress applied to the composite surface, and the tensor is expressed by the subscript m for the PP matrix and w for textiles.

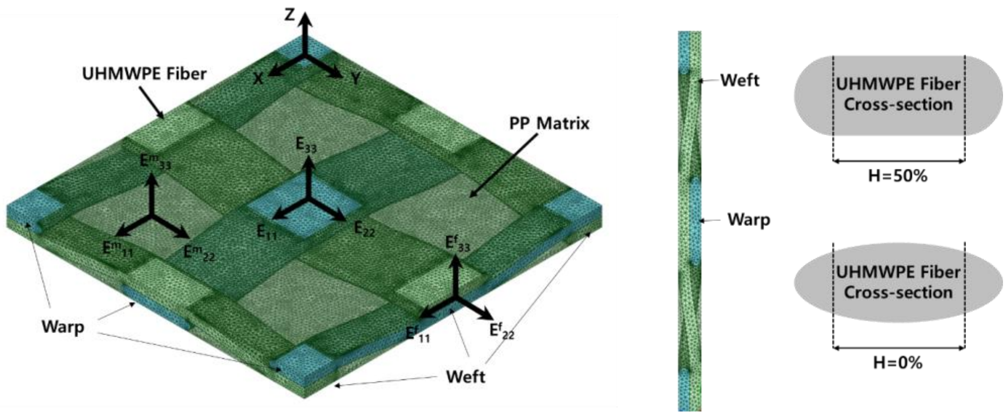

Figure 1. Three-dimensional model and tensor notations.

The properties of PP and UHMWPE used in this study are listed in Table 1 [12,38]. The measured physical properties were based on commercial products. The physical properties of PP were based on Adstif EA5074, manufactured by Polymirae Co., Ltd., (Seoul, South Korea) while those of UHMWPE were based on MIILON XM-220, manufactured by Mitsui Chemical. The materials used were characterized as linear isotropic materials according to their qualities. However, these isotropic materials may be used as anisotropic materials based on the geometry of UHMWPE in the textiles modeled using the ANSYS Material

Designer software. Consequently, depending on the modeled structure, the physical properties may appear as anisotropic material properties in FEA analysis.

Table 1. Properties of PP and UHMWPE.

	PP	UHMWPE
Modulus of elasticity (MPa)	1325	25,000
Shear modulus (MPa)	432.29	10,417
Poisson's ratio	0.43	0.20
Bulk modulus of elasticity (MPa)	3154.8	13,889.0
Density (kg/m^3)	904	950

FEA was used for 3D modeling of composites with UHMWPE textiles using the ANSYS Material Designer software and a homogenization approach. Homogenization theory was used to compute the effective properties of materials or composites with periodic structures. The simulations were performed based on the assumption that the structure is composed of a continuous network of infinitely small unit cells [39–41]. In the case of FEA using homogenization theory, the boundary conditions are symmetrical in all planes. Figure 2 shows the implementation of the 3D model of the composite material based on homogenization theory. A virtual RVE was constructed, and the volume was set to Matrix PP for 3D modeling of PP composites with UHMWPE textiles. The UHMWPE fibers were placed within the PP RVE. Subsequently, 3D modeling was conducted by determining the volume occupied by the UHMWPE textiles in the total composite and by adjusting the volume fraction from 45% to 75% in 5% increments. The fundamental modeling criteria were determined based on the volume fraction such that the oriented UHMWPE textiles were organized in the PP matrix. The element type used for FEA was SOLID187, with a mesh size of 0.5 µm. Because SOLID187 supports the implementation of secondary displacement, it is ideal for creating meshes inside irregularly shaped structures. To reduce the sensitivity of predicting physical properties based on mesh size, the elements used for the PP matrix and UHMWPE fiber were set to the same size. As shown in Figure 1, H corresponds to the horizontal area–length ratio in the fiber cross section. This value is what controls the volume of the fabric while maintaining its shape. In the 3D model used in this study, the final volume fraction of the fabric is controlled by the horizontal area–length ratio of the woven fibers. Consequently, the volume fraction reported in this study was calculated by varying the H values of the fiber. As shown in Figure 2, the H value of the yarn was varied and modeled. The Monte Carlo method was applied to realize a composite model in which the UHMWPE weave is evenly distributed inside the PP matrix. The Monte Carlo method is an algorithm that mathematically approximates a function in modeling through random sampling to implement an iterative model. The Monte Carlo method allows the UHMWPE weave to exhibit the same probability distribution for each location in the PP matrix and allows the model to be infinitely symmetric. Figure 2 shows the modeled shape based on the FEA mode.

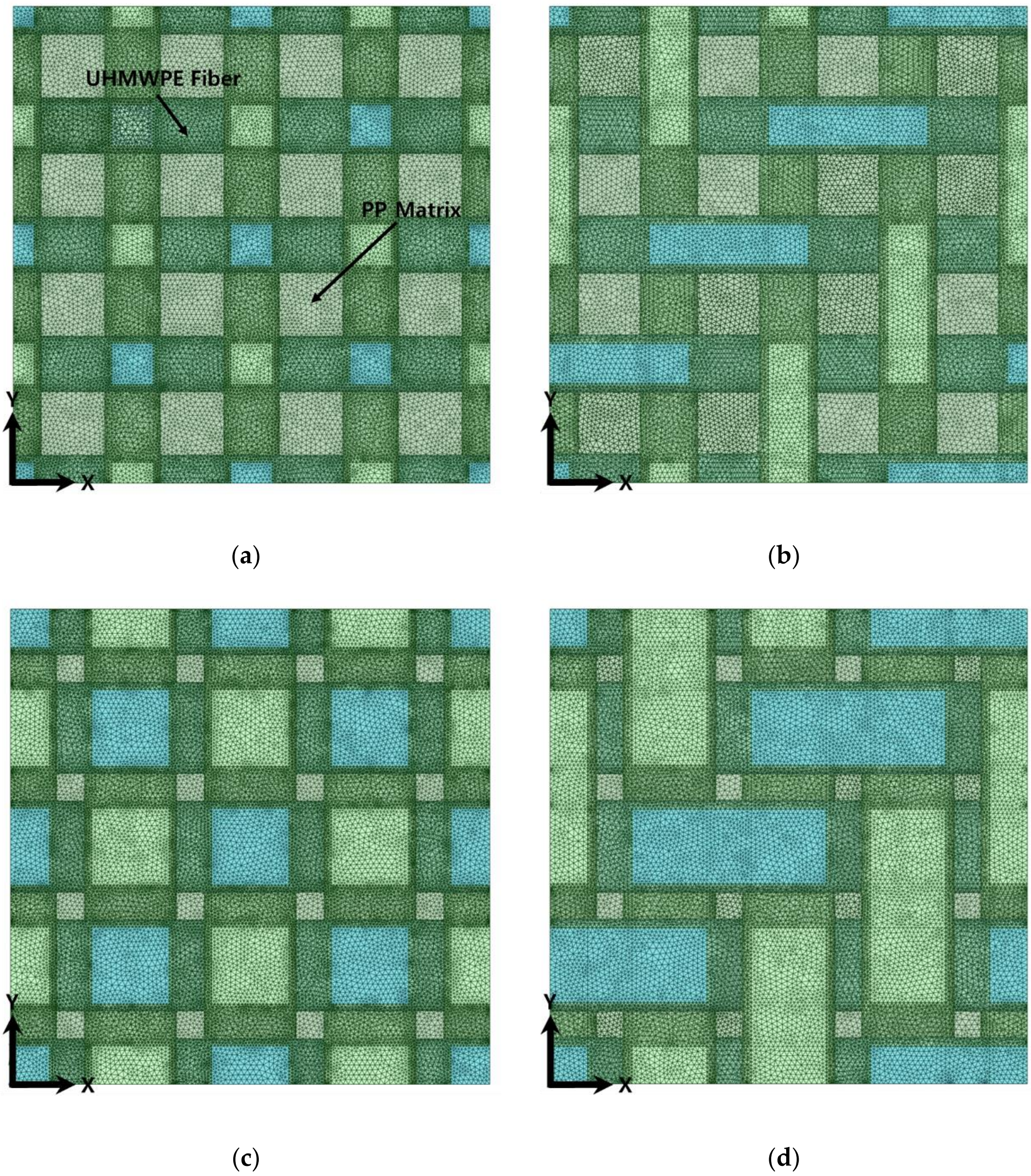

Figure 2. Textile compositions using the plain and twill weaving methods (**a**) Plain weave VF45, (**b**) Twill weave VF45, (**c**) Plain weave VF75, (**d**) Twill weave VF75.

3. Results and Discussion

The elastic properties of composite materials prepared with plain and twill-woven UHMWPE fibers were predicted using FEA, and the results are shown in Figure 3. Textile composites contain fabrics with their fibers arranged perpendicular to each other. Because these fibers are arranged at 90° and 0° angles to each other, forming interwoven textiles, E_{11} and E_{22} of the x- and y-axes of the composites exhibited the same results. In contrast, E_{33}, which is the thickness direction of the composites, has a more distinct trend than E_{11} and E_{22}. When the volume fraction of the UHMWPE fiber was 45%, Plain-E_{11} was estimated to be 9.2 GPa. The elastic modulus increased with increasing volume fraction, reaching 16.0 GPa at an UHMWPE fiber volume fraction of 75%. The Plain-E_{33} elastic modulus was estimated to be 7.7 GPa when the volume fraction of UHMWPE fiber was 45% and 15.4 GPa when the volume fraction was 75%. In contrast, the elastic modulus in the Twill-E_{11} direction was 8.6 GPa at 45% fiber volume fraction and 15.0 GPa at 75% fiber volume fraction. The elastic modulus in the Twill-E_{33} direction was 7.1 GPa at 45% fiber volume fraction and 14.8 GPa at 75% fiber volume fraction. The difference in elastic modulus between E_{11} and E_{33} with increasing fiber volume fraction was insignificant. Based on the findings of this study, the elastic modulus of the composites, including the textiles prepared by the plain weaving method, was demonstrated to be greater than that of the textile composites prepared by the twill weaving method. The elastic modulus is a value that represents the stiffness of a material and is defined as the stress-to-strain ratio. The elastic modulus may be calculated using the slope of the elastic section of the stress–strain curve obtained from tensile or shear experiments performed on material specimens. Notably, the elastic modulus can be used to calculate the response of a material to a load. For example, it is feasible to predict how much a steel wire will stretch under tension or how much a column will buckle under compression. Thus, when UHMWPE is woven into a plain weave and used for composite fabrication, the stress and strain under an axial load are minimal. However, this is not true in the case of tensile strength. Tensile strength is a force that reflects the strength of a material. It is calculated by dividing the largest load that a material can resist when pulled in the direction of its length by the cross-sectional area of the material. Thus, to precisely determine the tensile strength, tensile tests should be performed on plain and twill-woven UHMWPE/PP composites, and the maximum stress should be compared. Generally, it is concluded that tensile strength, abrasion resistance, stiffness, and pilling resistance are higher in plain-woven composites compared with twill-woven composites because these mechanical properties are enhanced by increasing the number of interlacements of the warp and weft yarns and decreasing the number of floats in the weave. However, tearing strength is higher in twill-woven composites because this property increases with an increasing number of floats in the weave and fewer interlacements [42]. Thus, plain-woven textiles are suitable for composites that require high flexibility.

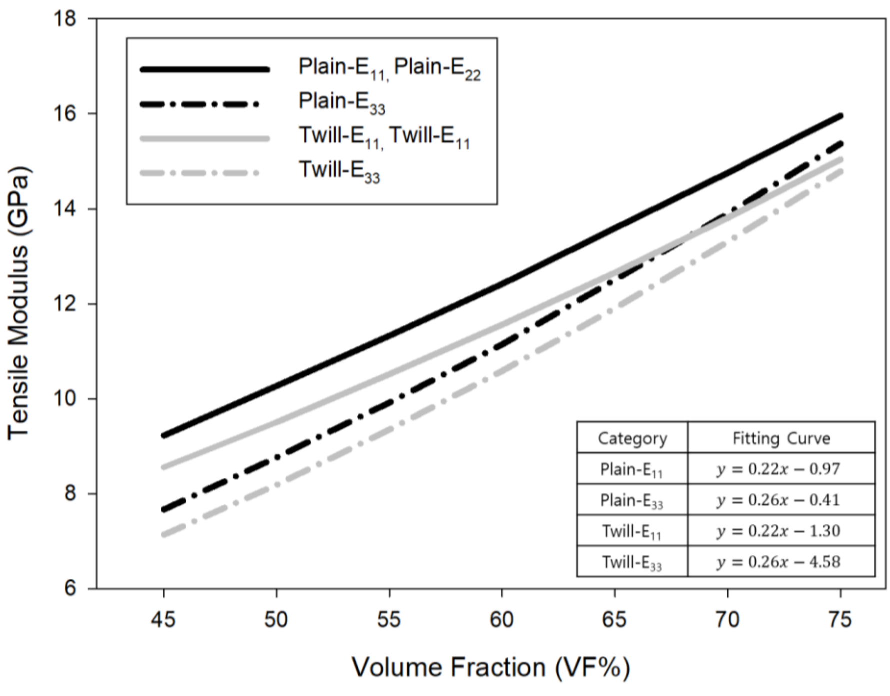

Figure 3. Comparison of the predicted values of elastic modulus.

Fabrics are generally constructed by the alternating arrangements of fibers; thus, G_{23} and G_{31} of the x- and y-axes of the composites exhibited the same results. Figure 4 shows the predicted shear modulus behavior of the composites in relation to the UHMWPE fiber volume fraction based on FEA. The shear modulus of Plain-G_{12} was estimated to be 1.8 GPa when the volume fraction of plain-woven UHMWPE was 45%, and it increased to 4.9 GPa when the UHMWPE volume fraction was 75%. The shear moduli of Plain-G_{23} and Plain-G_{31} were estimated to be 1.4 GPa when the UHMWPE volume fraction was 45% and 3.8 GPa when the UHMWPE volume fraction was 75%. When the twill-woven UHMWPE fibers were used as reinforcements in the composites, the shear moduli of Twill-G_{12}, Twill-G_{23}, and Twill-G_{31} were equivalent at approximately 1.6 GPa when the UHMWPE volume fraction was 45%. Even at a UHMWPE volume fraction of 75%, similar shear moduli were observed at 4.2 and 4.3 GPa. This trend appears to be the same as for isotropic materials, but it is not. The shear modulus is a measure of the elastic shear stiffness of a material and is defined as the shear stress-to-shear strain ratio [43–45]. Therefore, it is assumed that the shear stress applied to each shaft surface is identical in the shear elasticity section of the composites prepared with twill-woven UHMWPE fibers as reinforcements. This characteristic is applicable only in the elastic range of a material. If the plastic deformation of a real composite material is analyzed using the graph of the change in the breaking point of the material obtained by the shear test, it may appear as an anisotropic material depending on the orientation and characteristics of the fiber textiles. Therefore, additional tests are required to evaluate the isotropic and anisotropic properties of the material. Several investigations have demonstrated that locations with significant warp–weft intersections in fiber textiles induce stress concentration, which leads to cracks, and thus they serve as crack initiation points [46–48]. Consequently, there may be differences between the plain and twill-woven textiles. Thus, it is thought that the tensile and shear strengths of plain-woven textiles with multiple warp–weft intersections will be low.

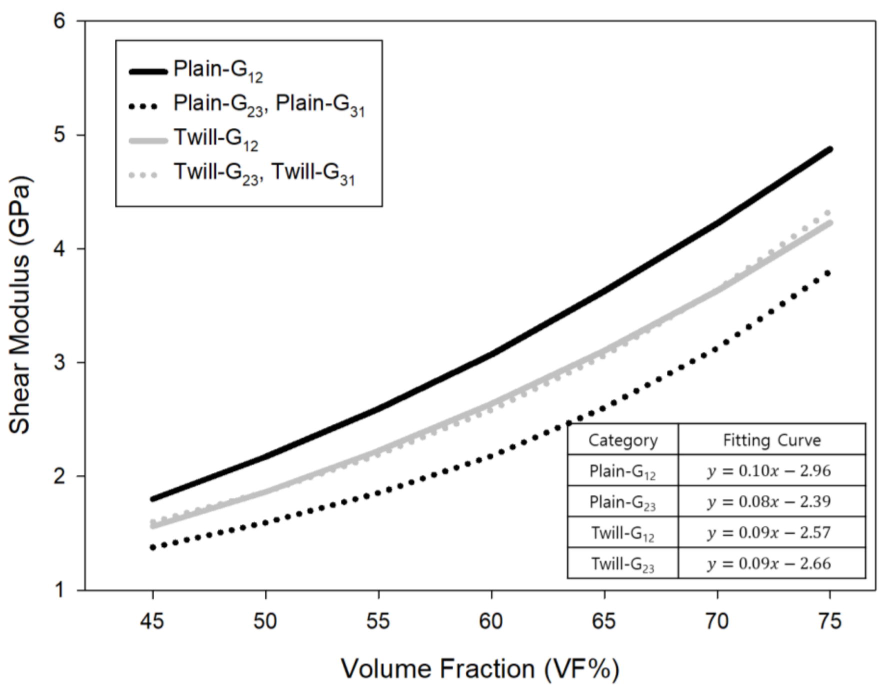

Figure 4. Comparison of the predicted values of shear modulus.

Figure 5 shows the Poisson's ratio results estimated by FEA for the composites prepared with UHMWPE textiles. Poisson's ratio is one of the fundamental properties of any engineering material and represents key mechanical characteristics for woven textiles in many applications, including in engineering systems that incorporate textiles as structural elements. The magnitudes of Poisson's ratios can reach unexpected values for woven textiles, which are significantly different from those for conventional engineering materials, leading to unusual stress–strain behavior [49,50]. The Poisson's effect in a woven textile originates from the interaction between the warp and weft yarns and can be expressed in terms of the structural and mechanical properties of the system. This characteristic is exclusive to textiles and different from a typical continuum, although their mechanical characteristics are relatively similar. The Poisson's ratio calculation result for the composites based on FEA revealed that when the UHMWPE volume fraction increases, the effect of UHMWPE in the composite increases and the Poisson's ratio decreases. Furthermore, a difference in the Poisson's ratio between the twill weave and plain weave was observed, and the Poisson's ratio of the twill weave was higher. The Poisson's ratio of Plain-$_{v12}$ was estimated to be 0.22 at 45% UHMWPE volume fraction and decreased to 0.20 when the UHMWPE volume fraction increased. As the UHMWPE volume fraction increased, the Poisson's ratio of the Plain-$_{v13}$ composite decreased from 0.31 to 0.23. Similarly, the Poisson's ratio of Twill-$_{v12}$ decreased from 0.21 to 0.19 as the UHMWPE volume fraction increased, while that of Twill-$_{v13}$ decreased from 0.34 to 0.24. These characteristics may be analyzed owing to the difference in the number of orthogonal points of UHMWPE fibers depending on the weaving conditions. In the plain weave, orthogonal fiber points are constantly generated, but in the twill weave, fewer orthogonal fiber points are formed than in the plain weave. Thus, the strain from the external force is greater, resulting in the above-mentioned characteristics.

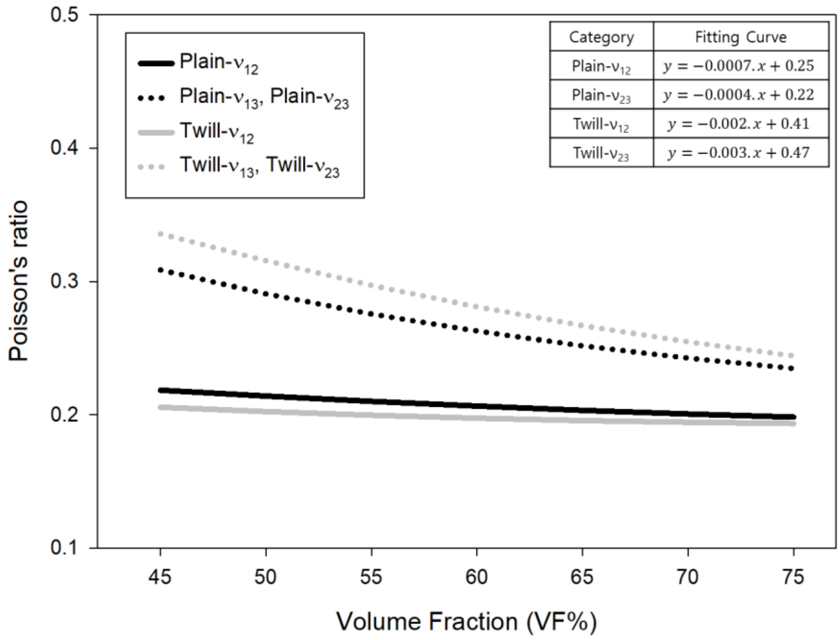

Figure 5. Comparison of the predicted values of Poisson's ratio.

Past research on the mechanical properties of woven materials through fibers has shown that the weave structure plays an important role. Among the composites tested, plain weave laminates have proven to have better properties than twill laminates. Plain weave fabrics are characterized by better resistance to deformation, and because they are less deformed, their modulus of elasticity and shear modulus are measured to be larger [51]. The results of the finite element analysis of the present study are as follows: the composites with plain weave fabrics have a higher property modulus and less variation in Poisson's ratio than the composites with twill weave fabrics, which is in good agreement with the finite element analysis conducted in this study.

4. Conclusions

In this study, preliminary research was conducted to develop PP-based, UHMWPE-reinforced, high-strength composites. FEA was used to estimate the elastic properties of the UHMWPE/PP textile composites. As a reinforcement, a textile woven with UHMWPE fibers was incorporated into the PP matrix. In terms of the weaving type, the reinforcements were fabricated by replicating plain and twill-woven textiles. A composite 3D model was generated based on these composite development requirements. Furthermore, the elastic properties of the composites were compared and analyzed by varying the volume fraction of UHMWPE fibers incorporated into the composites from 45% to 75%.

(1) The UHMWPE fibers were organized in the composites as reinforcements, which were positioned perpendicular to each other to form the textile composite. Consequently, E_{11} and E_{22} of the x- and y-axes of the composites exhibited the same results. In contrast, E_{33} (the thickness direction of composites) exhibited a different trend compared with E_{11} and E_{22}. Based on the comparative analysis of the estimated elastic modulus values, the elastic modulus of the composites with textiles fabricated using the plain weaving method was superior to that of the textile composites fabricated using the twill weaving method.

(2) Based on the comparative analysis of the calculated shear modulus values, G_{23} and G_{31} of the x- and y-axes of the composites exhibited the same results, owing to the interwoven fibers. The shear modulus calculation results for the plain-woven reinforcement textiles were different. In contrast, for the twill-woven textiles, the shear modulus in all directions exhibited similar values.

(3) The elastic properties of composites depend on the properties and volume fractions of the materials used. As the volume of the UHMWPE weave increases, the material's properties improve due to the superior properties of UHMWPE. Alternatively, if the volume fraction of UHMWPE is reduced, the material properties can be closer to PP.

(4) Based on the comparative analysis of the calculated Poisson's ratio of the composites, the strain caused by the twill weaving method was larger. Furthermore, it was confirmed that the plain-woven textiles with numerous weft and warp interlacements had a smaller strain.

Therefore, when fabricating composites with textile-type reinforcements, the type of textile reinforcement used may be determined based on the application and physical properties. Furthermore, for an accurate computation, the simulation for developing composites should be quantified by measuring the tensile and shear strengths of real composites.

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