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Multi-scale modeling and simulation of natural fiber reinforced composites (Bio-composites)

Jagath Narayana K

Multi-Functional Composites Lab, Mechanical Engineering Department, Shiv Nadar University, UP - 201314, India.

E-mail: `kn469@snu.edu.in`

Ramesh Gupta Burela

Multi-Functional Composites Lab, Mechanical Engineering Department, Shiv Nadar University, UP - 201314, India.

E-mail: `rameshgupta.iisc@gmail.com`

Abstract. This work presents the numerical analysis of natural fiber reinforced composites (from renewable sources), to evaluate the mechanical behavior of Bio-composites and elucidated the role of micro-mechanical analytical models (Rule of Mixtures and Halpin-Tsai models). Specifically, this study is carried out to perform the Multi-scale modeling and simulation of Bio-composite that constitute of sisal fiber reinforcement and Epoxidized Soybean-Oil (ESO) based matrix. In general, it is difficult to predict the effective properties of natural fiber reinforced composites due to its heterogeneous properties. The Representative Volume Element (RVE) model is capable to estimate the effective properties of Bio-composites. Therefore, RVE model is designed and analyzed based on micro-mechanics by taking the individual properties of fiber and matrix as an input. As a result, the effective properties of Bio-composite can be obtained. Subsequently, a 3-D model of Bio-composite laminated plate behavior is analyzed based on macro-mechanics by taking the effective properties of Bio-composite obtained from micro-mechanical analysis. The obtained effective properties of Bio-composite are validated with the theoretical (Rule of Mixtures) results. The micro-mechanical analysis is carried out using the Digimat (Multi-scale modeling and simulation tool) and macro-mechanical analysis is performed using Ansys software.

1. Introduction

In the last two decades, the dumping of waste from non-biodegradable materials has become a major problem; these are responsible for damaging the environment and causing the all types of pollutions. To keep the environment green, decreasing the use of such materials is compulsory for the pollution free future [1, 2]. The demand of composite materials is increasing in automobile and aeronautical industries, but synthetic fibers and non-biodegradable resins as matrix utilized to make composites are creating serious environmental problems due to its poor recycling and the characteristics of non-biodegradability. The natural fiber reinforced composites are used in specific applications such as car bumpers, door inner trim panels and aircraft interior structures [3–6].

In the last few years, the continuous development and usage of natural fiber reinforced composites has been increased in various commercial applications due to substantial advantages such as biodegradability, low specific weight, availability (derived from renewable sources), non-corrosive nature and low cost [7–9]. In the literature, there are few studies on design and numerical simulation of natural fiber reinforced composites compared to the experimental work. So there is a lot of scope to work on the modeling and simulation of these composites at different scales to determine its micro and macro-mechanical behavior using multi-scale modeling tools [10–12]. Through micro-mechanical approach one can find the effective mechanical properties of a composite and these properties are used as an input to macro-mechanical analysis. The micro-mechanical approach is an efficient and powerful tool to determine the linear and nonlinear behavior of composites in terms of its mechanical properties and stress-strain relations [13–15].

The accuracy in estimating the overall properties of composite materials depends predominantly on how precisely input constituents (fiber and matrix) are defined. Through experimental methods, understanding and estimating the mechanical properties is an expensive process. It is difficult to find the interface behavior between the constituents using experimental methods so as computational micro-mechanics based simulations are useful in these situations [16]. If the internal boundaries of composite materials are ignored, then one can use the macro-mechanics to model the composite material based on the homogenized or effective properties. On the other end, micro-mechanics attempts to consider the internal boundaries of composite material and accounts the effects of its internal arrangements by taking its individual constituent material phases [17]. From the literature, some of the text on natural fibers, bio-based resins and natural fiber reinforced composites are presented below.

Natural fibers such as jute, sisal, banana, flax and hemp have economical and ecological advantages over synthetic fibers, these are favor to go green technology in composite manufacturing system [18–20]. The biodegradable polymers such as starch, protein and cellulose are mostly used in the bio-applications [21]. Among the different verities of natural fibers available from renewable sources, the sisal fiber is the most promising reinforcement material due to its good mechanical properties and high cellulose content compared to the other natural fibers [22]. The researchers are showing enormous interest in the recent years to develop the bio-based resins along with the natural fibers to increase the bio content in the composite material. Among them, the incorporation of Epoxidized Soybean Oil (ESO) and Poly Furfuryl Alcohol (PFA) in composite resins are the prominent research interests, these resins can increase the bio-based content (as a constituent material) in the bio-based composite [23, 24]. The leading research work on natural fiber reinforced composites are presented below.

Khan et al. presented the development of Eco-friendly composites with woven jute fabric reinforced poly lactic acid composites and fabricated by hot press molding method. The investigation is carried out on the influence of woven structure and direction of jute fiber [25]. Zhu et al. presented the inexpensive and alternative manufacturing process (pultrusion) for epoxidized soy-based resin and illustrated the mechanical characterization of composites. By partially replacing the epoxy resin with the epoxidized soy-based resin leads to the significant cost reduction of composite based structural components. Soy-based resins are not only low cost resins but also biodegradable and renewable materials. Hossain et al. developed jute fiber reinforced composites that are fabricated using Vacuum Assisted Resin Infiltration (VARI) method with different stacking sequences with fiber volume percentage of 25%. They emphasized the difficulties in fabricating the unidirectional jute fiber reinforced composites [26].

Niedermann et al. described the influence of epoxidized soybean oil on the modulus of jute fiber reinforced epoxy resin composite. Epoxidized soybean oil is probably the most important one in the research area of epoxidized vegetable oils (EVO) based composite matrix [27]. Porras et al. illustrated the development (film stacking lamination) and characterization of natural fiber (bamboo) reinforced composite (Poly Lactic Acid as matrix), these constituents are used

to make the composite as fully biodegradable green composite laminate with their environmental friendly nature [28]. Hosseini et al. developed a micro-mechanical model to estimate the mechanical properties of flax fiber reinforced polyurethane matrix based composite [14]. Das et al. developed a micro structure-guided modeling technique to estimate the effective elastic properties of heterogeneous materials, in its applications periodic boundary conditions are used as a strain controlled numerical simulation [29]. Borovkov et al. presented the homogenization using finite element procedure [30].

The present paper provides the fundamental information about the constitutive materials of bio-based composite material (illustrated by its individual material properties). Subsequently, focused on the micro and macro (Multi-scale) analysis of bio-based composites specifically for sisal fiber reinforced composite (epoxidized soybean-oil resin as a matrix). The micro-mechanical analysis is carried out using Digimat and the macro-mechanical analysis by using Mechanical Ansys Parametric Design (MAPDL).

2. Multi-scale modeling
In the last few years, the material modeling of natural fiber reinforced composites is one of the challenging areas in bio-based composites. In general, both bio-based and synthetic composite materials are anisotropic and heterogeneous due to these properties it is very difficult to evaluate its homogenized properties and performing a reliable analysis is also difficult using traditional techniques based on macroscopic constitutive models. Therefore, it is necessary to adopt efficient procedures for the composite material characterization, the traditional procedures that are applied to metals are not sufficient due to the complexity involved in the micro structure of composites [31].

In this paper, Multi-scale approach can be seen in two scales, first is at micro-level and second is at macro level. The fiber and matrix behavior corresponding to its micro-level analysis is required due to the composite heterogeneous nature.In the current context, to predict the behavior of bio-based composites in a realistic way, it is necessary to model these composites at micro scale. Therefore, micro-mechanics is applied on bio-based composites to predict the characteristic behavior by analyzing the constituent materials (fiber and matrix). The detailed process of Multi-scale modeling and analysis is shown in Figure 1.
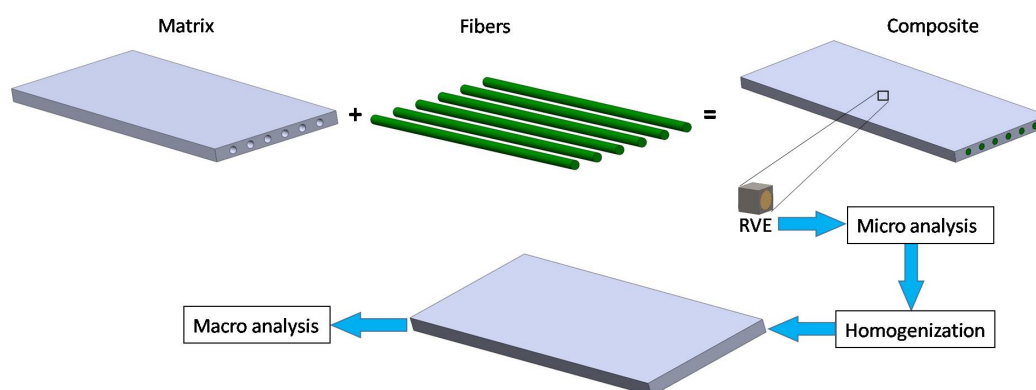

Figure 1. Process of Multi-scale modeling and analysis of composites.

CAE engineers and scientists in material science, uses the solutions obtained from these computational tools to accurately estimate the behavior (micro/macro level) of composite

materials and structural components. Thus, Multi-scale modeling tools help the end users to design an innovative composite materials and structural components.

3. Micro-mechanical analysis

Micro-mechanics is the study on behavior of constituent materials (fiber and matrix), influence of its volume fractions on the composite behavior and the detailed examination of interface behavior between the fiber and matrix [32]. The behavior of composite constituent materials can be represented based on its individual constitutive models. These models are adopted as the basis to develop homogeneous constitutive model of composite material [33]. Micro-mechanical analysis is an important and most common approach to assess the elastic constants of composite materials from known mechanical properties of their individual constituent materials through Representative Volume Element (RVE) model of a composite [16].

It is impossible to analyze the structural problem computationally at the micro-level. Therefore, one can consider RVE that comprise of heterogeneous micro structure and assume that each material point within the structural component is the center of RVE. Subsequently, the behavior of RVE can be considered as the basis for macro-level analysis by taking the effective mechanical properties obtained using homogenization process [34].

There are two powerful techniques in order to solve the RVE problem; those are Mean-Filed Homogenization (MFH) and Finite Element Homogenization (FEH). MFH approach is based on semi-analytical models such as Mori-Tanaka and Eschelby J.D models [35, 36] in order to estimate the volume average of stresses and strain fields. Another approach FEH is based on finite element formulations [37, 38]. In this context, Digimat-MF based on MFH and Digimat-FE based on FEH are used to solve RVE problem. Digimat-FE is used to solve realistic RVE models, the resulting model can be solved by FEA solver but it has two major drawbacks; meshing difficulties for realistic models of RVE and computationally expensive for nonlinear problems. Digimat-MF is easy to model and takes less computational time. To illustrate these approaches or practicing these techniques one can observe the influence of fiber length, volume fraction of fiber, fiber orientation in the micro structure, this information is the basis for microscopic responses of the Bio-composites.
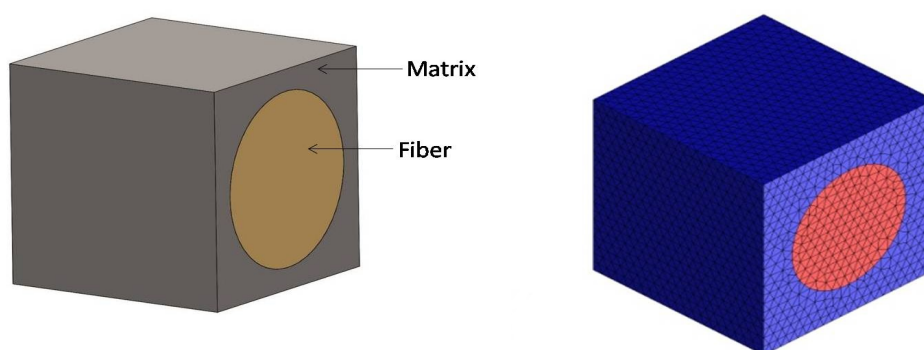

Figure 2. Design model (left) and mesh representation (right) of RVE.

The analyzed RVE design model and mesh model is shown in the Figure 2, the dimensions of RVE are shown in the Figure 3. The RVE length $L_m = 0.3$ mm, width $W_m = 0.3$ mm, height $H_m = 0.3$ mm. The fiber diameter $D_f = 0.2$ mm and the fiber length is same as RVE length [39–41]. It is necessary to provide constituent material properties to perform the micro-mechanical analysis in order to evaluate the effective properties. The constituent materials of adopted
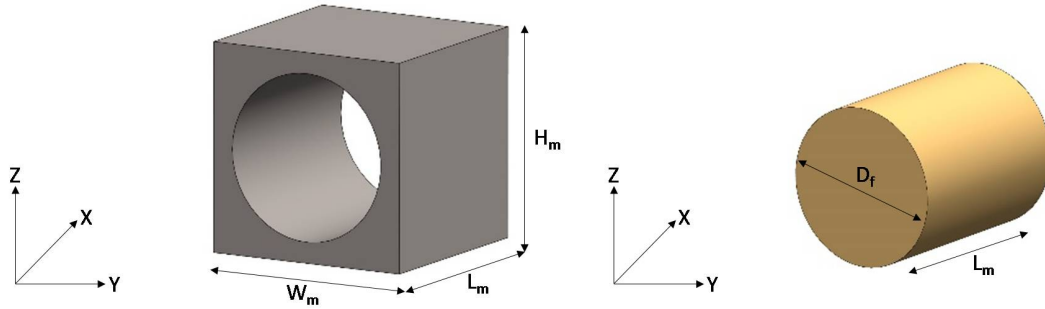
Figure 3. Dimensional representation of RVE.

Bio-composite are sisal fiber and Epoxidized Soybean-Oil based epoxy matrix (ESO) , these individual constituent mechanical properties [42, 43] are specified in the Table 1. Generally, the basic description of composite material can be specified based on the volume fraction of constituent phases. Typically for two-phase fiber-reinforced composites, it is sufficient to specify the fiber volume fraction (V_f) where the matrix volume fraction (V_m) can be determined using, $V_m = 1 - V_f$, because the sum of two phases must be equal to one.

Table 1. Mechanical properties of sisal fiber and ESO matrix [42, 43].

Material	Youngs modulus (GPa)	Poisson's ration	Density (Kg/mm^3)
Sisal fiber	12	0.2	1.60e-6
ESO matrix	1.353	0.4	1.45e-6

The Periodic Boundary Conditions (PBC) are applied to the RVE model of bio-based composite micro structure. Since, these boundary conditions shown that the better approximation in estimating the effective properties for even relatively small size of RVE models [44]. To apply PBC on RVE model one has to impose the continuity criteria at the RVE boundaries connected to the neighbor RVE in order to ensure the combination of all individual RVEs as a structural continuum body. In detail, the continuity criteria applied in terms of displacements so that the adjacent RVEs cannot be separated or penetrate each other [45]. The periodic boundary conditions are expressed as:

$$u_i = \bar{\epsilon}_{ij} x_j + v_i \tag{1}$$

where ϵ_{ij} are the average strain components, v_i is the displacement components of the periodic part (local fluctuation on boundary surfaces), u_i displacements of RVE in x_j direction. The displacement components on opposite boundary faces are represented as:

$$u_i^{n+} = \bar{\epsilon}_{ij} x_j^{n+} + v_i^{n+} \tag{2}$$

$$u_i^{n-} = \bar{\epsilon}_{ij} x_j^{n-} + v_i^{n-} \tag{3}$$

where $n+$ and $n-$ are representing the positive and negative direction of x_j respectively. In RVE model, the periodic parts of displacement components v_i^{n+} and v_i^{n-} are identical on the opposite boundary faces. The difference between Equation (2) and (3) is calculated as:

Table 2. Elastic constants of Bio-composite obtained from Digimat.

Elastic constants	Values	Units
E_{11}	5095.8	MPa
E_{12}	2519.8	MPa
E_{23}	2519.8	MPa
G_{12}	875.17	MPa
G_{13}	831.53	MPa
G_{23}	831.53	MPa
ν_{12}	0.324	-
ν_{13}	0.492	-
ν_{23}	0.492	-

$$u_i^{n+} - u_i^{n-} = \overline{\epsilon}_{ij}(x_j^{n-} - x_j^{n+}) = \overline{\epsilon}_{ij}\Delta x_j \tag{4}$$

where Δx_j is the RVE edge length. To solve the RVE problem under the defined boundary condition, volume averaging over the RVE of micro strain and stresses within the RVE is equal to the strains and stresses at micro-scale. Further, relating these obtained mean values of strains and stresses for a linear elasticity problem can provide the effective stiffness (macro-scale) of the composite (Bio-composite). The stress-strain relation of a RVE model is typically expresses as:

$$\overline{\sigma}_{ij} = C_{ijkl}^* \overline{\epsilon}_{kl} \tag{5}$$

$$\overline{\sigma}_{ij} = \frac{1}{\Omega} \int_\Omega \sigma_{ij} \, d\Omega \tag{6}$$

$$\overline{\epsilon}_{ij} = \frac{1}{\Omega} \int_\Omega \epsilon_{ij} \, d\Omega \tag{7}$$

where $\overline{\sigma}_{ij}$ and $\overline{\epsilon}_{ij}$ are the average stresses and average strains respectively. Ω is the volume of periodic RVE. The finite element based formulation is expressed as:

$$\overline{\sigma}_{ij} = \sum_{k=1}^{N} \sigma_{ij}^k \, \Omega^k \tag{8}$$

$$\overline{\epsilon}_{ij} = \sum_{k=1}^{N} \epsilon_{ij}^k \, \Omega^k \tag{9}$$

where k is the finite element label, N is the total number of finite elements in the RVE model. The obtained elastic constants using Digimat tool is presented in the Table 2.

Various micro-mechanical analytical models have been implemented and applied to evaluate the effective properties of bio-based composite materials, those are Rule of Mixture (RoM), Halpin-Tsai etc [46]. RoM is used rigorously for synthetic composite materials and this model can be applicable for natural fiber reinforced composite materials [47, 48]. The RoM is the simplest and effective analytical model for micro-mechanical analysis; this can be used to predict the overall properties of bio-based composites. The equation that relates the composite axial elastic modulus to the fiber and matrix axial elastic modulus using their volume fractions is written as:

$$E_1^c = E_1^{(f)}V_f + E_1^{(m)}V_m = E_1^{(f)}V_f + E_1^{(m)}(1 - V_f) \tag{10}$$
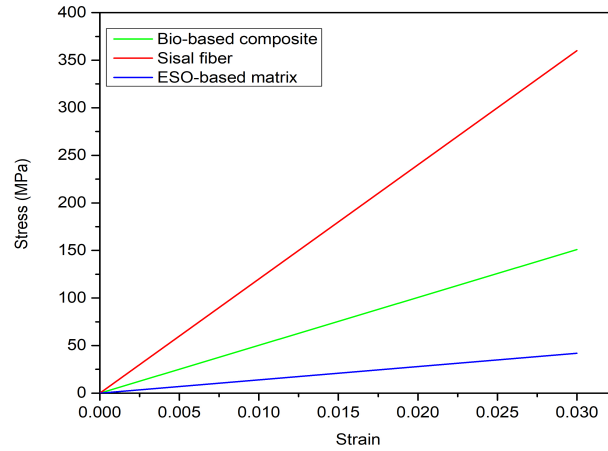
Figure 4. Stress-strain relation of sisal fiber, ESO matrix and bio-based composite.
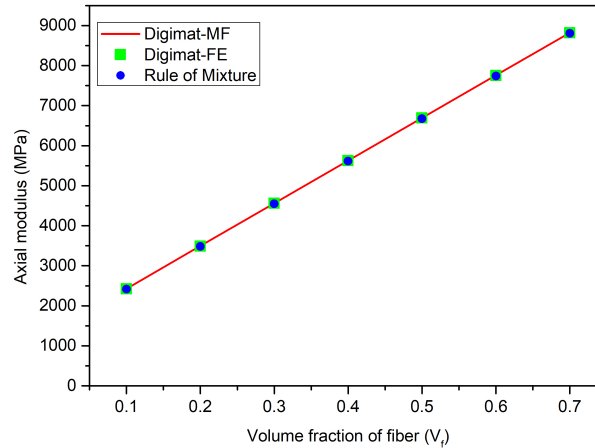

Figure 5. Axial modulus comparison with different fiber volume fractions.

where E_1^c is the axial elastic modulus of composite; E_1^f and E_1^m are the axial elastic modulus of fiber and matrix respectively. The equation used to calculate the effective in plane Poisson's ratio of composite based on the RoM is expresses as:

$$\nu_{12}^c = \nu_{12}^{(f)} V_f + \nu^{(m)} V_m = \nu_{12}^{(f)} V_f + \nu^{(m)}(1 - V_f) \tag{11}$$

where ν_{12}^c, $\nu_{12}^{(f)}$ and $\nu^{(m)}$ are the Poisson's ratios of composite, fiber and matrix respectively. The equation that relates the composite transverse elastic modulus to the fiber and matrix elastic modulus using their volume fractions is written as:

$$\frac{1}{E_2^c} = \frac{V_f}{E^{(f)}} + \frac{V_m}{E^{(m)}} = \frac{V_f}{E^{(f)}} + \frac{(1 - V_f)}{E^{(m)}} \tag{12}$$

where E_2^c is the effective transverse elastic modulus of composite; E^f and E^m are elastic modulus of fiber and matrix respectively.One of the assumption made in using the RoM model is the interface between the fiber and matrix is perfectly bonded. The assumption made for this RoM model may be unrealistic for some of the real life structural components, for those situations it is reasonable to adopt Hapin-Tsai model, this is a semi-empirical model and can be used to predict the effective properties of composites for non-perfectly bonded fiber-matrix interface conditions. The estimation of axial youngs modulus using Halpin-Tsai analytical model for a unidirectional composite is expressed as:

$$E_1^c = \frac{E^{(m)}(1 + \eta \xi V_f)}{1 - \eta V_f} \tag{13}$$

where η is specified as:

$$\eta = \frac{E^{(f)} - E^{(m)}}{E^{(f)} + \xi E^{(m)}} \tag{14}$$

In the Equation (13) and (14), the parameter ξ is referred as a shape fitting variable that fit the Halpin-Tsai equation to the extracted data from experimental work. This parameter describes the geometry and the packing arrangement of the reinforced fibers in the composite.

$$\xi = \frac{E^{(f)}(E_1^c - E^{(m)}) - V_f E_1^c (E^{(f)} - E^{(m)})}{E^{(m)}(E^{(f)} - E_1^c) - V_m (E^{(f)} - E^{(m)})} \tag{15}$$
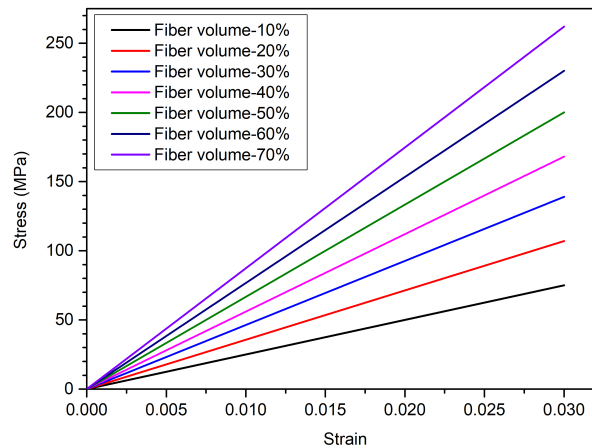

Figure 6. Stress-strain relation of Bio-composite with different fiber volume fractions.

The obtained bio-based composite stress-strain relation and its individual constituents stress-strain relation are shown in the Figure 4. Apart from the micro-mechanical analysis the comparative analysis is also presented for axial modulus of adopted bio-based composite with respect to the volume fraction of fiber. The analysis results (Digimat) are validated with the analytical model, is shown using Figure 5. The comparison of stress-strain relation of bio-based composite with different volume fractions of fiber is shown in the Figure 6.
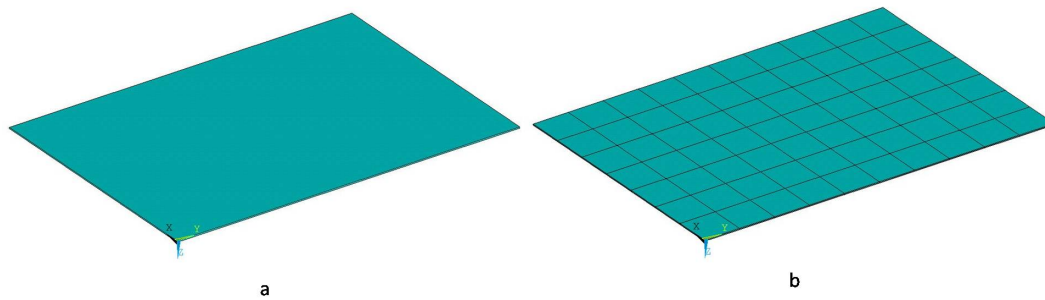
Figure 7. Bio-composite laminated plate a) design model b) finite element mesh.

4. Macro-mechanical analysis

Macro-mechanics is the study on behavior of composites at lamina level based on the effective properties of composite material obtained from micro-mechanical models [49]. In this section, finite element model of composite structure is constructed where the composite constitute of homogeneous effective properties that are determined in the earlier section.

Let us consider a bio-based composite laminated plate under compressive load. The dimensions are; length of the plate is L = 400 mm, the width of the plate is W = 300 mm, the plate thickness is t = 1.4718 mm and the thickness of each lamina is same. A cross-ply laminate [0/90/0] is taken for the analysis with material properties provided in the Table 2. The overall properties of composite are calculated by homogenization simulation tool Digimat. The cantilever boundary conditions are applied to analyze the plate in terms of its displacements, strains and stresses. The designed model and finite element mesh of composite plate is shown in the Figure 7. The mechanical behavior of a composite laminate depends not only on its material properties but also on its structural parameters such as laminate thickness and ply stacking sequence.

5. Conclusion

The presented paper illustrated the Multi-scale modeling and simulation of natural fiber reinforced composites. As an example of bio-based composite, evaluation of composite effective properties are carried out for sisal fiber reinforced with epoxidized soybean-oil based matrix. Subsequently, the influence of volume fraction of reinforcement fiber on the stress-strain relation of Bio-composite is analyzed. The emphasis of Multi-scale analysis is elucidated by coupling micro and macro-analysis using Digimat and Ansys (modeling and simulation) tools. In addition, extraction of individual constituent phase behavior along with the Bio-composite structural component behavior is carried out at different scales (micro and macro scales). The mechanical behavior of a laminated composite plate is analyzed using macro mechanical analysis. It is clearly noted that the material parameters provided to the macro analysis are not treated as constant input but these are obtained through a rigorous micro-scale analysis. The obtained effective properties are validated with the theoretical (RoM) results.

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