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ARTICLE

Multi-scale Modeling of Carbon Fiber Reinforced Magnesium Laminates (C_f/AZ91D) for Young's Modulus Prediction

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Abstract: Multi-scale models for carbon fiber reinforced magnesium laminate were established according to the characteristics of its realistic microstructure, including the crosswise and lengthwise unit cell model in microscale and structural unit cell model in mesoscale. The macro mechanical property Young's modulus was predicted according to the mesoscale model. The required properties for mesoscale model during simulation were obtained from microscale simulation. The Young's modulus for C_f/AZ91D laminates in different layup modes was predicted by multi-scale modeling technique and verified by corresponding experiments. The results show that multi-scale models can be used to predict the Young's modulus of laminate composites in different layup modes, and they show the same trend as but larger values than the experimental results. It is caused by the assumption of no degradation for matrix alloy and fiber during fabrication and perfect interface bonding. The multi-scale modeling technique proposed in this paper is meaningful for the laminate composite design.

Key words: multi-scale modeling; laminated composite; magnesium matrix composite; Young's modulus

Composite materials are ideal candidates as a structural material for automobile, aerospace and other applications [1-3]. Composites reinforced with carbon fiber have good resistance to crack propagation. The greatest advantage for composites is that its properties can be tailored by different microstructural designs [4-7].

Young's modulus is the most important property of advanced composites [8,9], and is indispensable for designing any structures. Although modulus is an intrinsic material property and a key parameter in engineering design and material development, the current mechanical test methods for measuring it are not well established [10]. ASTM E111 [11] is currently the only standard covering the measurement of Young's modulus, tangent modulus and chord modulus in a tensile test, although a number of proprietary procedures exist. Obtaining modulus values from the uniaxial tensile test relies on the measurement of stress and strain. Modulus measurements based on the tensile test show larger variation compared with dynamic measurements, and issues such as specimen installation alignment, strain measurement and data analysis are important affecting factors[10, 12]. Fortunately, an alternative method for determining macroscopic properties of advanced composites is applied by analytical or numerical methods [13-17]. Prediction of the Young's modulus of composite materials has been the subject of extensive research over half a century [18]. Calculation with commercial software allows corrections of equations and defining of special coefficients [19]. The finite element method is in use and is proved by scientific research that it can lessen the burden for engineers and save money [20, 21]. Lusti et al [22] compared the predictions of the thermoelastic properties of misaligned short glass fiber reinforced composites, calculated using the finite-element-based numerical approach of Gusev[23, 24], with experimental measurements. Agreement between the measurements, in particular the longitudinal Young's modulus

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E_{11} and the longitudinal and transverse thermal expansion coefficients α_1 and α_2, and the numerical predictions was found to be excellent. Lu et al [25] proposed a new multi-scale model to investigate the relationship between the mechanical properties and microstructure of fiber-reinforced silica aerogel composites and proved that the multi-scale model can be extended to study the mechanical properties of other composites. Drathi et al [26] presented a multi-scale framework for PMCs in order to predict the mechanical properties of PMCs. The framework coupled three different models over three length scales.

The structural modeling in multi-scale was supported by finite element method effectively. The multi-scale modeling allows decomposition of complex heterogeneous structure into the partial levels from the simplest composition to the composition of whole sample body. The accuracy of the simulation is better because specifications and properties from each scale are combined during processing. The simulation in this paper presents a two-dimensional model of lengthwise and crosswise unit cell model of fiber bundles surrounded by matrix alloy in the microscale and structural unit cell model in mesoscale. Experimental measurement is compared to the simulation for a validation of results. A multi-scale analysis technique for a composite structure is illustrated in Fig.1. More detailed description about the multi-scale simulation for the C_f/AZ91D laminates is provided subsequently.

1 Experiment

1.1 Preparation of C_f/AZ91D laminates

AZ91D magnesium alloy was chosen as matrix material, reinforcement was 12K T700 carbon fibers fabricated by Toray in Japan. The elastic modulus and the strength of carbon fiber are 5 and 17 times higher than those of magnesium alloy, respectively, while its density is the same as that of magnesium. So carbon fiber can be an excellent lightweight reinforcement. The chemical composition of the AZ91D magnesium matrix is shown in Table 1 and some typical properties of both AZ91D and T700 carbon fiber are summarized in Table 2.

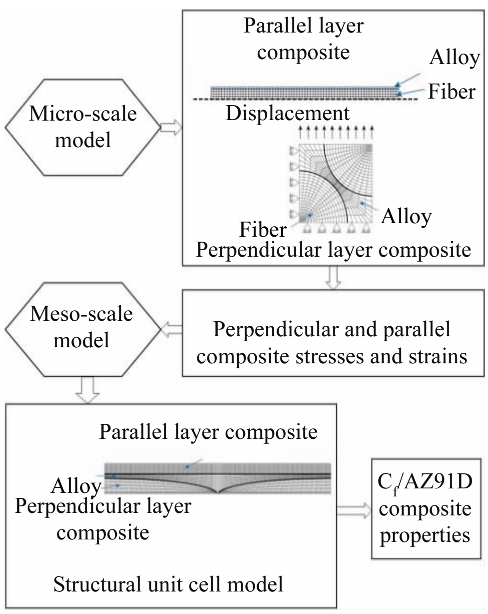


Fig.1 Schematic diagram for multi-scale analysis of C_f/AZ91D laminates

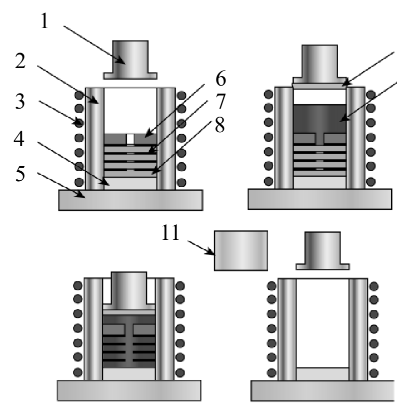
C_f/AZ91D laminates were fabricated by laminate squeeze casting process, as illustrated in Fig.2. Laminate squeeze casting setup was installed at the hydraulic machine which can supply 350 t forming load at most. The pressure applied by punch is determined by the load applied and head area of the punch. T700 carbon fiber and graphite sheets were cut to discs with 140 mm in diameter, placed into the die in a layered configuration, and then heated to 600 °C. The heating time was 2 h. Die and sample were maintained at 590 °C for 30 min. The pressure of 30 MPa was applied by the punch downward-moving and kept until cooling below the solidus of the magnesium matrix to allow molten magnesium to infiltrate and wet the carbon fiber layers.

Table 1 Chemical composition of magnesium alloy AZ91D (wt%)

Al	Zn	Mn	Si	Cu	Ni	Fe	Mg
8.5~9.5	0.45~0.9	0.17~0.4	≤0.05	≤0.025	≤0.001	≤0.004	Bal.

Table 2 Typical properties of magnesium alloy AZ91D[27] and T700 carbon fiber

Constituent	Yield strength/ MPa	Ultimate tensile strength/ MPa	Young's modulus/ GPa	Elongation/ %	Density/ $g\cdot cm^{-3}$
AZ91D	94	157	45	4	1.82
T700	-	4900	230	1.5	1.76



1-punch; 2-container of die; 3-preheating furnace of die; 4-pad; 5-heel block; 6-mould component; 7-graphite sheet; 8-preform; 9-sealing module; 10-liquid magnesium alloy; 11-C_f/AZ91D laminates

Fig.2 Schematic diagram of laminate squeeze casting process

Layup configuration for C_f/AZ91D laminates was designed according to Fig.3 with parameters m_1, n, and m_2. Five different layup modes were selected, as shown in Table 3, with the codes of L1-1-1, L3-3-3, L3-2-3, L4-1-4, and L0-9-0. These layup modes of laminate composites were predicted and tested for Young's modulus.

1.2 Experimental determination of Young's modulus for C_f/AZ91D laminates

A tensile mechanical test was used for the evaluation of elastic modulus in the experiment. Dog-bone specimens were prepared by electric-discharge machining (EDM) from the fabricated C_f/AZ91D laminates along the longitudinal axis of the surface layer of the laminates according to the standard of HB 7616-1998 and GB/T228-2002. The specimens were finely polished to the final dimension, as shown in Fig.4.

Strain gauge was attached to the middle of the specimen to monitor the strain change during tensile test. Tensile test was conducted at the speed of 0.5 mm/min on the universal test machine (CMT5304-30 kN) from Shenzhen Sans Inc. Strain gauge (YJZA-32) was used to measure strain change.

1.3 Microstructural observation

Metallographical samples were ground, polished and finally etched for 2 min using a Keller solution. The microstructure was observed using a XJP-3A optical microscope for the analysis of fiber configuration and distribution as well as porosity.

2 Multi-scale Modeling of C_f/AZ91D Laminates

Fig.5 shows the detailed schematic diagram of multi-scale modeling for C_f/AZ91D laminates. Laminate composite can be regarded as a combination of three different mesoscale phases, i.e. matrix alloy, crosswise section of the fiber bundle (named as composite 1), and lengthwise section of the fiber bundle (named as composite 2). Composite 1 and composite 2 are composed of matrix alloy and fiber in microscale.

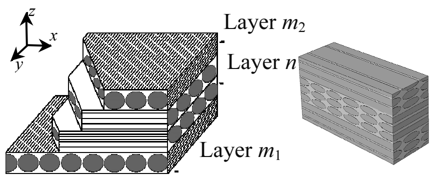


Fig.3 Layup configuration for C_f/AZ91D laminates

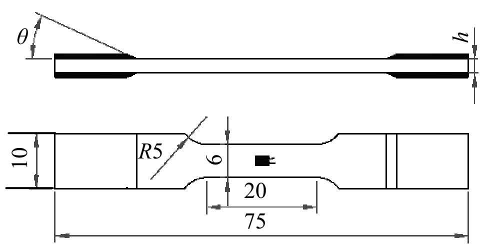


Fig.4 Dimension for tensile test specimen (h is specimen's thickness, h=2～3 mm; θ is strengthening plate chamfering, θ≥15°)

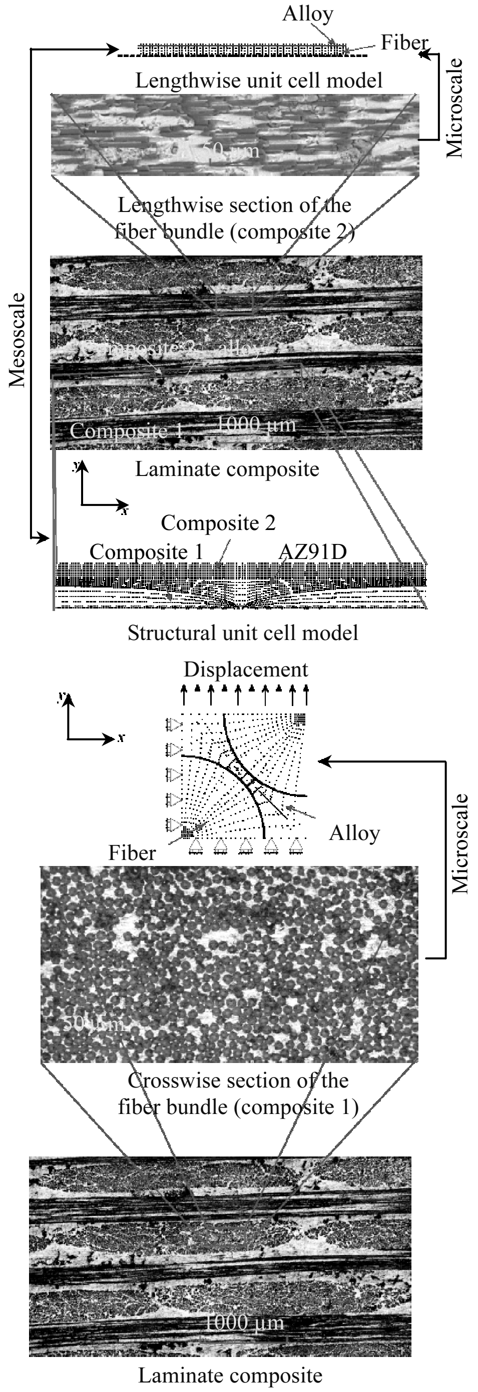


Fig.5 Detailed schematic diagram of multi-scale modeling for C_f/AZ91D laminates

The representative volume element (RVE) in different scales is based on realistic microstructure. So there are three different RVEs. The crosswise and lengthwise unit cell models in the microscale were constructed based on the local average volume fraction of carbon fiber in the crosswise section or lengthwise section of the carbon fiber bundle. Composite 1 and composite 2 should have the same volume fraction of fibers. The structural unit cell in the mesoscale was constructed from the mesoscale phases of composite 1, composite 2, and alloy AZ91D. Repeating of structural unit cell forms a whole macroscale unidirectional laminate composite.

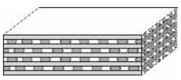
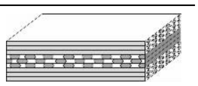
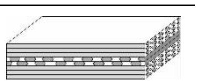
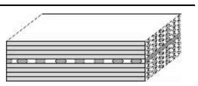
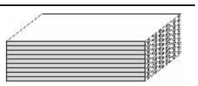
In the simulation, macroscale composite structures are idealized as a brick with identical properties in each brick counted from lower scale (micro unit cell → structural unit cell → macro composite bricks). Properties of the crosswise and lengthwise unit cell model were first predicted which were used as the property inputs for mesoscale phase composite 1 and composite 2 in the laminate composite. The crosswise and lengthwise unit cell models were meshed by plain strain element CPE8R and axisymmetric stress element CAX4R respectively. Structural unit cell model was meshed by plain stress element CPS4R.

Boundary and loading condition were exampled through crosswise unit cell model. Based on the symmetry, left edge of crosswise unit cell model can move freely along *y*-direction, and bottom edge can move freely along *x*-direction. Top edge was loaded by displacement along *y*-direction. For lengthwise unit cell model, displacement was applied along the fiber axial direction at one end of the model and the other end was fixed. Center line was set as the axisymmetric condition.

For clarifying the effect of layup of carbon fiber on the Young's modulus, layup modes in Table 3 were modeled based on the above mentioned multi-scale modeling methods. Structural unit cell models for layup mode in the Table 3 are illustrated in Fig.6.

Boundary and loading conditions for structural unit cell models were applied as the following rules. For L3-2-3 mode, left side was fixed in the direction of *x*, and right side was loaded along *x* direction by displacement boundary condition. For modes in Fig.6b~6d, considering the symmetry, left side was fixed in the direction of *x*, bottom edge was fixed in the direction of *y*, and right side was loaded along *x* direction by displacement boundary condition.

Table 3 Layup modes

Layup modes	m_1	n	m_2	$\frac{N_{center}}{N_{sides}}$	Illustration
L1-1-1	1	1	1	1:1	
L3-3-3	3	3	3	1:2	
L3-2-3	3	2	3	1:3	
L4-1-4	4	1	4	1:8	
L0-9-0	0	9	0	Unidirection	

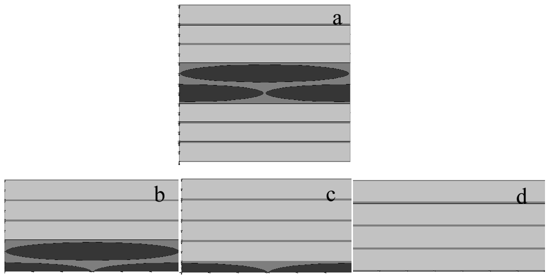


Fig.6 Structural unit cell models for predicting Young's modulus of Cf/AZ91D laminates in different layup modes: (a) L3-2-3, (b) L3-3-3, (c) L4-1-4, and (d) L0-9-0

3 Results and Discussion

3.1 Comparison between experiments and simulated results of L1-1-1 mode

69 tensile tests were conducted for C_f/AZ91D composites in the mode of L1-1-1. The probability distribution function (PDF) for 69 tensile tests is shown in Fig.7, and Weibull distribution function was used to fit the probability distribution function of tensile tests:

$$F(x) = 1 - \exp\left[-\left(\frac{x}{\eta}\right)^{\beta}\right]$$

where β is the shape parameter, and η is the scale parameter. The fitting parameters obtained by Wolfram Mathematica code are β=3.54 and η=97 GPa. It is shown that there is a large data dispersion for experimental Young's modulus results. Nevertheless, Weibull distribution with parameter of β=3.54 is close to normal distribution. It can be ascertained that the modulus for L1-1-1 mode of composite is about 97 GPa. If the corresponding simulation result shows a good agreement with 97 GPa, the proposed method will be proved to be effective in predicting the Young's modulus of C_f/AZ91D laminates.

Fig.8 shows the discrete data points (blue cross signs) in the elastic range of stress-strain curve for 69 C_f/AZ91D composite tensile specimens in L1-1-1 mode. It is clear that some unregular points deviate from the whole sample points. They should be removed during the modulus determination by linear fitting. Unregular points include points outside the modulus range between matrix alloy modulus and the carbon fiber modulus. The maximum value and minimum value of elastic modulus are determined to be 140 and 55 GPa, respectively, according to the edges of reasonable points by linear fitting. The focus of whole sample points is calculated to be 97.5 GPa by averaging the maximum and minimum, very close to the Weibull parameter η of 97 GPa. So 97 GPa is regarded as the experimental modulus of composite. The simulation result is 105 GPa, which is between the maximum

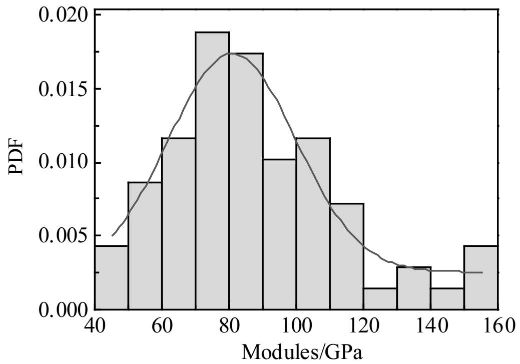


Fig.7 Probability distribution function (PDF) for tensile tests and fitting Weibull distribution function

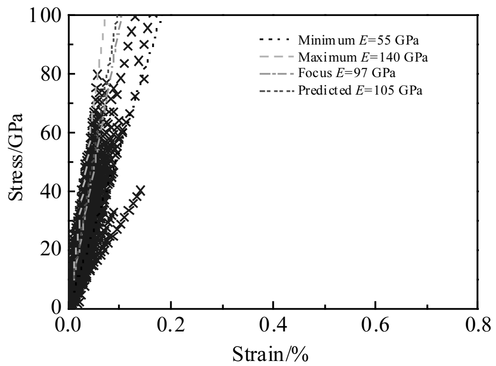


Fig.8 Fitting results of elastic modulus of 69 Cf/AZ91D composite tensile specimens in L1-1-1 mode

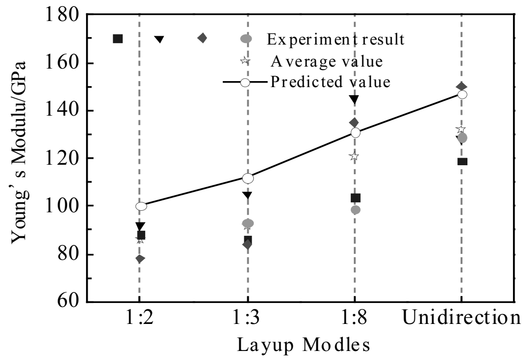


Fig.9 Predicted and experimental elastic modules in different layup modes

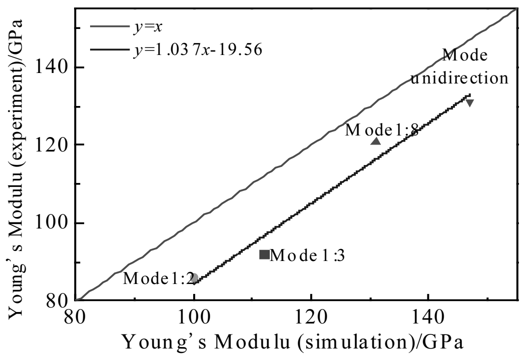


Fig.10 Comparison between experimental and simulated Young's modulus of Cf/AZ91D laminates

and the minimum and similar to the experiment result of 97 GPa. It verifies the effectiveness of the multi-scale modeling method.

3.2 Predictions for other layup modes except L1-1-1 and verifications

Three or four tensile specimens for each layup mode except L1-1-1 were prepared for determining the Young's modulus and the experimental results were plotted together with predicted values in the same figure for comparison, as shown in Fig.9.

Comparisons between simulation results and the average of actual testing results are shown in Fig.9, and the regularity of the results of FEM and testing is the same. However, experimental results for L3-3-3 (1:2) mode and L3-2-3 (1:3) mode are lower than the corresponding simulation result, and experimental results for L4-1-4 (1:8) and L0-9-0 (unidirectional) modes distribute in a certain reasonable scope close to the corresponding simulation result. By plotting experimental results and finite element simulation results in the same plot, the relationship between them is further explored, as shown in Fig.10, and the reliability and accuracy of the numerical analysis can be verified again.

The fitting function is y=1.037x−19.56, so we can confirm that there is a good agreement between the finite element results and the experimental values, indicating that the finite element simulation is feasible and acceptable, and the simulation result is closer to the actual Young's modulus.

However, the finite element simulation results are larger than the corresponding test results by about 20 GPa, for which there are several reasons. On the one hand, even though the model is based on the realistic microstructure, it is simplified to some extent. Different internal defects affecting the performance of the material were not considered in the finite element model, which causes the error between the simulation results and tests. On the other hand, the preparation of the composite material itself has certain inhomogeneity. Property such as elastic modulus is likely to change, and carbon fiber performance may be degenerated due to the high temperature during the preparation of C_f/AZ91D laminates. The perfect interface bonding was assumed during simulation. The generation of the finite element model does not take these factors into account.

Considering the actual situation, Young's modulus of C_f/AZ91D laminates is often influenced by some complex factors such as porosity, crack, damage, defect, residual stress, imperfect interface bonding. The trend of the theoretical simulation is proved to be the same as the experiments, and the finite element modeling is valid. The multi-scale modeling method proposed in this paper can be a reference in predicting Young's modulus of C_f/AZ91D laminates.

4 Conclusions

1) The Young's modulus of C_f/AZ91D composite laminates with a layup mode of L1-1-1 is tested by experiments, which verifies that the simulation results using multi-scale modeling methods proposed in this paper is valid.

2) The multi-scale modeling method has a reasonable capability for predicting the Young's modulus of C_f/AZ91D laminate with other different layup modes.

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碳纤维增强镁基复合材料（C_f/AZ91D）层压板杨氏模量的多尺度模拟及预测

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摘　要：根据碳纤维增强镁基复合材料层压板的真实微观结构特点建立了其多尺度微观力学模型，包括微观尺度下的横向及纵向单胞模型以及介观尺度的结构单胞模型。宏观力学性能弹性模量根据介观模型进行计算。介观模型中用到的性能参数通过微观模型计算获得。采用多尺度建模方法预测了不同铺层模式的碳纤维增强镁基复合材料层压板弹性模量，并采用对应的实验方法进行了验证。结果表明，多尺度建模方法可以用于不同铺层方式层压复合材料弹性模量的预测，与实验结果具有相同的变化趋势，但较实验结果偏大。这主要是由于模拟过程中忽略了实验中真实存在的合金、纤维性能退化及界面结合问题而造成的。本文所提出的多尺度建模方法对于复合材料层压板设计具有重要意义。

关键词：多尺度建模；层压复合材料；镁基复合材料；杨氏模量

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