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Material Behaviour

# A mesoscale study of thermal expansion behaviors of epoxy resin and carbon fiber/epoxy unidirectional composites based on periodic temperature and displacement boundary conditions

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ABSTRACT

The thermal expansion behaviors of neat epoxy resin and carbon fiber/epoxy unidirectional (UD) composites were experimentally and numerically studied in this paper. The dynamic mechanical analysis (DMA), thermogravimetric analysis (TG), differential scanning calorimetry (DSC) and thermal conductivity measurement were used to measure the thermo-mechanical properties of epoxy resin at different temperatures. The dilatometer was used to measure the thermal strains and linear CTEs of neat epoxy resin and UD composites. In addition, a mesoscale finite element model based on the periodic temperature and displacement boundary conditions was presented to analyze the thermal expansion behaviors of UD composites. The resin-voids representative volume element (RVE) was used to calculate the thermo-mechanical properties of several kinds of resin-voids mixed matrix. From the results it can be found that the glass transition temperature of epoxy resin, porosity and fiber orientation angle have significant effects on the thermal expansion behaviors of UD composites. The mesoscale finite element analyses (FEA) have obvious advantages than various existing analysis models by comparing their predictive results. The distributions of thermal displacement, thermal stress and thermal strain were extracted between the carbon fiber, resin-voids mixed matrix and their interface, and also between the front and back surfaces of the loading direction, to further investigate thermal expansion structure effects of UD composites. This paper revealed that the mesoscale FEA based on periodic temperature and displacement boundary conditions can be also used for thermal expansion researches of other complex structure composites.

## 1. Introduction

Carbon fiber-reinforced composites are currently more and more used in structural applications that involve various temperature ranges [1]. When excessive temperature differences occur in a composite structure or its surrounding, the disequilibrium of the potential volumetric changes or mismatch of structural deformations in this kind of composite are very complicated. A large rise in device temperature can lead to the fracture, delamination, melting, creep, electro-migration and even burning of packing materials [2]. The resistance capacity to these thermal failure modes of composites is always attributed to their thermal properties, such as thermal conductivity, specific heat and coefficient of thermal expansion (CTE). And CTE is an imperative property to define the end use application that should be firstly considered in these occasions. An understanding and ability to predict the CTE in composites is an important design criterion for producing dimensionally stable structures, especially if they are assemblages of many different types of materials [3]. Recently, many novel experimental methods have been developed to measure the CTE of polymeric materials, such as electronic speckle pattern interferometry [4], digital image correlation method [5], fiber bragg grafting sensor [6], infrared thermography [7], atomic force microscopy [8] and Raman spectroscopy [9], etc. Although they each have advantages in the measurement of CTE, all of them need sophisticated equipments, longer measuring time and more number of repeated trials and will also lead to larger error variations. Furthermore, the internal structure effects of thermal expansion, thermal-mechanical coupling relationship and thermal failure mechanisms of composites cannot be revealed from them.

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Therefore, a more convenient and more comprehensive analytical model is urgently needed to characterize thermal expansion behaviors of composites in a wide range of temperatures.

Considering the internal structure effects of UD composites on the thermal expansion, the thermal expansion properties of its constituents should be firstly determined and analyzed. It is well known that carbon fiber-reinforced composites are manufactured by carbon fiber reinforced body impregnated with resin matrix. And during their processing, there will also be some voids existing in composites. Therefore, to a great extent, the CTEs of these composites depend on the CTEs of its constituents. From this perspective, some researchers studied the CTEs of carbon fibers and epoxy resin. For example, Sauder et al. [10], Rupnowski et al. [11] and Pradere et al. [12,13] studied the CTEs of carbon fiber in a wide temperature range, which showed that the effective longitudinal and transverse CTEs of carbon fibers almost maintained stable during the temperatures from room temperature to 300 °C. However, the fiber orientation angle [14,15] may have a remarkable effect on the thermal expansion behaviors of UD composites. Due to the high temperature sensitivity of epoxy resin, its CTE may have a significant effect on the final thermal expansion behaviors of carbon fiber/epoxy composites. For example, Glavchev et al. [16], Tognana et al. [17] measured and analyzed the CTEs of pure epoxy resin matrix as well as its compounds. Both of their research found that the glass transition temperature $T_g$ had a great influence on the CTE of epoxy resin and the CTE of epoxy resin had an important role in the final CTEs of composite materials. Although the porosity of voids [18] in composites is very little, its effect on thermal expansion is very noteworthy. Therefore, effective determination the CTEs of epoxy resin, investigation the effects of fiber orientation and porosity are also important parts to accurately analyze the thermal expansion behaviors of composite materials.

For the numerical analytical models about the thermal expansion of composites, many researchers conducted a series of works. At the beginning, various kinds of micromechanical analytical models have been presented to predict the CTEs of UD composites, such as rule of mixture (ROM), Turner [19,20], Kerner [20,21], Levin [22], Schapery [23], Van Fo Fy [24,25], Chamis [26], Chamberlain [27], Geier [28], Schneider [27], Rosen & Hashin [29] and so on. However, due to many idealistic assumptions, these analytical models may have more or less shortcomings in terms of the CTE predictive ability. In addition, the structure effects and interfacial effects cannot be illustrated from these models. In this paper for facilitating comparisons, the detailed analyses about these micromechanical models are also made in Appendix A. Recently, with the improvement of computation capability of computer, many complicated numerical solutions, including perturbation-based stochastic homogenization analysis method [30], effective thermoelastic approach [31], Mori-Tanaka (M-T) method [32] and the finite element method (FEM) [33–38], are more and more used to predict the thermal expansion behaviors of composites. Among these, the finite element method is the most widely used for the CTEs prediction of carbon fiber-reinforced composites. For example, Karadeniz et al. [33] used the FEM to study the effective CTEs of fiber reinforced composites by micromechanical modeling. Their results showed that the FEM and existing analysis models were in good agreement with experimental for longitudinal CTEs, while for transverse CTE the FEM results showed better agreement with experimental data. Similar research was also done by Ran et al. [34], who not only analyzed the longitudinal and transverse CTEs of UD composite, but also indicated that the CTEs were mostly affected by the fiber to matrix stiffness ratio and the fiber to matrix CTE ratio. Dong [35] developed a regression-based model combined with FEM for predicting the transverse CTEs of UD composites. The result showed that the developed model offered excellent accuracy while reduced complicated computation process. Xu et al. [36] developed a strain energy model based on the relationship established between strain energy of the microstructure and that of homogenized equivalent model under specific thermo-elastic boundary conditions to predict the effective CTEs of composite materials. Accordingly, Abueidda et al. [37] investigated the effective CTE of novel interpenetrating phase composites by generating several three-dimensional unit cells models. Wang et al. [38] investigated the distribution and development of the thermal-shock-induced stress in ceramic-matrix composites by FEA. They found that the thermal stress failure always occurred at or near the heat part of the fibers. Although the prediction of FEM showed great advantages over other analytical models, most of them didn't consider the effect of temperature or ignored the temperature dependence of thermal and mechanical properties of carbon fibers and epoxy resin. In fact, the elastic modulus, thermal conductivity, specific heat capacity and CTEs of carbon fibers and epoxy resin are all temperature dependent. Therefore, both the thermal and mechanical properties of materials at different temperatures must be incorporated in finite element analysis for accurately predicting the CTEs of UD composites. Although some studies [39–42] may have already taken the temperature effects into account during the thermal expansion analysis of composites, the thermal-mechanical coupling effects on CTEs of composites have never been revealed. The thermal stress induced by the temperature variations, due to the CTEs mismatch between the fiber and the matrix, can greatly affect the mechanical properties of composite. On the contrary, the change of mechanical properties may also lead to the change of temperatures. Therefore, a more comprehensive thermal-mechanical coupling finite element analysis should be conducted.

Based on the above unsolved problems, we constructed a mesoscale finite element model in the present work to analyze the thermal expansion behaviors of epoxy resin as well as carbon fiber/epoxy UD composites at the temperature range of 20–300 °C. The thermal-mechanical coupling relation is realized by applying the periodic temperature and displacement boundary conditions to the mesoscale RVE. This study helps for further understanding the thermal expansion behaviors of epoxy resin and UD composites, but it can also provide an efficient method for thermal expansion research of complex structure composites. The paper is structured as follows. In section 2, the involved materials and experimental methods for temperature-dependent thermomechanical of neat epoxy resin and UD composites were presented. In section 3, the detailed finite element analyses were made, including the mesoscale microstructure model, the computing method of thermal strain/stress, the periodical boundary condition and the meshing scheme. The detailed experimental and FEA results as well as their comparisons are given and discussed in section 4. In section 5, a few concluding marks are provided.

## 2. Experimental

### 2.1. Materials and sample preparation

An epoxy resin JC-02A based on diglycidyl ether of bisphenol A (Changshu Jaffa Chemical Co., Ltd) with hardener JC-02B (improved methyl tetrahydrophthalic anhydride) and accelerant JC-02C (tertiary amine) was used as matrix material. The mixed proportion of resin, hardener, and accelerant was 100:80:0.5 by weight. The uncured epoxy resin was first vacuumed to remove the air bubbles before being used to make composites. The neat epoxy resin was cured by directly injecting them into rectangular mold. The curing temperature for neat resin was 90 °C for 2 h, 110 °C for 1 h and finally 130 °C for 4 h. The unidirectional carbon fiber pre-impregnated (prepreg) that was made up of carbon fibers