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Evolution of curing residual stresses in composite using multi-scale method

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ABSTRACT

Residual stresses occur in composite structures during curing process which play an important role in the deformation and mechanical properties of composite, especially for thick laminates. However, the experimental measurement of curing residual stresses is often costly and complicated. Alternatively, computational tools are used to predict the curing residual stresses. Considering the effect of multi-scale in composites, this paper proposes a multi-scale model to predict the residual stresses of composites during the curing process. At the part level, a macro-scale three-dimensional model, which incorporated the thermo-chemical model and residual stress model, is developed by considering the time-dependent properties of material performances during curing process. The two sub models are mathematically coupled to solve for the process with variables interactively to obtain part-level temperature, degree of cure gradients and macro curing residual stresses. At the reinforcement level, a representative volume elements (RVE) is employed to calculate the micro-scale residual stresses by using the results of macro-scale simulations. The results show there is a significant difference in the calculation of micro residual stresses by introducing the effect of multi-scale model. Subsequently, the effect of different boundary conditions and fiber arrangement are discussed.

1. Introduction

Fiber reinforced thermosetting composites, combined with different thermosetting resins (epoxy [1,2], phenolic [3], polyimide [4] and cyanate ester [5], etc) and different fibers (glass fiber [6], carbon fiber [7] and PBO fiber [5,8], etc), have been widely used in many fields where good mechanical properties and weight savings are required for their high specific strength and stiffness-to-weight ratios. The strength and the integrity of the final composite structure deeply rely on the curing process. Thus, the great need of the composites in the industries requires sufficient technologies to study the curing process of such materials. However, during the curing process of composites, residual stresses invariably arise due to chemical shrinkage of matrix, tool-part interaction and thermal expansion [9,10]. In terms of the resources, residual stresses in composites are classified into two categories: macro and micro residual stresses. At the length scales of composite part, macro residual stresses will generate in the laminates and result in shape distortion [11]. On the micro-mechanical level, the micro residual stresses develop in a single fiber-matrix reinforcement due to the differences in the coefficient of thermal expansion (CTE) and elastic modulus between the fiber and the matrix, which may have an adverse effect on the mechanical properties of the final product by developing micro-cracks or fiber-matrix debonding [12–14]. Therefore, the residual stresses of composite should be taken into consideration in both design and manufacturing process in order to meet the requirement of dimensional accuracy and good property performance at the same time.

Many experimental methods are used to measure residual stresses in composites which are divided into two categories: measuring residual stresses during curing process and after curing process of composites. The first category monitors the development of residual stresses during manufacturing process, such as using embedded strain gauges [15], fiber optic sensors [16,17], or interrupted warpage test [18]. The second category usually uses relaxation or destructive methods, such as slitting method [19,20], indentation method [21], hole drilling method and deep hole method [22,23]. However, the experimental approaches are often costly and complicated to monitor the evolution of residual stresses, especially for the micro residual stresses. Nowadays, using numerical model has been an alternative way to study the development of residual stresses in composites, especially when the composite structure becomes more and more complex. Meanwhile, these proposed models provide a deeply insight and an inexpensive way to understand the physics of the problem and the effects of curing parameters, part

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geometry and microstructure on the development of residual stresses. Despite all existing knowledge about these materials, the accurate prediction of the residual stresses in composite has been an elusive task due to the complexity of the curing process. For a typical composite, it is composed of two or more than two kinds of materials with different physical and chemical properties, and then cured by high temperature and high pressure with different structural scales (microscopic and macroscopic level). Various methods, including elasticity solution, finite element method, and cylinder theory, have been proposed to provide an insight to the macro residual stresses [6,16,24–26] and micro residual stresses [12,27–31]. Regular or random fiber packing has been assumed, typically, in a square or hexagonal layout. Although micro residual stresses due to the thermal mismatch of the fiber and matrix system has been extensively studied in composite, the connection between the macro and micro scale has not been studied clearly. The effects of macro level factors on the micro residual stresses, such as temperature, macro residual stresses have not been deeply addressed yet. Zhao et al. [12,31] presented perfect bonding model to calculate the residual stresses, which means that the composites only includes two phases, matrix and fiber. Herráez et al. [32] investigated the effect of fiber shape on the residual stresses and the transverse strength of unidirectional composites. Shokrieh et al. [30,33] investigated the influences of imperfect bonding between fiber and matrix on the micro residual stresses in composites. Then, Hen et al. [34] used a microscopic computational model of single fiber composite to research the micro residual stresses distribution. Although the above researches have been conducted to study the residual stresses mechanisms of composites, the connection between the macro and micro scales have not been discussed. Meanwhile, the third phase, interphase, has also been considered in many numerical models to investigate the effect of the interphase properties on the mechanical behaviors of composites [35–38]. In this work, the effect of interphase on the micro residual stresses is also taken into consideration in the multi-scale method.

To ensure high-performance, reliability and safety of engineering design, the exact measurements or prediction of micro residual stresses is critical. Multi-scale modeling is an new tool to study both the macro and micro behaviors of composite. One main advantage of multi-scale modeling is that complicated initial and boundary conditions at the macro-scale model can be studied for real life engineering problems, such as heat treatments and resin flows. In addition, it shares both the efficiency of the macro-scale model and the accuracy of the micro-scale model [39]. This study proposes multi-scale method to bridge the connection between the part and fiber-matrix level to obtain more realistic micro residual stresses. First, a three-dimensional (3D) macro-scale model is established to solve the temperature, degree of cure, macro residual stresses and strains at part level. Then, this information calculated by part level simulation is employed in the RVE model as boundary conditions in the micro-scale model to estimate the micro residual stresses, with resin viscoelastic behavior into consideration. This work mainly focuses on the effects of macro-level factors on the micro residual stresses of composite.

2. Theoretical modeling and numerical formulation

2.1. The multi-scale model

The general 3D multi-scale thermo-mechanical framework for composite to predict the curing residual stresses is applied in this work. In this work, the composite system chosen is Hexcel AS4/3501-6, which is commonly used in aerospace structures and investigated in literature. The properties of fiber and resin, such as glass transition temperature, cure shrinkage strains, thermal expansion coefficients and modulus have been summarized by many researchers [40–43]. The main ideas of the framework are:

At the macro-scale model, the governing equations for heat transfer and macro residual stresses are solved with respect to the initial and boundary conditions corresponding to real engineering problems. Composite are assumed as a continuum media at the macro-scale model. The temperature, degree of cure, macro residual stresses and strains will be calculated using the macro-scale model.

At the micro-scale, the temperature and cure of degree are assumed to be constant in each volume element according to the results calculated by the macro-scale model. The micro residual stresses are developed by the interaction between the three phases: matrix, fiber and interphase. The simulated results calculated by macro-scale model, such as temperature, degree of cure and macro residual strains, are employed in the RVE model as boundary conditions in the micro-scale model. The fiber reinforcement and interphase undergo only elastic deformation and the matrix uses a linear viscoelastic constitutive equation for predicting the residual stresses.

2.2. Macro-scale models

2.2.1. Thermo-chemical model

The thermo-chemical model is composed of heat conduction and reaction kinetic of resin. During the curing process of composite, the heat generation and conduction is from a nonlinear heat source in resin curing reaction. Considering this problem, transient heat conduction model contains both internal heat source and external heat flux, as follows [44]:

$$\lambda_x \frac{\partial^2 T}{\partial x^2} + \lambda_y \frac{\partial^2 T}{\partial y^2} + \lambda_z \frac{\partial^2 T}{\partial z^2} + Q = \rho_c C_c \frac{\partial T}{\partial t} \tag{1}$$

where λ_x, λ_y and λ_z are the anisotropic thermal conductivities of the composite in the x, y and z directions, respectively; ρ_c and C_c are the density and the specific heat capacity of the composite, respectively; T is the transient temperature of the composite at time t, and Q is the interior heat source, which can be expressed as follows:

$$Q = \rho_r (1 - V_f) H_r \frac{d\alpha}{dt} \tag{2}$$

where ρ_r is the density of the resin matrix; V_f is the fiber volume fraction of the composite; a is the curing degree of the resin matrix; da/dt is the curing rate of the resin matrix; H_r is the total release heat during curing.

During the curing process, complex chemical reactions occur in the resin matrix with a massive source of heat release. Thus, a phenomenological model of the cure kinetics is developed to represent the curing process by a rate equation. For 3501-6 epoxy resin, the internal heat generated due to the exothermic cure reaction is described as follows [45]:

$$\frac{d\alpha}{dt} = \begin{cases} (K_1 + K_2\alpha)(1-\alpha)(0.47-\alpha) & (\alpha \le 0.3) \\ K_3(1-\alpha) & (\alpha > 0.3) \end{cases} \tag{3}$$

where K_i $(i = 1,2,3)$ are the curing rate constants which can be defined generally by the Arrhenius equations:

$$K_\mathrm{i} = A_\mathrm{i} \exp\left(\frac{-\Delta E_\mathrm{i}}{RT}\right) \quad (i = 1,\ 2,\ 3) \tag{4}$$

where R is the universal gas constant; A_i are the frequency factors obtained from experiments; ΔE_i are the activation energies.

The composite specific heat capacity C_c and density ρ_c are calculated using the following equations [46]:

$$C_c = \frac{V_f \rho_f C_f + (1 - V_f)\rho_r C_r}{\rho_c} \tag{5}$$

$$\rho_c = V_f \rho_f + (1 - V_f)\rho_r \tag{6}$$

where ρ_f is the density of the fiber; C_f and C_r is the specific heat capacity of fiber and resin, respectively.

Assuming isotropic resin conductivity and transversely isotropic fiber conductivities, the rule of mixture is used to calculate composite