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MULTI-SCALE NUMERICAL SIMULATION OF THE THERMAL-MECHANICAL PROPERTIES FOR CERAMIC COMPOSITES REINFORCED WITH NANO-FIBER

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Key words: Ceramic Composites Reinforced with Nano-fiber; Multi-scale Numerical Simulation; Effective Thermal Expansion Coefficient; Thermal Stress; Homogenization method

Summary: In this paper, the analyzed equations are established by using the multi-scale macro-microscopic homogenization methods (HM) to analyze the main factors to affect the mechanical behaviors of ceramic composites reinforced with nano-fiber. The changes of the material parameters for nano-fiber are considered in the model. The effective elastic modulus, residual stress and the thermal expansion coefficient are calculated, and the results are compared well with those from the classical theoretical models, which show that the length, thermal expansion coefficient, and elastic modulus of the nano-fiber have obvious influences on the mechanical properties of ceramic composites reinforced with nano-fiber, and the transverse and longitudinal mechanical properties have great differences for the change of materials parameters of nano-fiber. The finite element method is effective to analyze the influence of more factors on the mechanical properties of ceramic composites reinforced with nano-fiber.

1 INTRODUCTION

The intrinsic brittleness of ceramic is a main problem in their applications. In order to improve their strength and toughness, the ceramic materials are designed by mixing the particles, short fibers and long fibers into the ceramic matrix. In fact, the combination of brittle matrix (ceramic, cement) with fibrous reinforcement provides the possibility to design composites with tuned properties [1]. However, the ceramic composites are typical non-homogeneous materials, and the qualitative and quantitative characteristics of composites depend on the mechanical, geometrical and statistical properties of the constituents and their interface [2]. Extensive research work has been performed on the development of multi-scale models, and micromechanical models have been developed to evaluate elastic constants of composites with respect to volume fraction [3] and shape [4] of the reinforcements. Eshelby's equivalent inclusion concept [5] and the Mori-Tanaka mean-field theory [6] are classical theories to verify the reliability of the results, and the existing studies have been focused on the stiffness and strength of ceramic composites [7-8], relatively few research have dealt with the thermal–mechanical coupling of these composites in the presence of temperature change.

In this paper, the analyzed equations are established by using the multi-scale macro-

microscopic homogenization methods (HM) to analyze the main factors to affect the mechanical behaviors of ceramic composites reinforced with nano-fiber. The changes of the material parameters for nano-fiber are considered in the model. The transverse and longitudinal effective elastic modulus, thermal stress and the thermal expansion coefficient are calculated, and the results are compared well with those from the classical theoretical models, which show that the length, the elastic modulus and the thermal expansion coefficient of nano-fiber have obvious influences on the mechanical properties of ceramic composites reinforced with nano-fiber, and the transverse and longitudinal mechanical properties have great differences for the change of the above factors.

2 HOMOGENIZATION METHOD FOR EFFECTIVE ELASTIC MODULUS

Homogenization theory adopts a multi-scale perturbation technique was applied to derive the effective elastic modulus for ceramic composites in literature [9]. According to the solution of the macro-microscopic controlling equation, the homogenized effective elastic modulus is:

$$D_{ijkl}^{H}(\boldsymbol{x}) = \frac{1}{|Y|}\int_Y E_{ijpq}\frac{\partial \tilde{\chi}_p^{kl}}{\partial y_q}dY \tag{1}$$

where, D_{ijkl}^{H} denotes the homogenized stiffness tensor and is usually called as macroscopic stiffness tensor, and Y represents the volume of the unit cell, and E_{ijkl} denotes the elastic constants tensor for each constituent, $\tilde{\chi}_p^{kl}$ is defined as the characteristic function which is solved by using the homogeneous integral equation with a simple periodic displacement boundary condition as follows:

$$\int_Y E_{ijkl}\frac{\partial \tilde{\chi}_k^{pq}(\mathbf{x},\mathbf{y})}{\partial y_l}\frac{\partial v_i(\mathbf{y})}{\partial y_j}dY = 0 \tag{2}$$

The homogenized elastic constants in Eq. (2) can be easily calculated by some Fortran program performed by the authors.

Halpin and Tsai[10] found that three Herman's equations for stiffness could be expressed in a common form:

$$\frac{P}{P_m} = \frac{1+\xi\eta v_f}{1-\eta v_f}, \text{ with } \eta = \frac{(P_f/P_m)-1}{(P_f/P_m)+\xi} \tag{3}$$

Here, P represents any one of the composite moduli, P_f and P_m are the corresponding moduli of the fibers and matrix, while ξ is a parameter that depends on the matrix Poisson ratio and on the particular elastic property being considered.

Tandon and Weng[11] derive explicit expressions for the elastic constants of a short fiber composite using the Mori-Tanaka approach.

$$E_{11} = \frac{E_0}{1+v_f(A_1+2v_0A_2)/A} \tag{4}$$

$$E_{22} = \frac{E_0}{1+v_f[-2v_0A_3+(1-v_0)A_4+(1+v_0)A_5A]/2A} \tag{5}$$

Where A, A_1, etc. are auxiliary constants given in their paper, and v_f is the fiber volume fraction.

3 CALCULATIONS OF THERMAL EXPANSION COEFFICIENT

According to the definition of thermal expansion coefficient, for the change of the temperature ΔT, the thermal expansion coefficient of ceramic composites along different direction is defined as:

$$\alpha_i = \frac{\Delta l_i}{l_i}\frac{1}{\Delta T} \tag{6}$$

In the classical Turner model[12], the thermal expansion coefficient for composites without internal stress is described as

$$\alpha_c = \frac{\alpha_m K_m V_m + \alpha_p K_p V_p}{K_m V_m + K_p V_p} \tag{7}$$

For composites reinforced with spherical inclusions, if there are interfacial shear stress and hydrostatic stress simultaneously, then the thermal expansion coefficient follows Kerner model [13]

$$\alpha_c = \alpha_m - (\alpha_m - \alpha_p) \times \frac{K_p(3K_m + 4G_m)V_p}{K_m(3K_p + 4G_m) + 4(K_p - K_m)G_m V_p} \tag{8}$$

Where, α_c、α_m and α_P is the thermal expansion coefficient of the composites, matrix and the reinforcements, respectively; and V_m and V_P is the volume fraction of matrix and reinforcement, respectively; K_m、K_p is the volume modulus of matrix and reinforcement, respectively, and G_m is the shear modulus of the matrix.

4 RESULTS AND DISCUSSION

Finite element analysis with homogenization method is performed using the commercial software CODE ANSYS. The typical representative volume element is shown in Fig.1, and the materials properties are shown in Table 1.

Table 1 The material property for ceramic composites

Materials / Material property	Nano-fiber	Ceramic matrix
Elastic modulus（GPa）	700	402
Thermal expansion coefficient（$\times 10^{-6}$/K）	4.7	8.2
Poisson ratio	0.23	0.23

Figure 2 shows the influence of the volume fraction of nano-fiber on the effective thermal expansion coefficient ($\times 10^{-6}$/K) for different methods, and the result from Tumer's model is far from those from the other methods for its simplicity. The longitudinal and transverse effective elastic modulus is shown in Fig.3 and Fig.4. It shows that the results from finite element with homogenization method are consistent with those from Halpin-Tsai, but Mori-Tanaka method gives a higher transverse elastic modulus, especially for the longer carbon

nano-fiber.

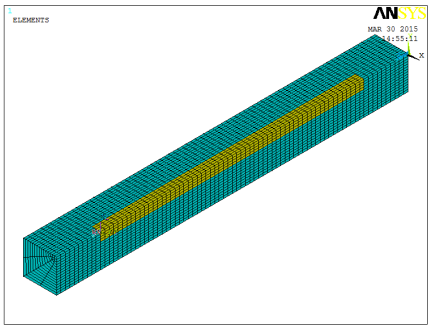

Fig.1 Typical representative volume element

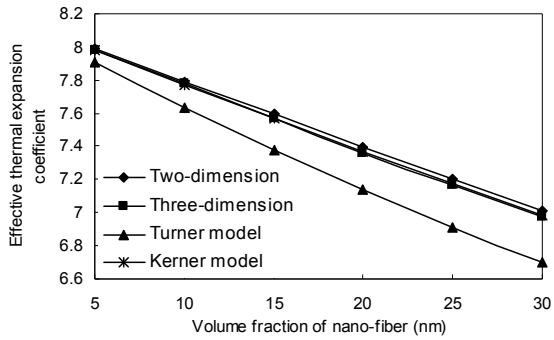

Fig.2 Influence of volume fraction of nano-fiber on effective thermal expansion coefficient

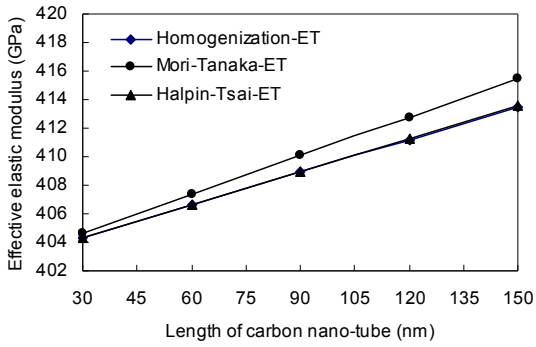

Fig.3 The relationship between effective transverse elastic modulus and length of carbon nano-fiber

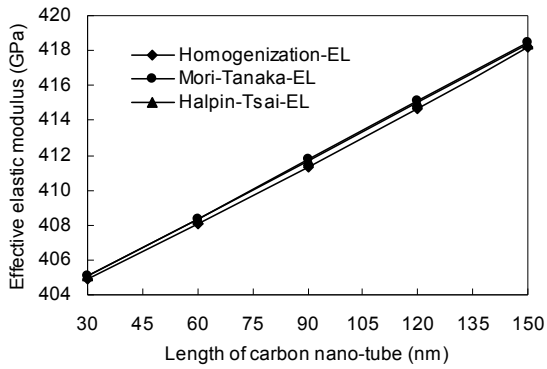

Fig.4 The relationship between effective longitudinal and length of carbon nano-fiber

Fig.5 and Fig.6 shows the changes of the minimum and maximum thermal stress with the length of nano-fiber, and the same tendencies are shown for theoretical method and finite element method, but the difference on values are obvious too. For the minimum stress, the difference is decrease with the increase of the length of nano-fiber, the results from theoretical model is higher than those from finite element method. On the contrary, for the maximum stress, the difference is increase with the increase of the length of nano-tube, and the result from theoretical model is lower than those from finite element method. FEM is reliable to analyze the effective elastic modulus, thermal expansion coefficient and thermal stress, and it is convenient to consider more factors to influence the mechanical behaviors of ceramic composites reinforced with nano-fiber.

Fig.7 and Fig. 8 shows the influence of the thermal expansion coefficient ($\times 10^{-6}$/K) of nano-fiber on the transverse and longitudinal thermal expansion coefficient of ceramic composites for different length of nano-fiber. Take the point that the thermal expansion coefficient of nano-fiber is the same with that of ceramic matrix as the critical point, the longitudinal and transverse thermal expansion coefficients decrease with the increase of the length of nano-fiber before the critical point, but the contrary tendency is occurred after the critical point, that is the effective thermal expansion coefficient of ceramic composites increase with the length of nano-fiber, and the same tendency is observed for longitudinal and transverse thermal expansion coefficient, but the transverse thermal expansion coefficient is lower than longitudinal thermal expansion coefficient.

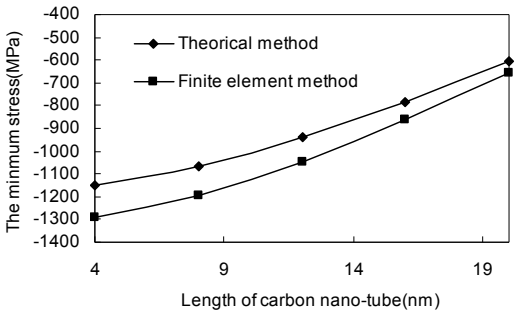

Fig.5 The influence of length of carbon nano -fiber on the minimum thermal stress

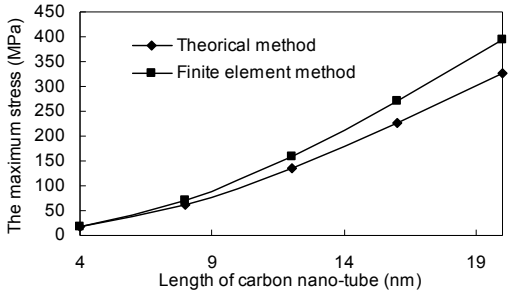

Fig.6 The influence of length of carbon nano -fiber on the maximum thermal stress

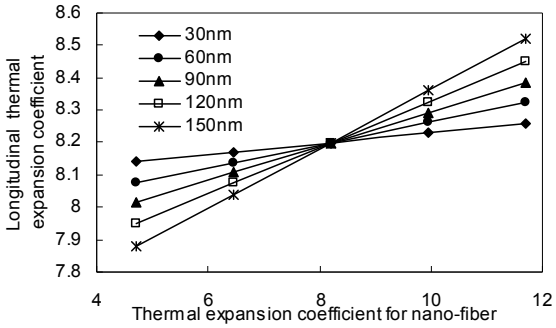

Fig.7 Thermal expansion coefficient of nano-fiber Vs transverse thermal expansion coefficient

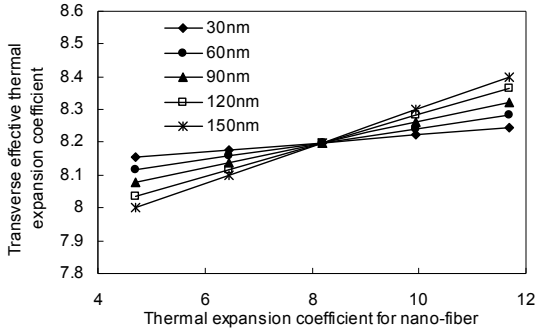

Fig.8 Thermal expansion coefficient of nano-fiber Vs longitudinal thermal expansion coefficient

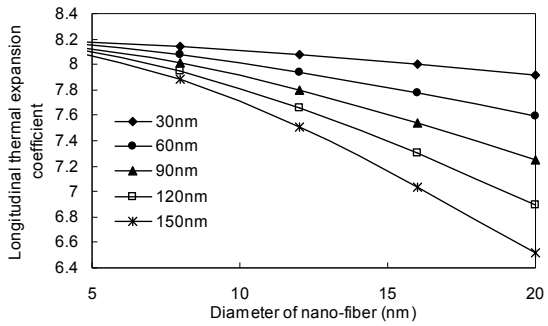

Fig.9 Influence of length of nano-fiber on transverse thermal expansion coefficient

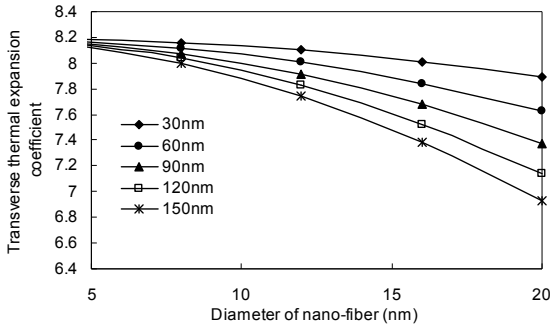

Fig.10 Influence of length of nano-fiber on longitudinal thermal expansion coefficient

Fig.9 and Fig.10 show the influence of the diameter of nano-fiber on effective thermal expansion coefficient of ceramic composites. The results show that the longitudinal and transverse thermal expansion coefficient decrease with the increase of the diameter of nano-fiber, and the longitudinal thermal expansion coefficient is more sensitive on the diameter of nano-fiber than transverse thermal expansion coefficient. It also shows that the nano-fiber with larger diameter is beneficial to improve the stability to resist on the temperature difference for the ceramic composites with nano-fiber.

6 CONCLUSIONS

In this paper, the mechanical properties of ceramic composites reinforced with nano-fiber are analyzed by the homogenization method and classical theoretical methods, and the results are consistent for different methods. Some important conclusions are summarized as followings.

(1) Finite element with homogenization method is reliable to analyze the effective elastic

modulus, thermal expansion coefficient and thermal stress, and it is convenient to consider all kinds of factors to influence the mechanical behaviors of ceramic composites reinforced with nano-fiber by using this method.

(2) When the thermal expansion coefficient of the nano-fiber is lower than the ceramic matrix, the longer nano-fiber is effective to decrease the effective thermal expansion coefficient of ceramic composites, and when it is higher the ceramic matrix, the shorter nano-fiber is effective to improve the effective thermal expansion coefficient.

(3) The longitudinal thermal expansion coefficient is more sensitive on the properties of nano-fiber than transverse thermal expansion coefficient.

(4) The lower thermal expansion coefficient for ceramic composites with the larger diameter of nano-fiber are obtained, which show that it is effective to improve the ability to resist against the temperature difference for ceramic matrix by taking the longer nano-fiber as the reinforcement.

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