Composites Part B 110 (2017) 178–184

Contents lists available at ScienceDirect

Composites Part B

journal homepage: www.elsevier.com/locate/compositesb

Analysis of the tensile moduli affected by microstructures among seven types of carbon fibers

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ARTICLE INFO

Article history:
Received 4 August 2016
Received in revised form
18 September 2016
Available online 16 November 2016

Keywords:
Carbon fiber
Micro-mechanics
Mechanical properties
Microstructures

ABSTRACT

A two-phase micromechanical model composed of crystallites and amorphous components can be employed to address the relationship between the microstructure and the tensile modulus of carbon fibers. It turns out that the tensile modulus increases with the increase of three factors: the aspect ratio of crystallites, volume fraction of crystallites and degree orientation of crystallites. Subsequently, seven types of carbon fibers are compared, and their differences of the tensile moduli affected by the three factors are calculated. The results show that the differences of the tensile moduli affected by the factors of microstructures between different types of carbon fibers can be discussed using the two-phase micromechanical model.

1. Introduction

Polyacrylonitrile (PAN)-based carbon fibers were first developed in 1959. Carbon fibers have high tensile modulus and strength, which play a significant role in civil engineering construction, aerospace field, automotive materials, athletic equipment, among others. In order to penetrate into the relationships existing between mechanical properties and the structure of carbon fibers, Oberlin [1], Johnson [2,3], Donnet [4] and Chung [5] have had a close look at the structure and morphology of carbon fibers. The structure of high modulus carbon fibers has been studied by Montes-Moran [6,7], Huang [8], Fujie Liu [9] and Zan Han [10]. In order to explain quantitatively the association between the tensile modulus and the crystallite orientation, Ruland W [11], Northolt MG [12] and Shioya M [13], respectively introduced the uniform stress mechanical model and mosaic mechanical model. The uniform stress mechanical model serves to describe the behavior of graphitized carbon fibers, while the mosaic mechanical model can explain the measured increases of the tensile modulus and crystallite orientation dependence on tensile stress. Carbon fiber has a unique microstructure which consists of carbon crystallite layers, crystallite disorder regions (amorphous phase), and needle-like microvoids [5,14]. Moreover, there have been reports of the structure of carbon fibers consisting of both crystalline and amorphous phases [15,16]. On this basis, a series–parallel mechanical model that comprises crystalline and amorphous phase was introduced, which serves to evaluate the heterogeneous stress distribution in carbon fibers [17]. With properties of both the crystalline and amorphous components in the fiber structure taken into account, a two-phase composite micromechanical model was established to predict the tensile modulus of PAN-based carbon fibers [18]. Recently, a new three-phase composite micromechanical model composed of crystallites, amorphous components, and microvoids was introduced to predict the tensile modulus of carbon fibers [19].

However, it has been demonstrated that the aforementioned uniform stress mechanical model, mosaic model and series–parallel mechanical model ignore the disordered structure. Worse still, the uniform stress mechanical model and mosaic model are unable to predict the behavior of low modulus PAN-based carbon fibers. The content of microvoids is about 10% or below in the carbon fibers, and the effect of microvoids on tensile modulus is not palpable [19]. In response, this present study draws upon the two-phase composite micromechanical model composed of crystallites and amorphous components to address the relationship between the microstructure and the tensile modulus of carbon fibers. Also, the differences of tensile moduli affected by the factors of microstructures between seven types of carbon fibers are discussed and compared. The X-ray diffraction (XRD) method is employed to measure the experimental data of crystallites in carbon fibers [16].

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http://dx.doi.org/10.1016/j.compositesb.2016.11.032
1359-8368/

2. Theoretical model

The two-phase composite micromechanical model is described in this section. We assume that the amorphous components is an isotropic matrix. The crystallites are regarded as inclusions in the isotropic matrix. As is shown in Fig. 1. The Eshelby equivalent inclusion theory [20,21] and Mori–Tanaka method [22] are employed to address this two-phase composite micromechanical model. We have assumed that (1) the amorphous components has a Poisson's ratio of $\nu_a = 0.3$ [18]; (2) the coefficients of the elastic tensor of the crystallites are the same as those of graphite [23]; (3) the total volume fraction of crystallite and amorphous carbon is tantamount to unity; (4) as required by the theory, the shape of the crystallites is an oblate spheroid [18], as is shown in Fig. 1. The aspect ratio of the oblate spheroid ω is given by $\omega = L_a/L_c$; where L_a is the crystallite diameter and L_c is the crystallite thickness, both of which are measured by XRD.

In addition, the concept of representative volume element (RVE) V in carbon fibers is introduced. We assume that the RVE is subjected to remote boundary conditions, e.g., see Refs. [24,25]. A global coordinate system $O - x_1x_2x_3$ is established in carbon fibers to ensure that the axis x_3 coincides with the fiber axis. Also a local coordinate system $O - x'_1x'_2x'_3$ in the crystallite is established. The axis x'_3 is made to coincide with the rotation axis of crystallite, as is shown in Fig. 2.

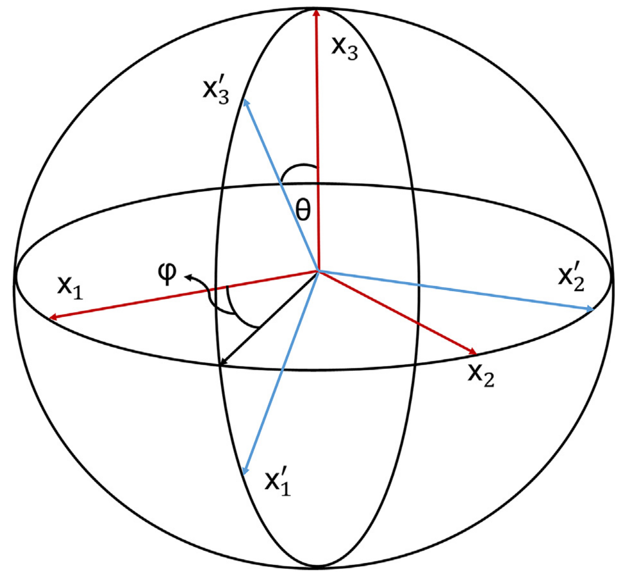

Fig. 2. Diagram of the global coordinate system and local coordinate system.

$\boldsymbol{T}$ is a transformation matrix between the local coordinate system and the global coordinate system. The elastic constants $\overline{\boldsymbol{C}}$ of the carbon fibers can be derived in the way of [18,19]

$$\overline{\boldsymbol{C}} = \left[f_0\boldsymbol{C}_0 + f\left\{\boldsymbol{T}\boldsymbol{C}_1[\boldsymbol{I}-\boldsymbol{A}]\boldsymbol{T}^T\right\}_{\text{angle}}\right]\cdot\left[\boldsymbol{I} - f\left\{\left(\boldsymbol{T}^{-1}\right)^T\boldsymbol{A}\boldsymbol{T}^T\right\}_{\text{angle}}\right]^{-1} \quad (1)$$

where $\boldsymbol{C}_0$ is the elastic coefficients of the amorphous components, $\boldsymbol{C}_1$ is the elastic coefficients of the crystallites, f is the volume fraction of crystallites, and the volume fraction of amorphous components is $f_0 = 1 - f$. $\boldsymbol{A} = \boldsymbol{S}(\Delta\boldsymbol{C}\boldsymbol{S} + \boldsymbol{C}_0)^{-1}\Delta\boldsymbol{C}$ and $\Delta\boldsymbol{C} = \boldsymbol{C}_1 - \boldsymbol{C}_0$. $\boldsymbol{S}$ is the fourth order Eshelby tensor of the crystallite inclusion which has an oblate spheroid shape [26,27]. The details of $\boldsymbol{C}_0$, $\boldsymbol{C}_1$, $\boldsymbol{S}$ and $\boldsymbol{T}$ can be seen in the appendix. $\boldsymbol{I}$ is the unit matrix, and $\{\cdot\}_{\text{angle}} = \int_0^{2\pi}\int_0^{\pi}\cdot\eta(\theta)\sin\theta\mathrm{d}\theta\mathrm{d}\varphi/2\pi\int_0^{\pi}\eta(\theta)\sin\theta\mathrm{d}\theta$, $\eta(\theta)$ is the distribution densities of the crystallites [19,28]. In the case of carbon fibers with a high degree of crystallite orientation in the present study, the distribution density function $\eta(\theta)$ of the orientation angle θ between the normal of the carbon layer and the fiber axis can be closely approximated by an orientation distribution function in the form of $\eta(\theta) = K\sin^{\alpha}\theta$ [29], where $K = \Gamma[(\alpha+3)/2]/\{2\pi^{3/2}\Gamma[(\alpha+2)/2]\}$, and $\alpha = -\ln 2/\ln[\sin(\pi\Pi/2)]$. $\Gamma(x)$ is a gamma function boasting the following property

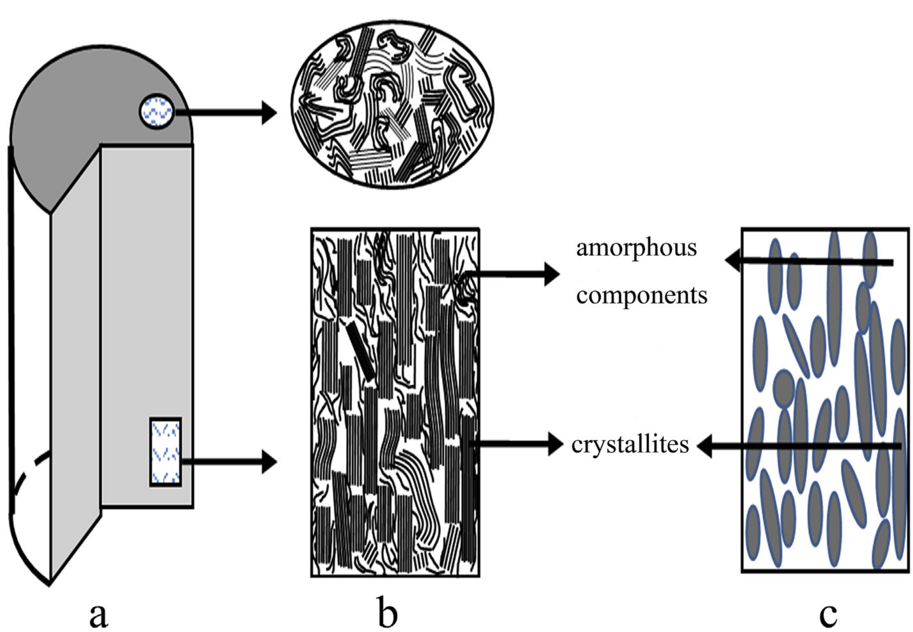

Fig. 1. (a) Model of the carbon fiber, (b) the structure of (a), (c) the modeling of (b).