Available online at www.sciencedirect.com
SCIENCE DIRECT®
Carbon 43 (2005) 1400–1406
CARBON
www.elsevier.com/locate/carbon

Texture modeling in carbon–carbon composites based on mesophase precursor matrices

Gaurav Gupta, Alejandro D. Rey *

Department of Chemical Engineering, McGill University, 3610 University Street, Montreal, Que., Canada H3A 2B2

Received 6 December 2004; accepted 6 January 2005
Available online 25 February 2005

Abstract

A computational modeling study of texture formation in carbon–carbon composites based on carbon fibers and carbonaceous mesophase precursors is presented. The modeling predictions on texture formation and disclination structures are quantitatively validated with extensive experimental data. The number and type of disclinations displayed by the carbonaceous mesophase matrix is shown to be governed by the elasticity of the mesophase, the carbon fiber–mesophase interfacial energy, the size of the fibers, and positional arrangement of the fibers. The simulations provide new insights on the fundamental principles that govern texturing and disclination nucleation, and on how to control the structure of carbon–carbon composites through fiber concentration, fiber cross-section, and fiber–matrix interaction.

Keywords: Mesophase pitch; Carbon composites; Modeling; Microstructure

1. Introduction

Carbon/carbon (C/C) composites are industrial materials used in the defense, sports, and transportation industries [1–3]. Tailoring mechanical property profiles and transport functionality usually leads to uses of different precursors as well as different processing techniques. The use of carbonaceous mesophases (CM) as matrices has the potential to offer advantages in the development of advanced C/C composites, since the matrix microstructure can be manipulated during the formation stage. This paper presents a computational study of texture development during the formation of C/C composites consisting of carbon fibers embedded in carbonaceous mesophase precursors. Experimental data in C/C composites based on carbon fiber–mesophase carbon precursors, related to the present study, has been widely documented by Zimmer and White [4,5]. Optimization, control of property profiles and functionality, as well as science-based manufacturing requires a better understanding of the fundamental principles that control microstructural features of the composite. As shown below, a unique feature of using CM precursors is the fact that inserting micron-size fibers has a structuring effect on the mesophase. In this paper we simulate textures in the mesophase, while the experimental textures [4,5] are obtained after carbonization. The premise of the present work is that significant textural features present in the mesophase state are preserved after carbonization. Since the simulation results are in excellent agreement with experimental textures, it is more than reasonable to conclude that our modeling premise is correct. Moreover previous simulations of texture development in the fiber spinning of mesophase precursors [6] are in excellent agreement with experiments, giving additional evidence to the assumption that significant aspects of mesophase texture are retained after carbonization.

* Corresponding author. Tel.: +1 1514 398 4196; fax: +1 514 398 6678.
E-mail address: alejandro.rey@mcgill.ca (A.D. Rey).

0008-6223/$ - see front matter © 2005 Elsevier Ltd. All rights reserved.
doi:10.1016/j.carbon.2005.01.009

Carbonaceous mesophases are discotic nematic liquid crystals, characterized by orientational order and positional disorder. Mesophases flow like viscous liquids but due to their orientational order, they are anisotropic as crystalline solids. A unique characteristic of liquid crystals including CM is their orientational response to surfaces, interfaces, flow fields, and electromagnetic fields. In C/CM composites the carbonaceous mesophase comes in contact with a dispersion of carbon fibers that affect the orientation of the mesophase based on their characteristic size. The intensity of the texturing process, such as the number of disclinations and the orientation gradients in the mesophase, depends on the nature of the fiber–mesophase interface and on the diameter of the fiber. The fiber–mesophase interfacial interaction is characterized by the anchoring coefficient γ_{an}([=] energy/area), whose sign determines whether the mesophase orientation is edge-on ($\gamma_{an} > 0$) or face-on ($\gamma_{an} < 0$). The effect of substrate chemistry on mesophase interfacial orientation has been characterized [7]. For the present case, it has been found that the mesophase orients face-on with respect to the carbon fiber [4,5]. The orientation gradient elasticity [8] of carbonaceous mesophases is due to basic distortion modes known as splay, bend, and twist [8], and is characterized by the Frank modulus of elasticity K ([=] energy/length). Embedding a circular fiber of radius R in an infinite mesophase will result in an orientational distortion only if:

$$\ell_{\text{extrapolation}} = \frac{K}{|\gamma_{an}|} < R \tag{1}$$

where $\ell_{\text{extrapolation}}$ is the extrapolation length and is a property of the interface (γ_{an}) and the mesophase elasticity (K). The magnitude of the extrapolation length indicates whether the distortion created by immersing an object in the mesophase is absorbed by the bulk or by the interface. When $\ell_{\text{extrapolation}} < R$ it is energetically favorable to distort the matrix, and when $\ell_{\text{extrapolation}} > R$, it is energetically favorable to distort the relative orientation between the mesophase and the object. The regime $\ell_{\text{extrapolation}} < R$ is known as "strong anchoring", and $\ell_{\text{extrapolation}} > R$ is known as "weak anchoring" [9]. In addition when $\ell_{\text{extrapolation}} < R$ the distortion is usually confined to a close region by the appearance of disclination lines (fibrous objects) or disclination points (spherical objects). Fig. 1 shows a schematic of a circular carbon fiber embedded in a carbonaceous mesophase for: (a) strong anchoring with face-on interfacial orientation, and (b) weak anchoring, the lines indicate the orientation of the directors. Fig. 1 shows that under strong anchoring two disclinations arise closer to the interface and the mesophase orientation displays bending distortions. For typical mesophases and micron-thick carbon fibers, experiments (see Fig. 2) shows that

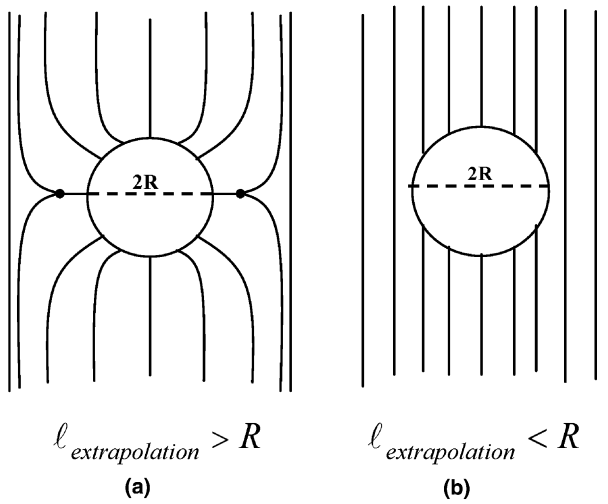

Fig. 1. Schematic of carbon fiber embedded in a carbonaceous mesophase matrix at different anchoring regimes: (a) strong anchoring with face-on interfacial orientation, when $\ell_{\text{extrapolation}} < R$, and (b) weak anchoring, when $\ell_{\text{extrapolation}} > R$. The lines in both plots represent a side-view of the molecular planes; see Fig. 2 for an actual composite structure under the strong anchoring regime.

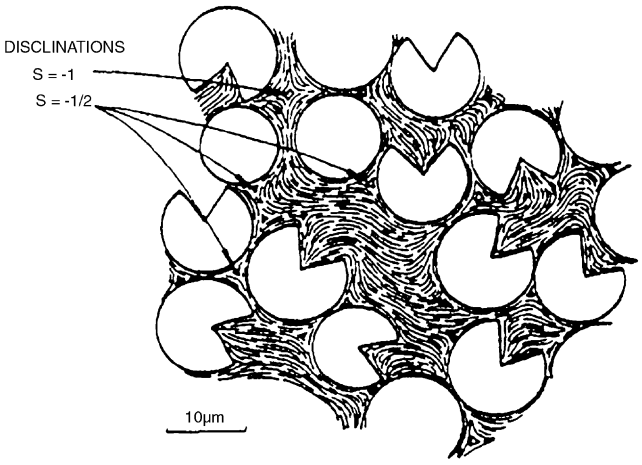

Fig. 2. Alignment of mesophase layers in a random arrangement of fibers. Disclinations of $-\pi$ and -2π are found in the matrix with $-\pi$ having a discontinuous core whereas -2π have continuous cores. Adapted from [5]. Reprinted with permission of Elsevier.

strong anchoring holds, and hence C/C composites will inevitably have a number of disclinations.

Texturing in C/C composites includes disclination nucleation phenomena from multiple fiber effects. At high fiber density three, four, and higher, multi-fiber clusters encircle mesophase domains and give rise to disclination nucleation from multiple surface anchoring. The rules of disclination nucleation in multiple fiber arrangements have been characterized experimentally [5], and will be discussed in Section 2.2 below. Fig. 2 shows a typical texture in C/CM composite [5]. The figure shows the random arrangement of circular and wedge carbon fibers and the texture in the mesophase.