Composite Structures 204 (2018) 578–586

Contents lists available at ScienceDirect

Composite Structures

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

# Multiscale modeling of the mechanical properties of Nextel 720 composite fibers

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ARTICLE INFO

*Keywords:*
Nextel fibers
Multiscale modeling
Ultimate tensile strength
Bridging Cell Method
Mechanical properties

ABSTRACT

The mechanical behavior of Nextel 720 ceramic matrix composite fibers was modeled using a novel multiscale modeling technique called the Bridging Cell Method (BCM). The BCM divides the system into three domains: atomistic, bridging, and continuum; with seamless coupling between the atomistic and continuum domains. The BCM allows considering the effects of the nano- and micro-structural characteristics of the material when modeling a macro-scale bulk. It incorporates interatomic potentials and quasi-harmonic calculations to find the final state of the system. The mechanical properties of the as-received fibers were investigated in tension via microtesile testing. The experimental results – evaluated in terms of the ultimate tensile strength, failure strain, and elasticity of the fibers under uniaxial loads – stood within the range reported in the literature; these results were then used to validate the Nextel BCM model. The Nextel BCM was conducted in two steps. First, the atomistic structure was relaxed. Then, a nano-crack was introduced in the mullite/alumina interface and the structure was pulled under a uniaxial tensile load until failure occurred. The BCM results indicated a good match between the Nextel BCM model and the experimental results. The validated Nextel BCM model can be used for the structural analysis of fibers.

## 1. Introduction

Nextels are a type of oxide/oxide ceramic matrix composite fibers made up of metal oxides and identified by numbers. These fibers are converted into textiles that make up fabric, paper, tape, sleeving, and yarn that needs to meet demanding performance requirements in service conditions [1]. Among the different types of Nextels, Nextel 720 is a polycrystalline consisting of alumina and silica, with only three elements: aluminum, silicon, and oxygen. It is known to be the most environmentally stable Nextel up to temperatures as high as 1100 °C, mainly due to its microstructural properties, high alumina content, and crystalline nature [2]. Nextel 720 fibers have a high tensile strength of 2100 MPa and Young's moduli of 260GPa, along with a low creep rate and thermal expansion [3]. In addition, they have better strength retention – 70% up to 1300 °C – than any other type of fiber, due to their reduced grain boundary sliding [1,4]. The room temperature strength is reported to be almost completely retained by fibers exposed to 1000 h of 1100 °C. However, there is a significant drop in their strength between 1100 °C and 1300 °C, which is attributed to the grain growth of the alumina. This growth makes the fibers much more vulnerable when bearing tensile and cyclic creep loads [4].

Nextel 720 fibers consist of 85% wt $Al_2O_3$ and 15% wt $SiO_2$. Their microstructure consists of a secondary phase mullite with 55% volume fraction and elongated $\alpha$-$Al_2O_3$ grains with 45% volume fraction crystallites [5]. The $\alpha$-$Al_2O_3$ phase is the most stable structure of the alumina at all temperatures, and has a closed-packed hexagonal crystal structure [6]. The mullite phase is a solid solution phase of alumina and silica, which is the only stable intermediate phase in the $Al_2O_3$-$SiO_2$ system. The mullite's composition can be displayed as $Al_2(Al_{2+2x}Si_{2-2x})O_{10-x}$, where x is the number of oxygen vacancies per unit cell [7,8]. By increasing the x value, i.e. the vacancy density, the aluminum content increases. The mullite structure is complicated in terms of composition, oxygen vacancy density, and random distribution of Si and Al in tetrahedral spaces [9]. These structural features strongly affect the Nextel fibers' behavior. Therefore, it is crucial to consider the effect of the fibers' microstructure when analyzing their macroscale behavior in service conditions.

Nextel 720 fibers are being used either as textiles or composite reinforcements for thousands of hours at a time and in harsh, high temperature environments such as aircraft engines; at the same time, they bear high cyclic creep and tensile loads [1,2]. However, there have been no specific models developed to identify the mechanical properties and failure origins of these fibers, either at room temperature or after exposure to high temperatures. The goal of this paper is to develop

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https://doi.org/10.1016/j.compstruct.2018.08.001
Received 21 November 2017; Received in revised form 3 July 2018; Accepted 1 August 2018

a model to predict the mechanical behavior of Nextel 720 fibers in terms of elasticity, ultimate tensile strength (UTS), and failure strain. An atomistic model could account for the microstructural properties of the fibers. However, purely atomistic models are computationally expensive and limited to minimal time steps and small scales. Conversely, multiscale models are capable of modeling larger scales of materials and incorporating atomistic models where necessary. Therefore, a multiscale modeling technique called the Bridging Cell Method (BCM) [10–15] was used to develop the model of the Nextel 720 fibers examined in this study. The BCM is one of the most efficient multiscale techniques developed to date. It divides the system into three domains: atomistic, bridging, and continuum, and solves the system of equations using numerical iterations based on finite element calculations in all domains. This makes the atomistic and continuum domains couple seamlessly through the bridging domain, leading to accurate predictions of bulk materials' behavior that also take the effect of the microstructure into account.

Iacobellis and Behdinan [13] studied the computational efficiency of BCM quantitatively. They applied BCM for three test cases of displacements of a one-dimensional chain of atoms, a two-dimensional void in copper, and a fracture model for copper. They compared the BCM's accuracy and its computational time with Molecular Mechanics and Molecular Dynamics approaches. They found that BCM is as accurate as purely atomistic models while it is at least ten times faster [13]. In another study, they showed that BCM's computational time is comparable with other concurrent multiscale methods such as Quasi-Continuum and Bridging Domain methods [10].

In the current paper, a BCM multiscale model of Nextel 720 fibers was applied to predict the mechanical properties of such fibers. This model was a combination of two BCM models of mullite and alumina, both of which had been previously generated, verified, and published by the authors [14,15]. The results of the combined model were then verified with the micro-tensile test results of the actual fibers in terms of ultimate tensile strength, failure strength, and elasticity, as described below.

## 2. Materials

The Nextel 720 ceramic matrix composite fibers used in this study were manufactured by 3M Company in St. Paul, MN, USA. The fibers had a polycrystalline mosaic structure with a mullite matrix and needle-shaped alumina grains of 50 nm and smaller, which were randomly oriented. The entire chemical composition was uniform in all grains, as confirmed by the TEM images. Fig. 1a and b show the TEM images of the as-received fibers with a mosaic microstructure on a scale of 500 nm, and the $< 50$ nm alumina grains on a scale of 20 nm, respectively. In the Figures, the white matrix is the mullite phase, and the gray grains are alumina. The fibers had a 10–12 μm diameter with a density of 3.03–3.94 g/cm$^3$, and were grouped together in yarn. The room temperature strength of a single filament was 2100 MPa at a 25 mm gauge length, with an elastic moduli of 250GPa, as reported by the provider [1].

## 3. Experimental procedure

The mechanical properties of the as-received fibers were investigated at room temperature. The single filament fibers were extracted from the yarn; great care was taken not to contaminate the fibers. Tensile strength tests were conducted on single-filament fiber samples using a Deben Microtest 20N machine. Before each tensile test, each fiber's diameter was measured using a high-resolution Zeiss Axio Scope A1 optical microscope. The samples were then mounted horizontally and clamped to a pair of jaws on the micro-tensile testing machine. Appropriate alignment of the filaments with the load axis was crucial to obtaining reliable load values. The tested gauge length was 10 mm, and the strain loads were applied with a displacement rate of 0.1 mm/min.

The microstructure of the as-received fibers was examined using a Titan 80–300 LB high resolution image-corrected HRTEM/STEM operating at 80 and 300 keV. The TEM samples were prepared via the FIB method described in the literature [16,17]. The external and fracture surfaces of the tested fibers were observed with a SU3500 Variable Pressure SEM in order to analyze the fracture morphology and failure behavior of the fibers.

## 4. Multiscale model

This study performed a novel multiscale modeling technique called the Bridging Cell Method (BCM) to model the mechanical behavior of the Nextel 720 fibers. The BCM divides the problem domain into a continuum zone to be solved on a larger scale, and an atomistic zone to be solved on a nanoscale where necessary [13]. There is also a bridging domain to transfer information between the atomistic and continuum domains. The atomistic and continuum domains are coupled via the bridging domain by mapping the displacements of the atoms to the nodes of the bridging cells. Then, the displacement of the continuum domain neighbouring the interface is constrained to follow the least square fit of atomistic displacement. In addition, the nonlocal interaction of the atoms in the bridging cells locally interacting with their nearest neighbours is approximated by a linearized potential function. In this way, spurious forces are eliminated, since there is no local/nonlocal mismatch. The whole system is solved using finite element calculations and an iterative approach to solving the problem, allowing the system to reach a minimum state of potential energy at finite temperatures [10,11].

In this study, a BCM model was developed for the Nextel 720 fibers

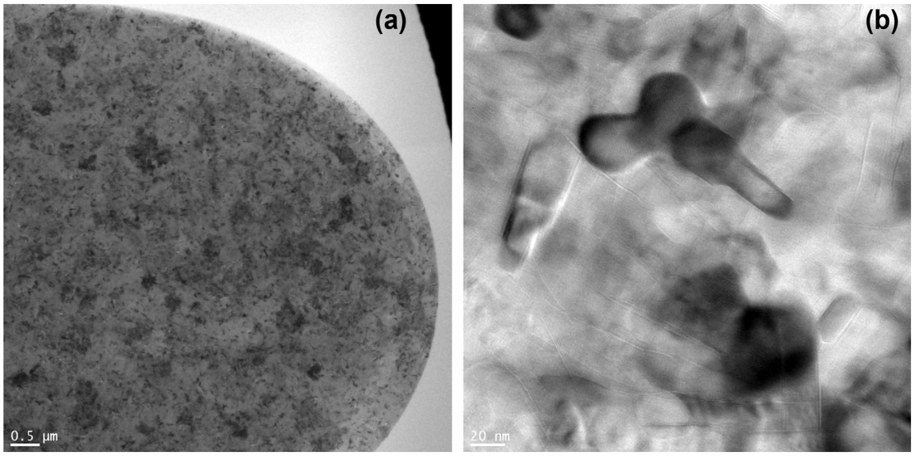

**Fig. 1.** TEM images of the as-received Nextel 720 fibers, highlighting a mosaic microstructure consisting of a white matrix (the mullite phase) and gray alumina grains. a) The 500 nm scale shows a single filament fiber and its structure; b) The 20 nm scale shows the grain boundaries between the alumina grains and mullite matrix.