Composites: Part B 60 (2014) 637–662

Contents lists available at ScienceDirect

Composites: Part B

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

Virtual testing of advanced composites, cellular materials and biomaterials: A review

M.I. Okereke *, A.I. Akpoyomare, M.S. Bingley

Department of Mechanical, Manufacturing and Design Engineering, University of Greenwich, Kent ME4 4TB, UK

ARTICLE INFO

Article history:
Received 23 September 2013
Received in revised form 3 December 2013
Accepted 3 January 2014
Available online 9 January 2014

Keywords:
A. Polymer–matrix composites (PMCs)
C. Computational modelling
C. Numerical analysis
E. Weaving
Virtual testing

ABSTRACT

This paper documents the emergence of virtual testing frameworks for prediction of the constitutive responses of engineering materials. A detailed study is presented, of the philosophy underpinning virtual testing schemes: highlighting the structure, challenges and opportunities posed by a virtual testing strategy compared with traditional laboratory experiments. The virtual testing process has been discussed from atomistic to macrostructural length scales of analyses. Several implementations of virtual testing frameworks for diverse categories of materials are also presented, with particular emphasis on composites, cellular materials and biomaterials (collectively described as heterogeneous systems, in this context). The robustness of virtual frameworks for prediction of the constitutive behaviour of these materials is discussed. The paper also considers the current thinking on developing virtual laboratories in relation to availability of computational resources as well as the development of multi-scale material model algorithms. In conclusion, the paper highlights the challenges facing developments of future virtual testing frameworks. This review represents a comprehensive documentation of the state of knowledge on virtual testing from microscale to macroscale length scales for heterogeneous materials across constitutive responses from elastic to damage regimes.

1. Introduction

The need to advance the understanding of the mechanics of many engineering materials has led to developments of analytical, computational and phenomenological methods for predicting the behaviour of such materials. About 10 years ago, Oden and co-workers [1] predicted that virtual design, in other words virtual testing, will be one of the key areas that will revolutionize computational mechanics research. According to the authors, this will require development of "*radically new computational tools, with the ability to handle multiscale phenomena, very heterogeneous materials, and discontinuous behaviour, such as fracture and assessment of the range of performance...*" [1]. As the authors predicted, in the last decade, the use of virtual testing methods as predictive tools for understanding the mechanics of engineering materials has become commonplace. Firstly this is encouraged by better understanding of the physics of microscale response of materials. Secondly, the improvements in computational powers have encouraged researchers to begin modelling a wide range of mechanical responses originating from atomic [2] and microscale length scales which serve as inputs for predicting constitutive behaviour at the structural level [3–6]. Therefore such developments have resulted in various forms of virtual laboratories that could eventually become substitutes to physical experiments under certain conditions [7]. Typical examples of *virtual experiments* [2,5,6] are described by the originating authors using various keywords as: *computational experiments* [8], *virtual laboratories* [9], *numerical testing machines* [7], *virtual frameworks* [10,11], *immersive virtual environments* [12], *in silico experiments* [13], etc. In the context of this work, the authors will make interchangeable use of any of the following terms to refer to a virtual testing framework: *virtual laboratory*, *virtual testbed*, and *virtual framework*.

The main driving factor towards the use of advanced materials for structural applications in engineering, healthcare, sports equipment manufacture industry, etc. is the possibility of engineering novel materials by altering the microstructural composition. According to Jones and Ashby [14], the possibility of developing novel and improved materials is the *underpinning technology which can stimulate innovation in all branches of engineering.* Advances in understanding of the physics of materials and improvements in computational capabilities have led to development of niche heterogeneous materials described as *tailored or designer* or *smart materials* [15]. These materials possess a combination of mechanical properties that can be adapted (by altering their microstructural composition) to make them suitable for different design

* Corresponding author. Address: Department of Mechanical, Manufacturing and Design Engineering, School of Engineering, University of Greenwich, Medway Campus, Chatham Maritime, Kent ME4 4TB, UK. Tel.: +44 (0) 1634 88 3580; fax: +44 (0) 1634 88 3153.
E-mail address: m.i.okereke@gre.ac.uk (M.I. Okereke).

1359-8368/$ - see front matter © 2014 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.compositesb.2014.01.007

requirements. The microstructural adaptation in some cases involves molecule-by-molecule assembly of their constituents [16,17]. The science of microstructural modifications has also led to development of many different categories of high performance materials like textile composites, functionally graded materials, 3D reinforced composites, tissue-engineering enhanced biomaterials, nano-composites, etc. For the purposes of this paper, all these advanced materials are broadly described as *heterogeneous systems*. The enhanced properties arise from the possibility of altering their multi-component microstructural compositions. However, this advantage also presents the predictive modelling challenge they pose to material modellers.

Research in virtual testing of heterogeneous materials is still relatively limited and to date there has been no structured compilation of the current state of knowledge. However, such information is necessary as a growing community of researchers are working on virtual testing of continuous fibre reinforced composites [3,18]. This paper aims to present a detailed review of the existing virtual testing approaches for a wide class of heterogeneous materials namely: composites, cellular materials and biomaterials. This is by no means an exhaustive list as other possible heterogeneous materials include: functionally graded materials, piezoelectric materials, etc. The paper also documents the challenges facing developers of virtual testing frameworks in order to make such methods realistic substitutes for physical experiments. Emphasis is on recent literature of virtual testing of heterogeneous materials; published in the last decade.

The term *virtual testing* is commonly used in aerospace industry to describe the extrapolation of coupon-level experimental data towards understanding the fracture mechanics of structural parts of the aircraft [19,20]. The aircraft industry uses virtual testing as a design tool thereby reducing the cost of expensive structural testing of new aircraft variants which can cost as much as $40 million [5]. Whilst such application of virtual testing theory is laudable and widespread, the scope of this review article does not encompass such structural level applications of virtual testing. The strategy of using coupon-level data for predicting structural response falls outside the scope of this paper. Rather this work deals with relevant literature on the application of virtual testing of heterogeneous materials by tracking the effect of microstructural modifications on macroscale predictions.

The paper first presents an overview of virtual testing before discussing the roles of lengthscale in designing virtual experiments. The structure of typical virtual testing laboratories is also presented and typical examples considered. Subsequently, the paper describes different virtual testing implementations for a wide class of heterogeneous materials, ranging from composites to biomaterials. Finally, the paper concludes with delineating the challenges facing the development of new virtual testing frameworks.

2. Virtual testing: an overview

Over the last two decades, virtual testing of heterogeneous materials has been generally accomplished by numerical modelling tools after the finite element method (FEM) [10,12,13]. Although the research investigation for virtual tests differs considerably from case to case, there are, however, several distinct steps typified by these strategies, necessary to execute a virtual test. Firstly, the virtual problem domain of interest must be defined: this involves developing a geometry/domain that represents the material to be investigated, or, defining a boundary within which the *virtual matter* of interest exists. Secondly, the constitutive behaviour of the declared virtual domain must be defined; for example, the material may exhibit a classical Hookean behaviour or a pre-defined non-linear constitutive behaviour, etc. Thirdly, boundary conditions must be imposed on this domain: this may be in the form of body forces, displacements or thermo-mechanical loading, etc. Fourthly, the constitutive response (i.e. stress–strain curves) of the virtual domain is obtained either directly or through appropriate homogenization techniques. The final, important step in the virtual testing framework is a *validation exercise* which involves comparing the constitutive response(s) obtained from the virtual tests with available experimental or analytical data.

Although the foregoing outlines the basic steps involved in performing virtual tests; in reality, several issues exists that present considerable challenges. The mechanical behaviour of any material is a consequence of synergistic combination of its constituents (i.e. atoms, crystals, crystal planes, etc.). For heterogeneous materials, this is particularly true because of the relationship that exists between its constituents (i.e. in composites the matrix and fibres) as well as the internal structure of its individual constituents (i.e. atomic structure of fibre or matrix, etc.). Thus, the features that are responsible for the behaviour of heterogeneous materials exist across several domains, spanning a spectra of length and time scales. There arises therefore the challenge of incorporating the physics behind each relevant feature, at each relevant length and time scale, which affects the constitutive behaviour of the virtual domain of interest. The next section considers the place of length scale in virtual testing, and in later sections different variants of virtual testing frameworks are considered.

3. Virtual testing and length scales

The determination of a relevant length scale is central to computation of properties of heterogeneous materials. Rudd and Broughton [21] stated that the central aim of computational materials physics is the accurate description of specific materials on length scales spanning the electronic to the macroscopic. Heterogeneity in these *designer materials* suggests that there will be microscale constituents whose composition, orientation and evolution influence macroscale properties. Therefore, at the onset, it is important that length scales be defined for common heterogeneous materials with a view towards understanding the development of virtual tests for such materials.

Typical length scales for describing the response of engineering materials range from atomic/molecular to structural length scales. At the atomic length scale, a typical length dimension, L is very much less than 10^{-9} m; whilst at the nanoscale, the length dimension is in order of a nanometre. The microscale is usually in orders of magnitude of a micron, while the mesoscale is a couple of millimetres. The macroscale is in dimensions of centimetres and structural length scales are in orders of meters. Fig. 1 shows the order of increasing length scales and the applicable area of computational experiments where each length scale can be used.

Current virtual testing research is based either on a bottom-up (hierarchical) or top-down (concurrent) modelling implementation. The bottom-up implementation determines constitutive behaviour of the heterogeneous material by building up a detailed understanding of the material's constitutive behaviour, from lower length scales through to higher length scales, by utilizing robust constitutive models of the constituents of the test material [22–24]. In the lower length scale regime, lower order behaviour can include crystal plasticity [25], macro-molecular mechanics [26,27], fibre rupture/kinking and matrix cracking in composites [28], bone tissue porosity [24], cell walls distortions in cellular materials [29], fibrillar and molecular deformation mechanisms of collagens[30], fibroblasts and tenocytes mechanics [31], etc.

Regarding the bottom-up approach, the differences in length scales present a challenge towards relating the predictions