
Damage Mechanisms of Hierarchical Composites: Computational Modelling

L. Mishnaevsky, Jr.*

Technical University of Denmark, Risø Campus, Roskilde, 4000 Denmark

* e-mail: lemi@dtu.dk

Received September 02, 2015

Abstract—Computational studies of damage mechanisms in hierarchical composites, including biocomposites, nanoparticle reinforced polymer composites and other materials are discussed. Different methods of the analysis of hierarchical effects in the multiscale composites are demonstrated, among them, hierarchical fiber bundle model, 3D multiscale finite element models, analytical studies. Considering wood as a gradient, cellular material with layered composite cell walls, one analyzed the effect of wood structure on damage resistance of wood. The influence of nanoparticles distribution in unidirectional polymer matrix composites with secondary nanoreinforcement on the strength and damage resistance of the composites is demonstrated. The concept of nanostructuring of interfaces and grain boundaries as an important reserve of the improvement of the materials properties is formulated.

DOI: 10.1134/S102995991504013X

Keywords: composites, hierarchical materials, strength, fracture, nanomaterials, biomaterials

1. INTRODUCTION

Hierarchical composites attracted large interest of the scientific community, due to several reasons. The ideas of biomimicking and investigations of biomaterials (wood, bones, etc) suggested that hierarchical architectures of the materials are among the main sources of their extraordinary mechanical properties (high strength, fracture toughness, etc.) [1–6]. Further, with the development of nanotechnology and nanomaterials, the idea of incorporate nanoengineered materials into common composites (thus, creating hierarchical materials, combining the advantages of composites and nanomaterials) was formulated and realized in several cases at laboratory level (see, e.g. [7–9]).

The potential advantages of hierarchical composites over common composites and materials include:

- synergy between structural elements at several scale levels (example: fibers control the tensile strength and stiffness in hierarchical composites, while secondary nanoparticles in the matrix control the shear and compression strength [7, 8, 10]);
- possibility to improve competing properties of materials (examples: hierarchical ceramics demonstrate both higher strength and higher toughness [9]);

- potential to improve the interface controlled properties, like compression and fatigue strength, by placing nanoparticles on interfaces or fiber sizing;
- combination of advantages of nanomaterials and composites, and so on.

In this paper, computational studies of the effect of hierarchical structures of several groups of multiscale composites on their damage mechanisms, carried out at the Department of Wind Energy, Technical University of Denmark, are summarized. The general effect of hierarchization on the damage resistance of composites, the roles of multiscale structures of wood and of carbon nanotube reinforcements in hierarchical unidirectional polymer composites are studied. Further, the concept of degradation scenario based multiscale material design and using the nanoengineered interfaces are summarized.

2. SYNERGY AND INTERPLAY BETWEEN STRUCTURAL ELEMENTS AT DIFFERENT SCALE LEVELS

Mechanisms of the peculiar properties of hierarchical composites are related to the interaction between structural elements at several scale levels. So, under mechanical loading, the load transfer between the levels takes

place, especially when the microstructure changes (i.e., due to damage or deformation). In order to study the effect of hierarchical structures of composites on their properties, taking into account the peculiarities of load transfer directly, the hierarchical load sharing models can be used [10]. According to this model, the load is transferred from the upper elements of the hierarchical “tree” (“roots”) to the lower (“branches”) and down to the lowest elements of the material (fibers, in the case of long fiber reinforced composites). The load is shared equally among all the sub-elements of a given branch (as long as they are intact) or among remaining intact sub-elements after some of them fail. In simplest case, this load rule can be directly introduced into the analytical fiber bundle models of composites [6, 11, 12].

Let us consider a multiscale self-similar composite model (Fig. 1a) subject to a tensile mechanical loading. The composite consists of elements which are either pure matrix or reinforcements at each level. The reinforcing elements at the different levels are self-similar: they, in turn, consist of pure matrix and the lower level reinforcing elements. Since the strain on the fibers and matrix in each element is constant, the load is distributed between the fiber (or strong elements at the given hierarchy level, which represent composites, in turn consisting of fibers and matrix) and matrix proportionally to the Young modulus of a given element [12].

At the lowest level, the strong elements (i.e., fibers) are assigned the strengths according to the Weibull law. If the strength of a given element is less than the applied load, the element (fiber, matrix or bundle) fails and the load is redistributed on the remaining fibers belonging to the same bundle/branch. After all the fibers in the branch fail, the higher level element is considered as failed, and the load is distributed among all the remaining elements belonging to the same higher level branch (“bundle of bundles”), and so on.

If the volume content (vc) of the reinforcing elements at each level is constant, the global volume content of lowest level fibers in the material is given by $vc_{\text{glob}} = vc^M$, where M —the amount of hierarchy levels. Thus, if we define the total volume content of glass in the composite, the volume content of stronger phase at each scale level is calculated as a M -degree root from this number. Determining the Young modulus of the material at each level using the rule of mixture, we have the Young module at the j th level as [12]:

$$E = vc^j E_f + (1 - vc) E_m \left(1 + \sum_{i=1, j-1} vc^i\right),$$

where E_f , E_m are the Young moduli of (lowest level) fibers and pure matrix respectively; vc —volume content of reinforcing elements at each level (assumed to be constant).

Using a program code for the analysis of damage evolution in the multiscale fiber bundle model [12], the effect of hierarchization and structure of the self-similar materials on their damage resistance was investigated. Figure 1b shows the critical stress (at which the damage in the whole fiber bundle exceeds 0.9) plotted versus the amount of hierarchy levels for the total damage, and separately for fibers and matrix, for glass fiber reinforced composites.

The important observation is that the damage resistance of the multiscale self-similar fiber reinforced composites increases with increasing the amount of hierarchy levels in the material (as differed from the case of “hierarchical tree” considered in [10, 12], where increasing the amount of hierarchical levels means reduced damage resistance).

This rather simple model of hierarchical composites allows to analyze the effects of hierarchical structures and hierarchical load transfer in pure form, paying attention only to the hierarchical structures and disregarding the

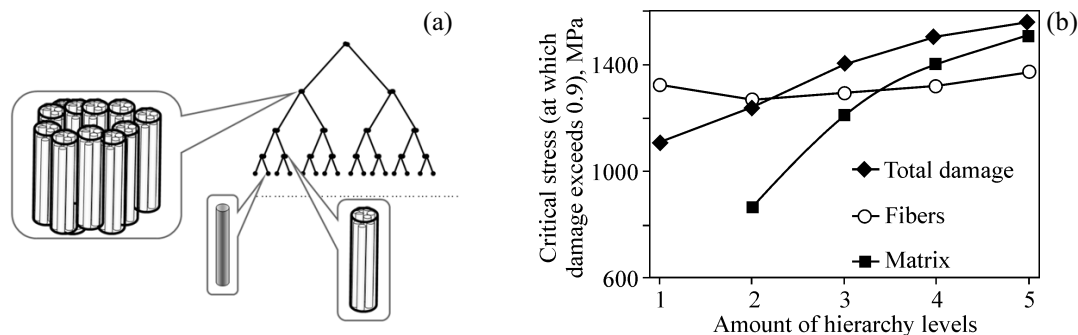


Fig. 1. Hierarchical fiber reinforced composite model (a) and critical stress plotted versus the amount of hierarchy levels for glass fiber reinforced composites (b). Reprinted from [12] with kind permission from Elsevier.

influence of more complex, inhomogeneous structures at each scale level.

3. HIERARCHICAL BIOCOMPOSITES: WOOD

Biological composites such as nacre, wood, bone have been widely studied both experimentally and numerically. For instance, extraordinary nacre strength is in clear contrast to the brittleness of its components. Among the microstructural peculiarities of nacre, responsible for its unusual properties, the brick and mortar structure, interlocking of platelets, layered configuration, thin organic layers, etc can be mentioned [13]. Bone is a porous, cellular materials consisting of multilayered lamellas, built in turn of fibrous layers with different orientations and thicknesses and with various microgeometries for different types of bones (cortical and cancellous). At the nanolevel, the bone is seen as the collagen fibers, surrounded by mineral [14]. Wood is characterized by layered and gradient structures at the macrolevel, cellular structure at microlevel, with multilayer cell walls, and fiber composite-like structures at the nanolevel (Fig. 2). As different from the idealized self-similar composites, natural hierarchical materials have different structures at different scale levels. In order to simulate such heterogeneous (over scale levels) structures, complex micro-mechanical models are required.

In [15–17], the computational model of wood which takes into account the different structural features of the wood at different scale levels, was developed. The model includes four levels of the heterogeneous microstructure of wood:

- macrolevel: annual rings are modeled as multilayers, using the improved 3D rule of mixture,
- mesolevel: the layered honeycomb-like microstructure of cells is modelled as a 3D unit cell with layered walls; the properties of the layers were taken from the microlevel model,
- submicro- and microlevel: each of the layers forming the cell walls was considered as an unidirectional, fibril reinforced composite. Taking into account the experimentally determined microfibril angles and content of cellulose, hemicellulose and lignin in each layer, the elastic properties of the layers were determined with the use of Halpin–Tsai equations

Figure 2 gives an example of the finite element unit model of earlywood. Using the developed model, the effect of microstructural parameters of wood on its deformation behaviour was studied. In particular, the influence of microfibril angle and wood density on the deformation behaviour was considered. From the computational studies, it was concluded that the variation of microfibril angles represents a rather efficient mechanism of the natural control of stiffness of the main shear load bearing layer of the cell wall. By increasing the microfibril angles, the drastic increase of shear stiffness in 1-2 direction is achieved, without any sizable losses of the transverse Young modulus and shear modulus in the 23 plane.

In order to analyze the effect of wood microstructure on the fatigue lifetime, the 3D hierarchical model was extended to include the damage process and combined with phenomenological approach toward the fatigue modeling [18]. The progressive damage models for wood were developed, taking into account the strength of the cell wall

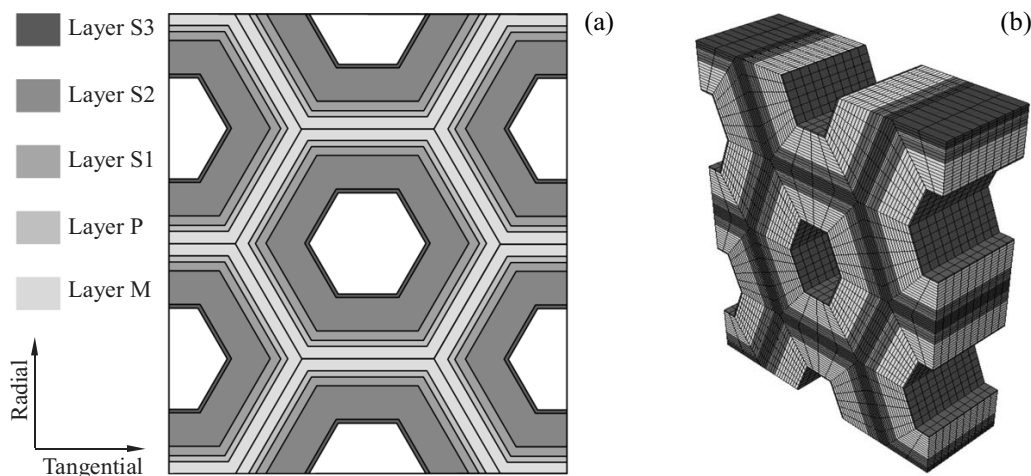


Fig. 2. 3D finite element unit cell model of wood as multilayered cellular material. Schema of layers (a) and 3D finite element model (b) [15–17].

layer components (lignin, cellulose, polymers) and different strengths of different layers (see [17] for more details).

Several unit cells with different predamage degrees (i.e., notch lengths) and different microfibril angle degrees in the cell wall layers S2 (largest and strongest layer) were generated and subject to cyclic tensile loading. The curves of fatigue damage accumulation rate plotted versus the damage density (crack length) were approximated by power laws, and the fatigue lifetime was calculated for given microstructures of the materials. The fatigue lifetimes calculated from these curves are given in [18].

With such multiscale models, the effects of different microstructural parameters and the synergy between microstructures at different scales can be studied in “virtual experiments”. The extension of the hierarchical material model to include the strength and fatigue effects demonstrate the possibilities of the “virtual testing” of hierarchical microstructures.

4. HIERARCHICAL POLYMER COMPOSITES WITH NANOSCALE REINFORCEMENT

The development of hybrid composites, with nanoengineered phases, is a very promising direction to design lightweight materials with improved properties. The fiber reinforced composites with nanoengineered matrix

have much higher strength and fatigue resistance than the neat composites. For instance, 80% improvement of fracture toughness of carbon fiber reinforced epoxy composites achieved as a result of 0.5 wt % addition of carbon nanotubes [19]. 30% enhancement of the interlaminar shear strength of woven carbon fabric in epoxy matrix due to the deposition of multi and single walled carbon nanotubes on fibers [7, 8].

In order to analyze the effect of the nanoparticle distribution in the matrix and in the interface on the strength of the composites, a computational multiscale model was developed, which includes the fiber/matrix interaction at the higher scale level (microlevel) and nanoclay/epoxy matrix interaction on nanolevel. A set of programs for the automatic generation of 3D multiscale models of composites was developed [20–22]. The programs generate command files for the commercial finite element software ABAQUS. The unit cell structures are divided into two levels. The macro (upper level) unit cells contain three phases: the matrix, fibers and “third phase” interface layers (which characterizes the interface roughness, interphases [6, 21]). Both matrix and the interface layer might contain nanoreinforcements. The microscale (lower level) unit cell includes the nanoreinforcement in matrix and/or interfaces, polymer matrix as well as the “effective interface layers” [23]. The macro-model analysis saves the time-dependent values of variables (i.e. stress and displacement field) of the “seed nodes” which

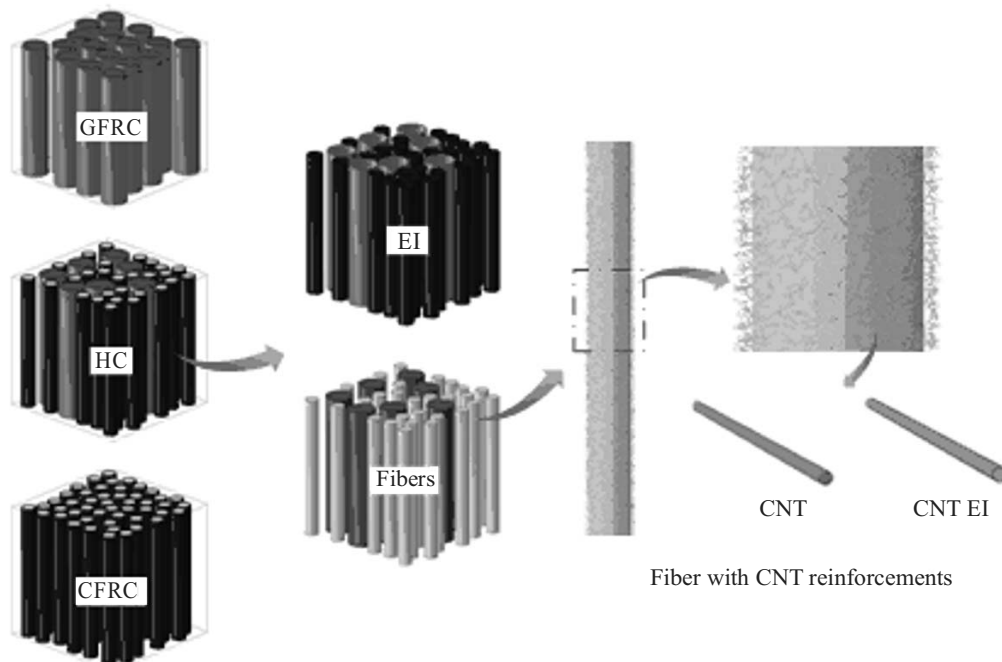


Fig. 3. Example of unit cell model of carbon nanotube reinforced hybrid composite. Reprinted from [24] with kind permission from Elsevier. GFRC—glass fiber reinforced composite, HC—hybrid composite, CFRC—carbon fiber reinforced composite, EI—effective interface.

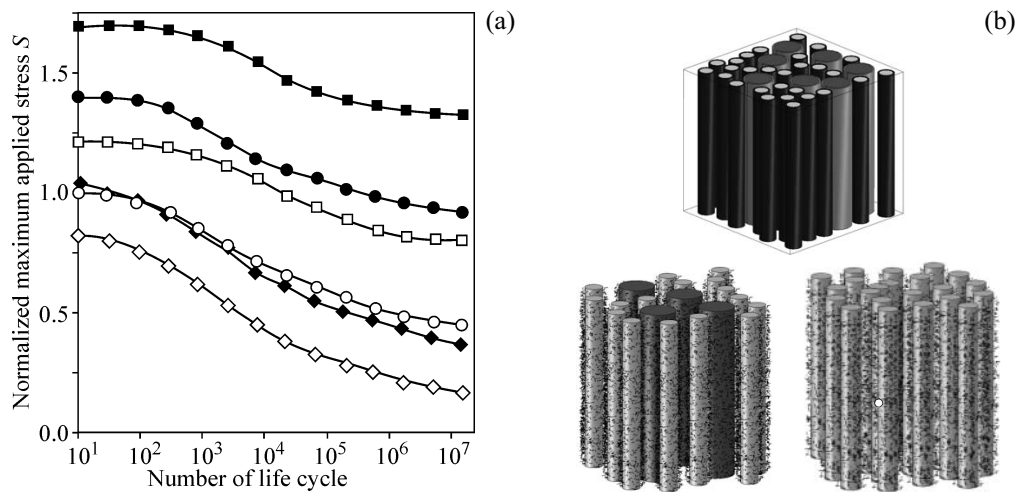


Fig. 4. S - N curves for hybrid composites under pure mechanical cyclic loading (tension-compression) with (■, ●, ◆) and without carbon nanotube reinforcement (□, ○, ◇) (a) and examples of unit cells (glass/carbon hybrid fiber composites without carbon nanotube, hybrid with carbon nanotube, and pure carbon reinforced with carbon nanotube composites) (b). Reprinted from [24] with kind permission from Elsevier.

located on the boundary between macromodel and micromodel after the macrolevel analysis. The micromodel inherits these data as the initial boundary condition and together with other added boundary condition (if needed) to go on the analysis. The mechanical properties and strength of fibers and epoxy were taken from [20, 24]. The mechanical properties of the “effective interface layer” between carbon nanotubes and epoxy in the micromodel were taken from inverse simulations in [25] (assuming that the “effective interfaces” between graphene and epoxy, and carbon nanotube and epoxy are similar). For simplicity, the carbon nanotubes were represented as cylinders.

A number of 3D multiscale unit cell models of carbon nanotube and fiber reinforced composites have been generated and used for the computational testing of structures of composites [21]. Figure 3 shows an example of a unit cell model. The aspect ratio of carbon nanotubes was 1000, and they were distributed in the sizing of the fibers. The volume fraction of the carbon nanotube reinforcement is 0.46%. The model was subject to cyclic compression-tension loading. In order to simulate the fatigue damage evolution, two step procedure was employed. Initial defects (with the sizes of the order of one-two finite elements) were introduced into the macroscale model by subjecting the unit cell to a quasi-static load before the cyclic loading.

Figure 4 shows the S - N curves of composites (under tension-compression loading with $R = -1$) with pure glass, pure carbon and hybrid (1 : 1) fibers, reinforced by carbon

nanotubes located in fiber sizing, and some examples of the unit cells. The vertical axis is normalized by the initial maximum stress of 1 : 1 hybrid fiber reinforced composite without carbon nanotube reinforcement under this loading (274.82 MPa).

It was demonstrated that the carbon nanotube enhances the fatigue performance (maximum stress and lifetime) in all considered composites. For the very low cycle loading, the carbon nanotube reinforcement leads to 25–43% increase in the stress, while for the millions of cycles, the carbon nanotube effect increases the stress by 64–120%. Similarly, the nanoclay particles located in the matrix or in the fiber sizing, ensure drastically enhanced fatigue lifetimes of composites [20]. Figure 5 shows a schema of model of hierarchical fiber composite with nanoclay reinforcements (a) and simulated crack paths in in-between platelets observed in the simulations (aligned and randomly oriented platelets (b and c) [20].

The composites with nanoclay reinforcement achieve the same fatigue life (taken exemplarily at 5.68×10^7 cycles) as neat composites, while subject to 2.0–3.5 times higher loadings. Composites with the nanoplatelets localized in the fiber/matrix interface layer (fiber sizing) ensure much higher fatigue lifetime than those with the nanoplatelets in the matrix: 43–49% higher applied stress corresponding to the selected lifetime of 5.68×10^7 cycles. Composites with exfoliated nanoplatelet reinforcement ensure the better fatigue lifetime than those with clustered particles. For instance, for the lifetime 5.68×10^7 , the applied compressive loading can be 17–25% (both for nanorein-

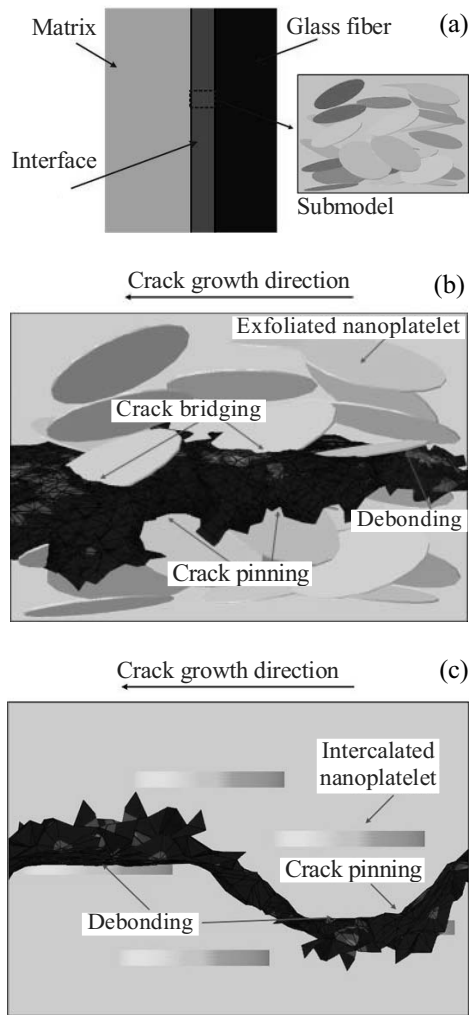


Fig. 5. Schema of model of hierarchical fiber composite with nanoclay reinforcements (a) and simulated crack paths in submodels (aligned (b) and randomly oriented platelets (c)). Reprinted from [20] with kind permission from Elsevier.

forcement in sizing and in matrix) higher for nano-reinforced composite with exfoliated structure than for that with clustered structure.

5. NANOSTRUCTURED INTERFACES: CONTROLLING THE DEFORMATION SCENARIO

Following [26], and analyzing the nanoarchitectures of biomaterials, nanometals and nanocomposites and their effects on the mechanical properties, one can observe the following common feature. Complex, graded, structured interfaces of biocomposites, like nacre and teeth, ensure the extraordinary toughness of the materials [27–30]. Layers of constrained disturbed polymers surrounding nanoparticles in polymer ensure the drastic enhancement

of nanocomposite properties (like 200% increase in stiffness or strength achieved at 0.5% nanoparticle content). As already noted above, nanoparticles (nanoclay or carbon nanotubes) located in fiber/matrix interfaces (fiber sizing) of unidirectional composites allow to increase the fatigue lifetime of the composites drastically [20, 24, 31]. One of reasons of extraordinary strength and toughness of nanocrystalline, ultrafine grained metals is the high content of grain boundary phases in these materials. Their properties can be further enhanced if the grain boundaries are non-equilibrium, with high density of dislocations and especially with foreign atoms/precipitates [32–34]. The availability of precipitates strongly delays the damage growth and ensures 83% increase in the critical strains due to the precipitates, and around 300% increase due to the precipitates located in grain boundaries.

Summarizing these results one can conclude that the purposeful nanostructuring of interfaces and grain boundaries represents an important reserve of the improvement of the materials properties [26]. Since the material deformation is often localized in and around defects (interfaces and grain boundaries), the structuring of these regions (adding specially arranged and oriented nanoreinforcements, or adding nanoscale defects, changing the local properties) allows to control the deformation and fracture behavior of these weak areas, thus, determining the degradation process in the whole material. Quite often, the interfaces with low stiffness lead to the localization of deformation, while the internal structures of the interfaces (like mineral bridges in nacre, or nanoplatelets in sizing of fiber reinforced composites) allow to control the deformation, damage initiation and fracture processes locally.

6. CONCLUSIONS

In this paper, computational studies of damage mechanisms in hierarchical composites carried out over last years at the Section of Composites and Mechanics of Materials, Department of Wind Energy, Technical University of Denmark, are summarized. Both analytical and numerical studies are presented. The main potential advantages of hierarchical materials with view on increased damage resistance as compared with common composites include the exploitation of the load transfer between micro- and nanoelements of the material, localization of strain and damage mechanisms, combination of structural elements paying different roles and controlling different properties. The concept of nanostructuring of interfaces and grain boundaries as an important reserve of the improvement of the materials properties is formulated.

ACKNOWLEDGMENT

The author gratefully acknowledges the financial support of the Danish Council for Strategic Research via the Sino-Danish collaborative project “High reliability of large wind turbines via computational micromechanics based enhancement of materials performances” (Ref. No. 10-094539). Furthermore, the author is grateful to the Danish Council for Strategic Research for its support via the Danish Centre for Composite Structures and Materials for Wind Turbines (DCCSM) (contract number 09-067212).

REFERENCES

1. Fratzl, P. and Weinkamer, R., Nature’s Hierarchical Materials, *Progr. Mater. Sci.*, 2007, vol. 52, no. 8, pp. 1263–1334.
2. Gao, H., Application of Fracture Mechanics Concepts to Hierarchical Biomechanics of Bone and Bone-Like Materials, *Int. J. Fract.*, 2006, vol. 138, no. 1–4, pp. 101–137.
3. Schmahl, W.W., Greisshaber, E., Merkel, C., Kelm, K., Deuschle, J., Neuser, R.D., and Goetz, A.J., Hierarchical Fibre Composite Structure and Micromechanical Properties of Phosphatic and Calcitic Brachiopod Shell Biomaterials. An Overview, *Miner. Mag.*, 2008, vol. 72, no. 2, pp. 541–562.
4. Lakes, R., Materials with Structural Hierarchy, *Nature*, 1993, vol. 361, pp. 511–515.
5. Mishnaevsky, L., Jr., Micromechanics of Hierarchical Materials: a Brief Overview, *Rev. Adv. Mater. Sci.*, 2012, vol. 30, pp. 60–72.
6. Mishnaevsky, L., Jr., *Computational Mesomechanics of Composites*, Wiley, 2007.
7. Bekyarova, E., Thostenson, E.T., Yu, A., Kim, H., Gao, J., Tang, J., Hahn, H.T., Chou, T.-W., Itkis, M.E., and Haddon, R.C., Multiscale Carbon Nanotube-Carbon Fiber Reinforcement for Advanced Epoxy Composites, *Langmuir*, 2007, vol. 23, no. 7, pp. 3970–3974.
8. Bekyarova, E., Thostenson, E.T., Yu, A., Itkis, M.E., Fakhrutdinov, D., Chou, T.-W., and Haddon, R.C. Functionalized Single-Walled Carbon Nanotubes for Carbon Fiber-Epoxy Composites, *J. Phys. Chem. C*, 2007, vol. 111, pp. 17865–17871.
9. Kanzaki, S., Shimada, M., Komeya, K., and Tsuge, A., Recent Progress in the Synergy Ceramics Project, *Key Eng. Mater.*, 1999, vol. 161–163, pp. 437–442.
10. Newman, W.I. and Gabrielov, A.M., Failure of Hierarchical Distributions of Fiber Bundles, *Int. J. Fracture*, 1991, vol. 50, no. 1, pp. 1–15.
11. Daniels, H.E., The Statistical Theory of the Strength of Bundles of Threads, *Proc. Roy. Soc. Lond. A*, 1945, vol. 183, no. 995, pp. 405–435.
12. Mishnaevsky, L., Jr., Hierarchical Composites: Analysis of Damage Evolution Based on Fiber Bundle Model, *Compos. Sci. Technol.*, 2011, vol. 71, no. 4, pp. 450–460.
13. Katti, K.S. and Katti, D.R., Why is Nacre So Tough and Strong? *Mater. Sci. Eng. C*, 2006, vol. 26, no. 8, pp. 1317–1324.
14. Rhoa, J.-Y., Mechanical Properties of Hard Tissues, in *Encyclopedia of Materials: Science and Technology*, Jürgen Buschow, K.H., Ed., Amsterdam: Elsevier Ltd., pp. 3723–3728.
15. Qing, H. and Mishnaevsky, L., Jr., 3D Hierarchical Computational Model of Wood as a Cellular Material with Fibril Reinforced, Heterogeneous Multiple Layers, *Mech. Mater.*, 2009, vol. 41, no. 9, pp. 1034–1049.
16. Qing, H. and Mishnaevsky, L., Jr., 3D Multiscale Micromechanical Model of Wood: From Annual Rings to Microfibrils, *Int. J. Solids Struct.*, 2010, vol. 47, no. 9, pp. 1253–1267.
17. Qing, H. and Mishnaevsky, L., Jr., 3D Constitutive Model of Anisotropic Damage for Unidirectional Ply Based on Physical Failure Mechanisms, *Comput. Mater. Sci.*, 2010, vol. 50, no. 2, pp. 479–486.
18. Qing, H. and Mishnaevsky, L., Jr., Fatigue Modeling of Materials with Complex Microstructures, *Comput. Mater. Sci.*, 2011, vol. 50, no. 5, pp. 1644–1650.
19. Godara, A., Mezzo, I., Luizi, F., Warriar, A., Lomov, S.V., van Vuure, A.W., Gorbalkin, L., Moldenaers, P., and Verpoest, I., Influence of Carbon Nanotube Reinforcement on the Processing and the Mechanical Behaviour of Carbon Fiber/Epoxy Composites, *Carbon*, 2009, vol. 47, no. 12, pp. 2914–2923.
20. Dai, G.M. and Mishnaevsky, L., Jr., Fatigue of Multiscale Composites with Secondary Nanoplatelet Reinforcement: 3D Computational Analysis, *Compos. Sci. Technol.*, 2014, vol. 91, pp. 71–81.
21. Mishnaevsky, L., Jr. and Brøndsted, P., Micromechanisms of Damage in Unidirectional Fiber Reinforced Composites: 3D Computational Analysis, *Compos. Sci. Technol.*, 2009, vol. 69, no. 7–8, pp. 1036–1044.
22. Qing, H. and Mishnaevsky, L., Jr., Unidirectional High Fiber Content Composites: Automatic 3D FE Model Generation and Damage Simulation, *Comput. Mater. Sci.*, 2009, vol. 47, no. 2, pp. 548–555.
23. Wang, H.W., Zhou, H.W., Peng, R.D., and Mishnaevsky, L., Jr., Nanoreinforced Polymer Composites: 3D FEM Modeling with Effective Interface Concept, *Compos. Sci. Technol.*, 2011, vol. 71, no. 7, pp. 980–988.
24. Mishnaevsky, L., Jr. and Dai, G.M., Hybrid Carbon/Glass Fiber Composites: Micromechanical Analysis of Structure-Damage Resistance Relationship, *Comp. Mater. Sci.*, 2014, vol. 81, pp. 630–640.
25. Dai, G.M. and Mishnaevsky, L., Jr., Graphene Monolayer Nanocomposites: 3D Simulation of Damage and Fracture, *Computat. Mater. Sci.*, 2014, vol. 95, pp. 684–692.
26. Mishnaevsky, L., Jr., Nanostructured Interfaces for Enhancing Mechanical Properties of Materials: Computational Micromechanical Studies, *Composites. B*, 2015, vol. 68, pp. 75–84.

27. Qi, H.J., Bruet, B.J.F., Palmer, J.S., Ortiz, C., and Boyce, M.C., Micromechanics and Macromechanics of the Tensile Deformation of Nacre, in *Mechanics of Biological Tissues*, Holzapfel, G.A. and Ogden, R.W., Eds., Graz: Springer-Verlag, 2005, pp. 175–189.
28. Marshall, S., Balooch, M., Habelitz, S., Balooch, G., Gallagher, R., and Marshall, G.W., The Dentin–Enamel Junction—A Natural, Multilevel Interface, *J. Eur. Ceram. Soc.*, 2003, vol. 23, no. 15, pp. 2897–2904.
29. Smith, B., Schaffer, T., Viani, M., Thompson, J., Frederick, N., Kindt, J., Belcher, A., Stucky, G., Morse, D., and Hansma, P., Molecular Mechanistic Origin of the Toughness of Natural Adhesives, Fibres and Composites, *Nature*, 1999, vol. 399, pp. 761–763.
30. Katti, D.R., Pradhan, S.M., and Katti, K.S., Modeling the Organic-Inorganic Interfacial Nanoasperities in a Model Bio-Nanocomposite, Nacre, *Rev. Adv. Mater. Sci.*, 2004, vol. 6, pp. 162–168.
31. Dai, G.M. and Mishnaevsky, L., Jr., Carbon Nanotube Reinforced Hybrid Composites: Computational Modelling of Environmental Fatigue and Their Usability for Wind Blades, *Composites. B*, 2015, 10.1016/j.compositesb.2015.03.073.
32. Mishnaevsky, L., Jr., Lavashov, E., Valiev, R.Z., Segurado, H., Sabirov, I., Enkeev, N., Prokoshkin, S., and Solov'yov, A.V., Nanostructured Titanium Based Materials for Medical Implants: Modeling and Development, *Mater. Sci. Eng. R*, 2014, vol. 81, pp. 1–19.
33. Liu, H.S. and Mishnaevsky, L., Jr., Gradient Ultrafine-Grained Titanium: Computational Study of Mechanical and Damage Behavior, *Acta Mater.*, 2014, vol. 71, pp. 220–233.
34. Liu, H.S., Pantleon, W., and Mishnaevsky, L., Jr., Non-Equilibrium Grain Boundaries in UFG Titanium: Computational Study of Sources of the Material Strengthening, *Computat. Mater. Sci.*, 2014, vol. 83, pp. 318–330.