# MULTISCALE SIMULATION OF DAMAGE AND HEALING OF COMPOSITE STRUCTURES.

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**Keywords:** Simulation, multiscale, composite, healing.

**Abstract:** It is known that reproducing material structures found in nature is an appealing strategy to develop smart and multifunctional solutions for novel composite materials [1]. The architectures of biomaterials are optimized for adaptation to the external environment and are of great interest in various engineering fields. In biologic structural materials, the arrangement of nano- to macro- components is generally organized in a hierarchical structure. Some well-known examples are spider silk, gecko toes, sea shells, bone, etc. The possibility of using bioinspired structural criteria leads to new possibilities in the field composite material design, in particular since the introduction of carbon nano-reinforcements, offering the possibility of creating truly multiscale engineering materials, which could potentially achieve tailor-made, simultaneously optimized mechanical properties, such as stiffness, strength, toughness, etc.

Organization of base biomaterials components is also linked to the self-healing capability of the structure, which is an extremely attractive feature that could be implemented in future industrial applications. To design such materials, a robust multiscale simulation approach, including both fracture and healing mechanisms, needs to be developed to aid in preparing experimental solutions.

Here, we develop a multiscale numerical model to simulate the mechanisms involved in damage progression and energy dissipation at different size scales in self-healing structures, considering all relevant parameters, including heterogeneity of the material, hierarchical structure, structural modifications, etc. All of these aspects are incorporated into a model based on a lattice model [2], which is able to simulate both damage and internal structure modifications. Nonlocality is implemented through interaction between multiple non-neighbouring nodes to simulate more realistic crack paths. The model is validated by comparing numerical results to continuum mechanics and fracture mechanics theories, and then employed to model the multiscale response, to various types of external loads.

The developed code could be a valuable support in the design and optimization of advanced composite materials, drawing inspiration and going beyond biological materials with exceptional mechanical properties.

*Excerpt from ISBN 978-3-00-053387-7*

## 1. Introduction

Mechanical properties displayed by biomaterials differs and outstand the traditional engineering materials in that they shows some optimized competing properties such as strength and toughness or stiffness and density [3, 4]. The mechanisms involved in those properties are usually linked to the biomaterials internal structures, which include some complex heterogeneous architecture, with a hierarchical arrangement of microstructural and base components [5, 6].
In order to obtain artificially created materials with similar properties, the challenge is therefore to capture the optimization criterions related to the internal structure and replicate them [7, 8]. Fibber based composite already combine lightweight and directional strengthening properties to optimize the material response to specific applications, but is still not able to obtain simultaneously the stiffness/density or strength/toughness combinations as in biocomposites. With the recent introduction of nano reinforcements such as carbon nanotubes, nano ribbons or grapheme [9, 10], new possibilities of artificial multiscale hierarchical composites have emerged and the present work could be a valuable support in the design and optimization of these advanced materials, drawing inspiration and going beyond biological materials with exceptional mechanical properties.
Therefore, we developed a numerical model to study the impact of the composite structures on global mechanical properties. Classic finite element models encounter difficulties to model crack growth, which is in the present study related to the determination of the composite toughness, and requires complex remeshing procedures. The LSM approach provides accurate solutions to the description of crack growth problems.

## 2. Numerical model

To simulate fracture propagation in heterogeneous media, the domain is discretized in a set of nodes that are connected with axial springs. Lattice Models approach is based on a discontinuous formulation which avoids singularity related issues. An example of the regular grid used to discretize a material portion is showed in figure 1. Springs properties (Elastic modulus and volume) are obtained through a homogenization procedure based on the equivalence of stored strain energy between the spring network and the continuum. The stored strain energy for the spring network is obtained as the sum of the spring's strain energy contributions in one node:

$$U = \frac{1}{2}\int_{V^*} \varepsilon_{xx}\sigma_{xx} + \varepsilon_{yy}\sigma_{yy} + \varepsilon_{zz}\sigma_{zz} + 2\sigma_{yz}\varepsilon_{yz} + 2\sigma_{xz}\varepsilon_{xz} + 2\sigma_{xy}\varepsilon_{xy}dV = \sum U_S \qquad (1)$$

$$U_S = \frac{1}{2}kl^2\left(\varepsilon_{xx}\alpha^2 + \varepsilon_{yy}\beta^2 + \varepsilon_{zz}\gamma^2 + 2\varepsilon_{yz}\beta\gamma + 2\varepsilon_{xz}\alpha\gamma + 2\varepsilon_{xy}\alpha\beta\right)^2 \qquad (2)$$

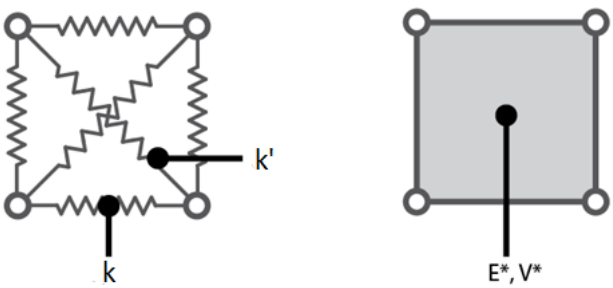


**Figure 1.** Spring discretization of elementary volume cell.

The regular lattice obtained can be local or non-local (one node is linked with his first neighbors or in a wider range). It has been showed that for fracture propagation simulations, the non-locality of the network avoid path dependency problems [11].

Excerpt from ISBN 978-3-00-053387-7

An iterative scheme is used to deal with the large rigid motion and large deformation deriving from fracture growth during simulations. The total Lagrangian formulation is employed at each simulation steps in order to obtain the equilibrium between internal and external forces.
Fracture is introduced by removing springs that exceed a maximum strain at each loading steps.
Figure 2 shows an example of the strain distributions in 2D samples around singularities, a centered crack in the first case and a rigid line inclusion in the second case.

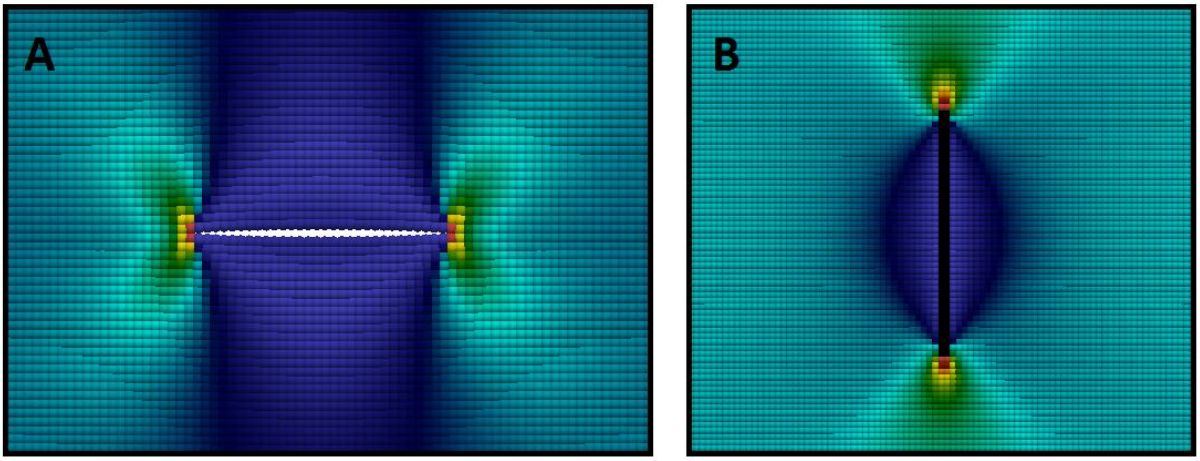


**Figure 2.** Strain fields around a cracked sample (A) and a line stiffener (B).

To simulate multiple scale levels, i.e. the hierarchical organisation of the composite, we apply a bottom up strategy. From the nano or micro scale, we derive mechanical properties and global material response to various loading cases and use them as input for the upper scale level (figure 3). If random structures are added at the bottom hierarchy level, the mechanical properties are defined in the upper level by a Weibull probability law, by the calculation of scale and shape parameters from the distribution obtained.

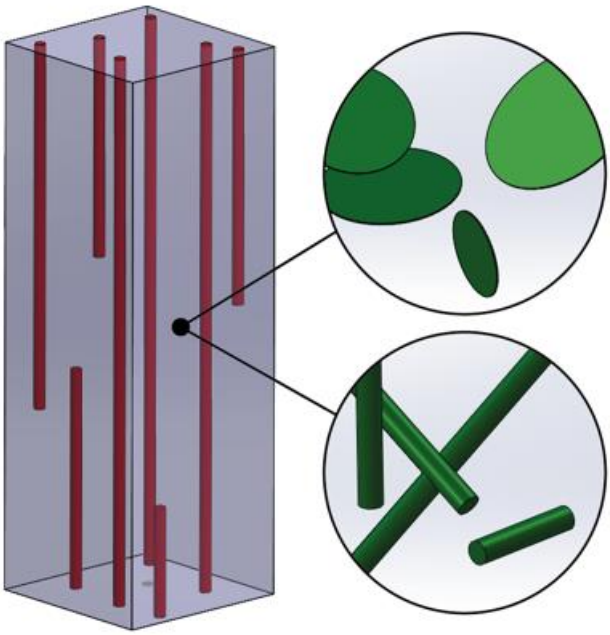

**Figure 3.** Hierarchical organisation of a multiscale composite material.

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## 3. Simulations

Deriving the material properties from the lower scale to the upper ones, the first step is to define the mechanical properties as a function of the reinforcement's shape, size and orientation (figure 4) at the lowest scale (nanotubes or grapheme embedded in the matrix). It is well known [12] that the presence of stiff inclusion gives in one hand a stiffening of the material, but in the other hand, to a stress concentration inside the material, which lead to a decreased toughness. Matrix properties also plays an important role here, such as the non-locality or the non-linear behaviour which is useful to spread the load around the most stressed domains and delay the crack nucleation.

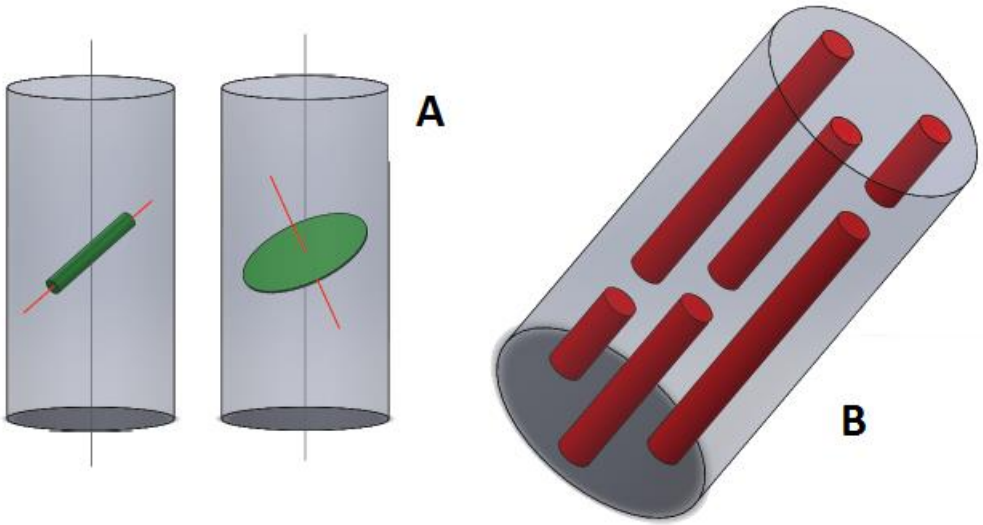


**Figure 4.** Geometry of the reinforcements inside the matrix (A), Organization of the reinforcments in the composite structure (B).

Then, at a single scale level, we derive some optimization criterion as a function of the pattern of the inclusions. Some organized structures with preferential orientation or/and overlapping of the reinforcements are likely to give different results respect to a fully random configuration. As a simple example, orientated line inclusion (such as nanotubes) will increase the stiffness of the composite in the direction of the lines, whereas the stiffness in the other directions almost remains unchanged respect to the matrix one. The challenge is then to create a structure at the upper scale level where the load transfer between the reinforcements trough the matrix take advantage of the lower scale optimized property.

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## References

[1] U. G. K. Wegst, H. Bai, E. Saiz, A. P. Tomsia and R. O. Ritchie. Bioinspired Structural Materials. Nature Materials, 4089 (2014).

[2] Ostoja-Starzewski, M. Lattice models in micromechanics. Appl. Mech. Rev. 55, 35–60.doi:10.1115/1.1432990 (2002).

[3] Gao, H.J., Ji, B.H., Jager, I.L., Arzt, E., and Fratzl, P. (2003). Materials become insensitive to flaws at nanoscale: Lessons from nature. Proceedings of the National Academy of Sciences of the United States of America 100, 5597-5600.

[4] Ritchie, R.O. (2011). The conflicts between strength and toughness. Nature Materials 10, 817-822.

[5] Zhang, Z.Q., Zhang, Y.W., and Gao, H.J. (2011). On optimal hierarchy of load-bearing biological materials. Proceedings of the Royal Society B-Biological Sciences 278, 519-525.

[6] Bosia, F., Abdalrahman, T., and Pugno, N.M. (2012). Investigating the role of hierarchy on the strength of composite materials: evidence of a crucial synergy between hierarchy and material mixing. Nanoscale 4, 1200-1207.

[7] Munch, E., Launey, M.E., Alsem, D.H., Saiz, E., Tomsia, A.P., and Ritchie, R.O. (2008). Tough, Bio-Inspired Hybrid Materials. Science 322, 1516-1520.

[8] Pugno, N.M., Bosia, F., and Abdalrahman, T. (2012). Hierarchical fiber bundle model to investigate the complex architectures of biological materials. Physical Review E 85.

[9] Coleman, J.N., Khan, U., Blau, W.J., and Gun'ko, Y.K. (2006). Small but strong: A review of the mechanical properties of carbon nanotube-polymer composites. Carbon 44, 1624-1652.

[10] Young, R.J., Kinloch, I.A., Gong, L., and Novoselov, K.S. (2012). The mechanics of graphene nanocomposites: A review. Composites Science and Technology 72, 1459-1476

[11] Hailong Chen, Enqiang Lin, Yang Jiao and Yongming Liu. (2014) A generalized 2D non-local lattice spring model for fracture simulation. Comput Mech. 54:1541–1558

[12] Bigoni, D., Dal Corso, F., and Gei, M. (2008). The stress concentration near a rigid line inclusion in a prestressed, elastic material. Part II. Implications on shear band nucleation, growth and energy release rate. Journal of the Mechanics and Physics of Solids 56, 839-857.

*Excerpt from ISBN 978-3-00-053387-7*