The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5 – 9 June 2022, Oslo, Norway

A COMPUTATIONAL FRAMEWORK FOR MODELLING GRAPHENE NANOPLATELETS

Panagiotis Gavallas[1], Dimitrios Savvas[1] and George Stefanou[1]

[1] Department of Civil Engineering, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
pgavallas@civil.auth.gr, dimitriosavvas@yahoo.gr, gstefanou@civil.auth.gr

Key Words: *Graphene Nanoplatelets, Multiscale, Homogenization, Random Fields.*

The present work aims at providing a computational framework for modelling graphene nano-platelet (GnP) reinforced composites, linking atomistic and macroscopic mechanical behaviour while taking microstructural uncertainty into account. GnPs, which consist of multiple graphene sheets connected by van der Waals forces [1], are modelled following the Molecular Structural Mechanics (MSM) approach [2] using energy equivalent beam and spring elements. Homogenization is applied to obtain the random spatially varying mechanical property fields of GnPs, which can contain various structural defects, such as Stone-Wales and single or double vacancies [3]. The homogenized mechanical properties are used in the formulation of an equivalent shell element model for the GnP reinforcements. It is shown that the proposed shell model can represent the membrane and bending behaviour of GnPs in an accurate and efficient way.

REFERENCES

[1] P. Cataldi, A. Athanassiou and I.S. Bayer, Graphene nanoplatelets-based advanced materials and recent progress in sustainable applications. *Applied Sciences*, Vol. **8**, pp. 1438, 2018.

[2] C. Li and T.W. Chou, A structural mechanics approach for the analysis of carbon nanotubes. *International Journal of Solids and Structures*, Vol. **40**, pp. 2487-2499, 2003.

[3] D. Savvas and G. Stefanou, Determination of random material properties of graphene sheets with different types of defects. *Composites Part B*, Vol. **143**, pp. 47-54, 2018.