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GENERAL MODELING OF THE BEHAVIOUR OF CARBON-NANOTUBES

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ABSTRACT

The paper presents a computational method for the simulation of carbon nanotubes, whose complexity is linear on the number of atoms. The regularity of a graphene lattice at its energy ground permits the definition of a tiling scheme that is applied to the surface of nanometric carbon pipes. The scheme employs elementary Y-shaped cells and proposes a coherent combination of a discrete approach with a continuous elastic beam reference for the numerical simulation of complex structures.

In the molecular region, the employed potential is obtained from the local harmonic approximation and leads to an explicit formulation of the acting forces, therefore permitting the dynamical prediction of large deformations as bending and torsion.

The study includes a numerical consistency check based on the conservation of the global energy of the molecular system. Comparisons are made with an abstract new material obtained by homogenization of the mechanical formulation of the material considered.

As a conclusion, future developments of the obtained homogenized material and some applications of the proposed scheme are presented.

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