Molecular dynamics simulation of three periodic auxetic entanglements

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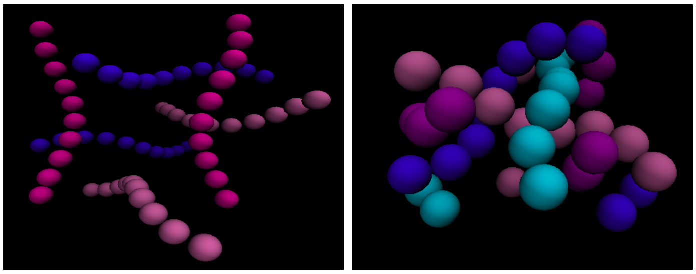
A material is said to be auxetic when its Poisson's ratio is negative, meaning that when it is stretched it becomes thicker in the directions perpendicular to the applied stress. Auxeticity occurs in a wide range of materials, both organic and inorganic, but this work only focuses on those structures in which the auxeticity is given by the arrangement of fibres within them. More in detail, the focus is on two three periodic cubic rod packings, namely Π^+ and Σ^+ [3], both with symmetry $I4_132$. They consist in an entanglement of rigid infinite and identical tubes aligned respectively along $\langle 100 \rangle$ and $\langle 111 \rangle$. The Π^+ is chiral and describes the chemical structure of $\beta - Mn$ [4] while Σ^+ describes the arrangement of keratin intermediate filaments in cells of the outer layer of the mammalian's skin, the *stratum corneum* [1]. To stretch the structures in order to explore their dynamics it is necessary to substitute the rigid rods with elastic elements [4], that means to switch from a framework to a tensegrity structure, which can be regarded as a set of beads and springs. This work focuses on the interplay between topology of the entanglement and mechanical properties explored with molecular dynamics techniques. The simulation has been carried out in LAMMPS and the initial coordinates have been retrieved from the rod packing represented in Houdini. The bonded interaction has been set according to [2] while the non bonded one, which is modeled with a WCA potential, has been chosen so that in the equilibrium configurations the chains are no longer straight but helical. The angle distribution, the Poisson's ratio, as defined in [4] and the energy are calculated with scripts in Python. Understanding how the topology influences the dynamics of the packing is essential to explore the behaviour of materials that already exist in nature and design new ones.



(a) (b)

Figure 1: Here are represented the unit cell of Π^+, in panel (a), and Σ^+, in panel (b) in VMD in the helical configuration, before the elongation of the box.

References

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