Modeling the mechanisms for formation of helices and perversions in elastic nanofilaments through molecular dynamics

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Abstract

Helices made of elastic filaments have been the target of considerable and growing interest in past years [1-3]. The formation mechanisms for such helices are still not well understood, but recent results have indicated they may be due to buckling instabilities that naturally emerge when primary interactions strength vary asymmetrically across the filament's cross-section. Several different treatments (e.g. thermal, friction or radiation), can induce such asymmetry, which means this can be easily obtained in practice [4-5]. In addition, these effects can be observed on filaments at different length scales; both micro-filaments and nano-filaments also form this sort of structure.

In this work, we present coarse-grained molecular dynamics (MD) simulations performed using the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) platform. We will also discuss in detail how perversions - regions where the helical handedness changes - occur. The simulations show it is possible to replicate the formation of helices and perversions, within certain conditions. Finally, we show how the helical radius can depend on the strength and the asymmetry of the interactions used, the filament's aspect ratio, and the recovery velocity.

The occurrence of a perversion has attracted considerable interest in a number of theoretical works, in which they are shown to occur in the stationary solutions of Kirchoff's equations [6-7]. However, the possibility of creating more than a single perversion has been given much less attention [8]. Understanding and being able to control the formation mechanisms of helices and perversions could enable many different practical applications. As next-generation nano-mechanical systems can be obtained by nano-patterning of soft materials, these simulations can provide importance input for the design of such systems.

References

[1] Gerbode S. J., Puzey J. R., McCormick A. G., Mahadevan L., Science, **337** (2012), 1087-1091.
[2] Shariatpanahi S.P., Irajizad A., Abdollahzadeh I., Shirsavar R., Bonn D., Ejtehadi R., Soft Matter, **7** (2011), 10548-10551.
[3] Godinho M.H., Canejo J.P., Feio G., Terentjev E.M., Soft Matter, **6**(2010), 5965-5970.
[4] Godinho M.H., Trindade A.C., Figueirinhas J.L., Melo L.V., Brogueira P., Deus, A.M., Teixeira P.I.C., The European Physical Journal E, **21** (2006), 319–330.
[5] Wilson D.K., Kollu T., Textile Progress, **21:3** (1991), 1-42.
[6] McMillen T., Goriely A., Journal of Nonlinear Science, **12** (2002), 241-281.
[7] Goriely A., Nizette M., Journal of Mathematical Physics, **40** (1999), 2830.
[8] Domokos G., Healey T. J., International Journal of Bifurcation and Chaos, **15** (2005), 871.

Figures

Fig.1 - Initial fiber configuration

Fig.2 - Final simulation configuration, exhibiting one perversion (D=5, L/D=100)

Fig.3 - Final simulation configuration, exhibiting several perversions (D=3 L/D=200)