

Mechanics of Chirality Transfer in Bio- and Nano-Materials

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Summary Many biomaterials and nanomaterials have hierarchy of chirality. The transfer of chirality among different structural levels is crucial for the morphologies, properties and even functions of these materials. In this paper, we theoretically and experimentally investigate the chirality transfer in polymer lamellae and paper sheets from the viewpoints of mechanics and physics. The physical mechanisms underlying these two chirality transfer phenomena are presented to elucidate why polymer lamellae and paper sheets can be twisted during the growth process and the wetting-drying process, respectively. The origins of the size effects of the twisting morphologies are also given. The results of the study is useful not only for understanding various interesting phenomena associated with chirality such as the chiral growth in biological world but also for optimal design and fabrication of novel materials and devices with enhanced properties and functions.

Introduction

Chirality, the configurational properties of an object that is not superimposable on its mirror image, is a key concept in biology, chemistry, materials science and engineering, physics and many other disciplines. According to Neumann's principle, the absences of mirror symmetry of molecules, arrangements of atoms and protein lattices, microstructures and even morphologies of biological and synthetic materials can have remarkable effects on their geometrical morphologies, physical and chemical properties. This is especially true for those biological and nanostructured materials with a hierarchy of chirality such as the twisting nanobelts of chiral polymer lamellae [1-3], twisted paper sheets [4], nanohelices of chiral carbon nanotube and so on.

Structural hierarchy of chirality is widely observable in a diversity of biomaterials, nanomaterials and self-assembly systems. For these materials and systems, different chiralities often exist on several structural levels, and a chirality on a lower level begets another one on a higher level. Thus, chirality is always transferred from the lower structural level to the higher level during the growth, fabrication process and self-assembly, i.e., chirality transfer, which often induces chiral morphologies and some unusual properties. In other words, chiral morphologies of materials and systems with hierarchy of chirality are often macroscopic reflections of chemical chirality (e.g., molecular and conformational chirality), microstructural chirality (e.g., helical monodomains) and material chirality at lower levels [5]. During the growth of chiral polymer lamellae, for example, chirality are transferred from the molecular level to helical chain structures, then to chain folding organization on the lamellar surface, and eventually to the macroscopic level (twisting lamellae and even clustering of crystals and polymer spherulites), as shown in Figure 1.

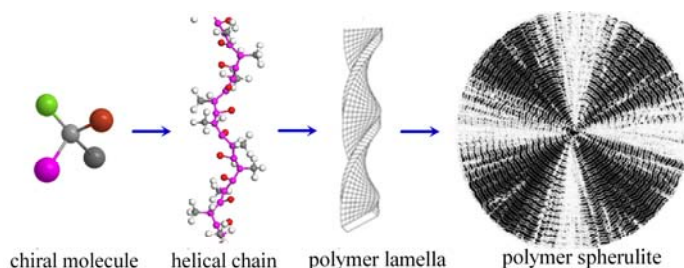


Figure 1. Hierarchical chiral structures in polymer lamella and chirality transfer

Chirality transfer is often a complicated process. The macroscopic morphology chirality and/or material chirality depend not only on the chirality of the basic constituent elements at lower structures levels but also on the interactions between chiral elements and other factors such as intermolecular forces, surface stresses and residual stresses. Furthermore, chirality transfer from the molecular or atomic level to macroscopic level involves complicated multiscale interactions of different chiralities at various structural levels. Thus, the macroscopic chirality of a material or system is closely but not unequivocally correlated with the lower level chiralities. In addition, it is worth mentioning that "chirality" itself is a multidisciplinary concept and has somewhat different definitions in different fields. Therefore, it is of great interest to study the underlying physical mechanisms of chirality transfer and the correlation between macroscopic morphologies chirality or materials chirality and the lower-level chirality.

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In this paper, we theoretically and experimentally investigated the multiscale chirality transfers in polymer lamellae and paper sheets, which are typical examples of nanomaterials and biomaterials, respectively.

Chirality Transfer in Nanomaterials: Polymer Lamellar Twisting

Using the coarse treatments, a continuum mechanics model is developed to phenomenologically rationalize the chirality transfer from the constituent molecules to geometric morphology of polymer lamellar twisting. We demonstrate that the competition or cooperative interactions between lower-level chirality and surface effects may lead to the formation of various asymmetric geometric shapes. The twisting handedness and pitch length of chiral morphologies of polymer lamella is derived in terms of materials chirality and anisotropic surface stresses. The inversion of morphology chirality and some size dependent phenomena can be interpreted by considering the interaction of the two mechanisms. We also provide a possible explanation for the observed conflicting experimental results on the correlation between lower-level chirality and morphology chirality.

Chirality Transfer in Biomaterials: Paper Sheet Twisting

Paper made of plant fibers has elegant hierarchy of chirality, as shown in Figure 2. Experiments have been done to investigate the effect of water content and paper sheet width on the twisting deformation of paper sheets during their wetting and drying processes. Based on the experimental results and the microstructure at different length levels of paper sheet, the physical mechanism of paper sheet twisting is revealed from the viewpoint of multiscale chirality transfer. Paper sheet twisting is mainly induced by the change of helical angle of cellulose chain twining in the cell wall during wetting and drying processes. The chiral morphology parameters of paper sheets are dependent on the water content, the paper sheets width and the cut direction. Furthermore, the twisting pitch also exhibits distinct size dependence due to the frustration effect.

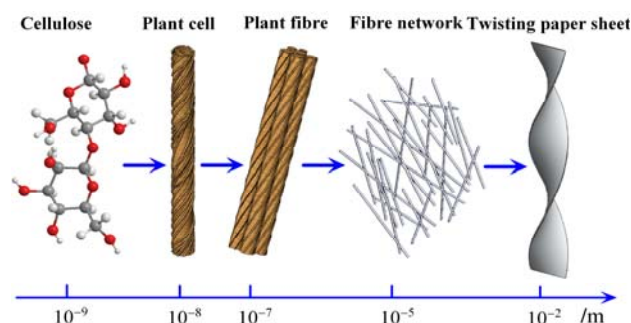


Figure 2. Hierarchical chiral structures in paper sheet and chirality transfer

CONCLUSIONS

In this paper, we have investigated two typical chirality transfer phenomena in biomaterials and nanomaterials. The physical mechanisms underlying these two chirality transfer have been proposed to correlate the morphology chirality and the lower levels chirality. Interestingly, the morphologies of both the polymer lamella and the paper sheet exhibit a distinct size effect. However, the former is mainly induced by surface effects, the non-local effect of the chiral microstructures and the frustration effect, and the latter is only derived from the frustration effect. This work is not only helpful for the control of the chiral morphologies and properties of nanomaterials during their self-assembly processes and three-dimensional fabrication but also shed light on the mechanisms of widely existing chiral growth in biological world.

Acknowledgements

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References

- [1] Wang J.S., Feng X.Q., Wang G.F., Yu S.W.: Twisting of Nanowires Induced by Anisotropic Surface Stresses. *Appl. Phys. Lett.* **92**: 191901-3, 2008.
- [2] Ye H.M., Wang J.S., Tang S., Xu J., Feng X.Q., *et al.*, Surface Stress Effects on the Bending Direction and Twisting Chirality of Lamellar Crystals of Chiral Polymer. *Macromolecules* **42**: 5762-5770, 2010.
- [3] Wang J.S., Feng X.Q., Xu J., Qin Q.H., Yu S.W.: Chirality Transfer from Molecular to Morphological Scales in Quasi-One-Dimensional Nanomaterials: A Continuum Model. *J. Comput. Theor. Nanosci.* **8**:1278-1287, 2011.
- [4] Dionne I., Werbowyj R.S., Gray D.G., Chiral Twisting Curl in Newsprint Sheets. *J. Pulp. Pap. Sci.* **15**: J123-J126, 1991.
- [5] Wang J.S., Ye, H.M., Qin Q.H., Xu J., Feng X.Q., Anisotropic Surface Effects on the Formation of Chiral Morphologies of Nanomaterials. *Proc. R. Soc. A*, *in press*, 2012. (doi:10.1098/rspa.2011.0451).