Structural transformation of cholesteric blue phases revealed by continuum simulation and machine-learning-aided structural analysis

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Cholesteric blue phases of a chiral liquid crystal [1] have been known as intriguing examples of exotic three-dimensional ordered structures exhibited by soft materials. They comprise a regular array of disclination lines (line defects of orientational order) and double-twist cylinders in which the orientational order is twisted along all the directions perpendicular to the cylinder axis. Two blue phases, BP I and BP II, show cubic order, and BP I has the space group $I4_132$, the same as that of a single gyroid (The space group of BPII is $P4_232$). The transition between BP I and BP II is an interesting example of transformation between ordered structures.

When a perfect lattice of BP II is cooled, it exhibits first-order phase transition to BP I. Recent experiments [2] revealed the formation of twinned structures that resembles those observed in martensitic transformation. However, the real-space dynamics of the transformation is still unclear. Here we carry out a simulation based on a Langevin-type equation for the dynamics of orientational order parameter, a second-rank tensor. The complex ordering of BP I and BP II makes the identification of local structures a non-trivial task. We overcome this difficulty by supervised machine learning that successfully distinguishes BP I and BP II.

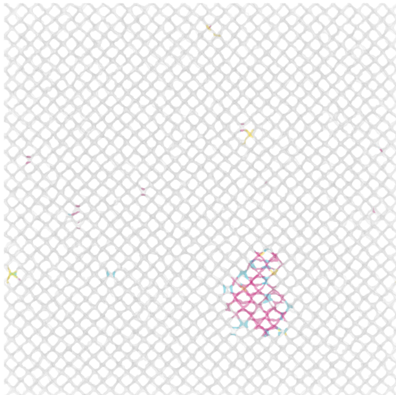

Figure 1 A snapshot of simulation exhibiting the formation of a BP I nucleus (magenta) Gray lines are disclinations forming BP II.

Figure 1 shows a snapshot of simulation with a BP I nucleus. We emphasize the difficulty of identifying the BP I region by the structure of the disclination network alone. Further growth of the nucleus is shown to lead to the formation of well-defined twin boundaries between BP I regions with different lattice orientation. We also find that by raising the temperature the twinned BP I structure almost reversibly recovers the perfect BP II ordering. Our simulation study with machine-learning-aided structure analysis successfully clarifies the transformation dynamics of blue phases involving twin boundaries, and will be applicable to other problems on complex structural transformation between ordered phases exhibited by a wide variety of soft materials.

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