Multiferroic hexagonal manganite YMnO$_3$ (YMO) has attracted extensive attention owing to its vortex-like domain patterns with ferroelectric, magnetic, and structural correlations and the resulting attractive physical properties. The complicated domain pattern of YMO has long been discovered. However, little is known about the real structure and origin of this domain pattern. Recent studies have shown that on the micro-scale, the typical domain pattern in YMO has a cloverleaf shape, and six interlocked ferroelectric and structural antiphase domain walls merge into a vortex core. However, the configuration of the domain pattern is still controversial. To gain insight into this problem, researches on nanoscale, particularly on the atomic-scale are necessary.

Using Cs-corrected transmission electron microscopy, we demonstrate the atomic details of a topological vortex-like domain pattern in multiferroic hexagonal manganite YMnO$_3$. We have demonstrated an example of the topological vortex-like domain pattern of YMO on the atomic-scale. The vortex-like pattern with domain configuration of $\alpha^+$, $\beta^-$, $\alpha^+$, $\beta^-$, $\alpha^+$, $\beta^-$ is revealed. We point out that distinguishing of six ferroelectric domains in the vortex-like pattern is not the sufficient condition to determine whether this pattern is a real vortex or not (Fig.1). The antiphase relationship must be carefully checked. Besides, the existence of domain walls (DWs) in two-dimensional projection is also a crucial point to be considered when discussing the vortex-like domain pattern. Our atomic detailed observations push forward the understanding of the intriguing vortex-like patterns in hexagonal manganites. Moreover, configurations of two kinds of interlocked DWs are revealed with the help of atomistic simulation (Fig.2). The antiphase domain boundary I (APB$_I$) and ferroelectric domain boundary (FEB) are overlapped while the antiphase domain boundary II (APB$_II$) and the FEB are separate on the atomic-scale, and surface hexagon of the hexagonal unit cell in the vicinity of the DW boundary suffers from slightly distortion. As more and more theoretical work are begin to focus on the interlocked DWs recently, such extensive investigations of the DWs can provide a reference for future theoretical studies. Finally, we should emphasize that all these fascinating results can be useful not only for this specific material but also as a guideline to envision domain behavior of other hexagonal multiferroics. The present study can throw further light on understanding of structure-property relation in multiferroic hexagonal manganites.


Acknowledgement: This work is supported by the National Science Foundation of China and the Ministry of Science and Technology of China.
Fig. 1: (a) Hexagonal crystal unit cell of YMO (red: Y, green: Mn, blue: O). (b) Atomic projection of YMO in the [110] zone axis. (c) HRTEM image of a multi-domain region. Areas with different polarization directions are indicated by arrows and different types of DWs are indicated by different color dot lines.

Fig. 2: (a), (b) The atomic displacements of Y ions near the APB$_1$ + FEB [region I in Fig. 1c] and APB$_2$ + FEB [region II in Fig. 1c], respectively. (c), (d) The [110] atomic structural model of APB$_1$ + FEB and APB$_2$ + FEB, respectively. (e), (f) Upper panels are the close-ups of the immediate vicinity of the DW boundary in (a) and (b), respectively.