Skyrmionic state in ferroelectric nanocomposites

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The topological invariance of nontrivial textures such as vortices and skyrmionic configurations against fluctuations and deformations triggers considerable interest for device applications [1–3]. Many advances have been achieved in predicting their formation and characterizing the new order they subtend in *magnetic* systems [4–6]. Whereas vortex configurations have already been revealed in ferroelectrics within nanoscale geometries [7–11], the search for a spontaneous formation of skyrmionic textures in *ferroelectrics* was somewhat hindered by the absence of chiral interactions that are known to stabilize such configurations in magnetic systems [12–14]. We here show that the anisotropy emanating from such interactions can be compensated for by that of confined geometries which can readily become the locus of thermodynamically stable skyrmionic configuration of polarization.

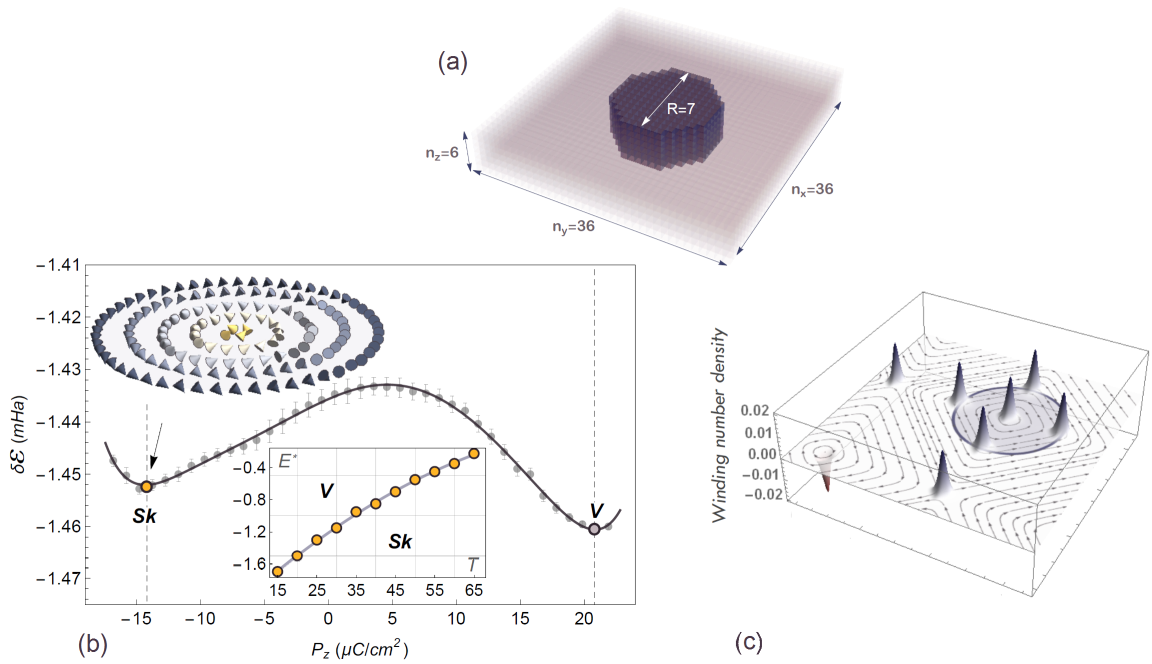

FIG. 1: (a) Schematic representation of the periodic supercell under study. The structure consists of a cylindrical $BaTiO_3$ nanowire embedded in a $Ba_{0.15}Sr_{0.85}TiO_3$ matrix. (b) Dependence of the internal energy on the P_z component of polarization showing the crossover between two stable minima: the one corresponding to the vortex configuration (V) and the one associated with the skyrmionic texture (Sk). Bottom inset provides the temperature dependence of the estimated threshold external electric field E^* needed to drive the system towards the skyrmion state. Pictorial inset depicts the polarization configuration within the skyrmionic state as obtained at 15 K. (c) Density of the winding number in an arbitrary z-plane of the shifted perdiodic supercell, showing the breaking of the skyrmion into fractions located at the junctions of domain walls. The location of the nanowire is indicated by a circle.

The considered structure is schematized in Fig.1(a). It consists of a cylindrical $BaTiO_3$ nanowire with a radius of 2.7 nm (7 lattice constant units) embedded in a $Ba_{0.15}Sr_{0.85}TiO_3$ matrix. We study this structure under periodic boundary conditions using Monte Carlo simulations of the first-principle-based effective Hamiltonian scheme of [11, 15], which has been shown to accurately reproduce various properties of (Ba,Sr)TiO_3 systems [15].

The procedure for getting a skyrmionic configuration involves the following steps. Firstly, we perform a temperature annealing under an electric field $E_{[001]}=10^8$ V/m. Secondly, we set the field to zero and further relax the priorly obtained 15 K configuration into a local minimum. The resulting configuration has been formerly observed [11]. It features a spontaneous polarization along the z direction coexisting with a flux-closure four-domain pattern formed by the components of polarization lying in the plane perpendicular to the wire axis. Within the wire, the in-plane components form a vortex occurring in order to reduce the depolarizing field stemming from the difference in polarizability between the wire and the matrix, while the matrix exhibits an additional vortex at mid-way between second-nearest neighbor wires and two anti-vortices at mid-way between first-nearest neighbor wires of the periodic supercell. These in-plane punctual topological defects all occur at the intersection of P_x and P_y domains and yield a zero net topological charge for the P_x and P_y component of polarization. Thirdly, we subject the obtained relaxed configuration under zero-field to a gradually increasing $E_{[00\bar{1}]}$ electric field. At a certain threshold value E^* of the field, the configuration is such that the P_z component of the matrix is anti-parallel to that of the wire, yielding a Bloch-like [16] skyrmionic configuration of polarization (pictorial inset of Fig.1(b)). Collecting the internal energies during this partial switching process enables us to access the internal-energy landscape as a function of P_z at 15 K (Fig.1(b)). The profile indicates the (meta)stability of the skyrmion state and reveals that the barrier's height is equivalent to approximately 6 K. Bottom inset of Fig.1(b) provides the temperature dependence of the estimated threshold external electric field E^* needed to drive the system towards the skyrmion state. Figure 1(c) provides the winding number density $\vec{P}_{ijk}.(\partial_x\vec{P}_{ijk}\times\partial_y\vec{P}_{ijk})$ where $\{ijk\}$ runs over the nodes of the lattice. The integration of the density over the supercell yields a winding number of 1 and it is thus seen that the skyrmion is broken into fractions located at the junctions of (P_x and P_y), (P_z and P_x) and (P_z and P_y) domain walls, as a genuine consequence of the considered nanocomposite structure.

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