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Electrical Control of Chiral Phases in Electrorotoroidic Nanocomposites

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System and Method

The 36x36x36 supercell (38,880 atom) of the BaTiO$_3$-SrTiO$_3$ nanocomposite$^{[5]}$ used in our simulations is schematized below. Each BaTiO$_3$ wire has (x, y, z)-plane cross-section (plane of [100] and [010]) of 4.8x4.8 nm$^2$ (12x12=144 sites) and adjacent wires are separated by 2.4 nm (6 sites) of SrTiO$_3$ medium with periodicity of 2.4 nm (6 sites) along x-axis or y-axis. 

- Order parameters of polarization ($P_z$) and toroidal moment ($G_z$) paralled to the nanowire axis
- Exhibits complex phenomena such as translational invariance and a vortex core transition
- Ferroelectricity and chirality vanish above Curie temperature $T_{C_2}$ = 240 K, vortices and $G_z$ vanish above electrostrictoronic transition temperature $T_{C_2}$ = 300 K
- $H_{app}$ for (Ba,Sr)TiO$_3$ alloys from $[7]$ used in MC to build electric-field phase diagram to see where $T_C ≃ T_{C_2}$; total energy consists of internal energy of hypothetical simple (A/B)O$_3$ system in virtual crystal approximation (VCA) and energy associated with alloy effects beyond VCA
- MC simulations heat from ground state at 5 K to 565 K while applying constant DC field along [001] for magnitudes from 0 to 1 × 10$^6$ V/m at each temperature; 10$^5$ sweeps to equilibrate, 10$^5$ sweeps for averages
- For some temperatures and DC electric fields, final MC configuration is used as input for MD simulations to calculate gyrotropy coefficient $g_{11}$

Phase Diagram (Monte Carlo)

Polarization $P_z$ is enhanced and toroidal moment $G_z$ is decreased when increasing applied DC field$^{[3]}$. Out-of-plane susceptiblity is used to identify $T_{C_2}$ for $P_z$ and $T_{C_2}$ for $G_z$.

Phase A: ferroelectric and $T < T_{C_2}$, this phase is chiral and encompasses the chiral phases at zero field

Phase B: ferroelectric and $T > T_{C_2}$, reducing to paraelectric but electrostrictoronic at zero field

Phase C: parastrictoronic and $T < T_{C_2}$, a new phase corresponding to no phases at zero field

Phase D: parastrictoronic and $T > T_{C_2}$, reducing to paraelectric and paratoroidic phase at zero field

PHENOMENOLOGY

Consider a Landau phenomenological model for this system under DC electric field $E = E_z$, and a biquadratic coupling$^{[5]}$ of constant strength $\lambda$ between polarization $P_z$ and toroidal moment $G_z$ = $G_{11}$. The free energy density is given by:

$$F = F_0(G, P, P_z) + A P_z^2 + \frac{1}{2} \lambda P_z^2$$

where $F_0(G, P, P_z)$ = $\alpha P_z^3 + \beta \lambda P_{13}^3 + \gamma G_{11}^2 + \delta G_{11}^4 + \cdots$

- Applying DC field favors $P_z$ via $-E_z$ term of Eq. (2), thus increasing $P_z$ (phase diagram) and increasing $P_z$ for any temperature below $T_{C_2}$
- Field-induced increase of $P$ strengthens repulsion between $P$ and $G$ as $\lambda$ in the coupling energy term is positive; then increasing DC electric field reduces $G_{11}$ (phase diagram) and decreases $G_z$ for any temperature below $T_{C_2}$

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