

A dynamical magnetic field accompanying the motion of ferroelectric domain walls: Supplementary Material

Dominik M. Juraschek,^{1,*} Quintin N. Meier,¹ Morgan Trassin,¹
Susane E. Trolrier-McKinstry,² Christian Degen,³ and Nicola A. Spaldin¹

¹*Department of Materials, ETH Zurich, Zürich, Switzerland*

²*Materials Research Institute, The Pennsylvania State University, University Park, PA, USA*

³*Department of Physics, ETH Zurich, Zürich, Switzerland*

Time evolution of Néel- and Bloch-type ferroelectric domain walls. In the following we review the derivation of the domain wall motion based on Refs. [17, 18], rewriting it in the notation used in this work. The Lagrangian for a ferroelectric domain wall separating domains of different orientation of polarization lying in the xy plane can be written as

$$\begin{aligned} \mathcal{L} = & \frac{1}{2}\mathcal{M}_x(\partial_t U_x)^2 - \frac{1}{2}S_x(\partial_r U_x)^2 - \frac{1}{2}A_x U_x^2 - \frac{1}{4}B_x U_x^4 \\ & + \frac{1}{2}\mathcal{M}_y(\partial_t U_y)^2 - \frac{1}{2}S_y(\partial_r U_y)^2 - \frac{1}{2}A_y U_y^2 - \frac{1}{4}B_y U_y^4 \\ & - C_{xy}U_x^2 U_y^2, \end{aligned} \quad (\text{S1})$$

where $U_{x/y}$ is the amplitude of the ferroelectric displacement along direction x/y , $\mathcal{M}_{x/y}$ is the effective mass of the ferroelectric distortion mode, $S_{x/y}$ are the gradient energies and $A_{x/y}$, $B_{x/y}$ and C_{xy} are the coefficients of the harmonic, quartic anharmonic, and coupling terms. The coordinate r denotes the position perpendicular to the domain wall in the xy plane of polarization. For a Bloch-type domain wall, we would require components perpendicular to the plane of polarization, $z \perp x, y$; for a Néel-type domain wall, we can express the change of ferroelectric displacement as simple rotation in the xy plane:

$$\mathbf{U} = \begin{pmatrix} U_x(t) \\ U_y(t) \end{pmatrix} = U_0 \begin{pmatrix} \cos(\phi(r, t)) \\ \sin(\phi(r, t)) \end{pmatrix}, \quad (\text{S2})$$

where U_0 is the amplitude of the bulk ferroelectric displacement. ($\mathbf{U} = U_0 \mathbf{Q}$ in Eq. (5) in the main text with $n = 1$.) Inserting this into the Lagrangian (S1), together with $\mathcal{M}_x = \mathcal{M}_y = \mathcal{M}$, $S_x = S_y \equiv S$, $A_x = A_y \equiv A$, $B_x = B_y \equiv B$, $C_x = C_y \equiv C$ we obtain

$$\mathcal{L} = \frac{1}{2}\mathcal{M}U_0^2(\partial_t \phi)^2 - \frac{1}{2}S U_0^2(\partial_r \phi)^2 - \frac{1}{2}A U_0^2 - \frac{1}{4}B U_0^4 - C U_0^4 \frac{1}{8}(1 - \cos(4\phi)). \quad (\text{S3})$$

The Euler-Lagrange equations for the Lagrangian (S3) yield after some rearrangements

$$\partial_t^2 \phi - c_0^2 \partial_r \phi + \kappa^2 \sin(4\phi) = 0, \quad (\text{S4})$$

where $\kappa^2 = C U_0^2 / (2\mathcal{M})$ and $c_0 = \sqrt{S/\mathcal{M}}$ is the characteristic velocity. A substitution $4\phi \rightarrow \theta$ and a transformation to a moving frame $r \rightarrow \xi = r - vt$, where v is the constant domain wall velocity yields

$$\partial_\xi^2 \theta - \alpha^2 \sin(\theta) = 0, \quad (\text{S5})$$

where $\alpha^2 = \kappa^2 / (c_0^2(1 - v^2/c_0^2))$. The solution to this equation is known for a 360° rotation of θ (corresponding to a 90° rotation of ϕ), see for example Ref. [18]:

$$\theta(\xi) = 4 \arctan(e^{\xi\alpha}) \quad (\text{S6})$$

$$\Rightarrow \phi(r, t) = \frac{1}{4}\theta(\xi(r, t)) = \arctan \left(\exp \left(\frac{1}{w} \frac{r - vt}{\sqrt{1 - \frac{v^2}{c_0^2}}} \right) \right), \quad (\text{S7})$$

where $w = c_0^2/\kappa^2 = S/(2C U_0^2)$ and $2w$ is the width of the domain wall. Eq. (S7) is the expression (4) given in the main text. $n\phi$ with $n = 1, 2, 4$ then corresponds to 90° , 180° , and 360° rotations of the ferroelectric polarization.

Stray field estimate. The vertical magnetic stray field B_z^s appearing at height h above a thin ($2w/\beta \ll h$), extended domain wall located (see Fig. 3a) is given by

$$B_z^s(r) = \frac{\mu_0 M_{2d} h}{2\pi(r^2 + h^2)}, \quad (\text{S8})$$

where r is the relative position of the domain wall with respect to the sensor, M_{2d} is the two-dimensional moment density of the domain wall, and where the material is assumed to be thick ($d \gg 2w/\beta, h$). The magnetic moment density is given by

$$M_{2d} = \frac{1}{V} \int_{-\infty}^{\infty} dr m_z(r) = \frac{1}{V} \int_{-\infty}^{\infty} dt v \gamma n \dot{\phi}(t) = \frac{\gamma}{V} v n \pi. \quad (\text{S9})$$

To detect the magnetic stray field, we repeatedly move the domain wall back and forth to create an oscillatory field $B_z^s(t)$ at the location of the NV spin sensor. When tuned to the spin resonance frequency f_0 , the oscillatory field induces a Rabi rotation of the spin providing an experimentally detectable signal. The Rabi field B_1 is given by the Fourier component of $B_z^s(t)$ at frequency f_0 ,

$$B_1 = \frac{4}{T} \int_{-T/4}^{T/4} dt \cos(2\pi t/T) B_z^s(t), \quad (\text{S10})$$

where $T = 1/f_0$ is the Larmor period of the spin. Because the Larmor period ($\sim 0.1 - 1$ ns) is typically much longer than the time taken for the domain wall to pass (~ 1 ps), $B_z^s(t)$ is non-zero only for a very short period of time around $t = 0$, and the integral can be approximated by

$$\begin{aligned} B_1 &\approx \frac{4}{T} \int_{-\infty}^{\infty} dt B_z^s(t) = \frac{4}{T} \frac{\mu_0 m h}{2\pi} \int_{-\infty}^{\infty} \frac{dt}{v^2 t^2 + h^2} \\ &= \frac{\gamma}{V} n 2\pi \mu_0 f_0, \end{aligned} \quad (\text{S11})$$

which is the expression used in the main text. Note that the expected signal is independent of domain wall width w , speed v and sensor height h as long as the geometric assumptions about the setup (a thick sample and thin moving domain wall) are satisfied and $vT \gg h$.

TABLE S1. Calculated diagonal Born effective charges $Z_{i,aa}^*$ in units of the elementary charge (a denoting spatial coordinates x , y , and z), and ferroelectric displacements $u_{i,x}$ in picometers for polarization along the x direction.

Atom	$Z_{i,xx}^*$	$Z_{i,yy}^*$	$Z_{i,zz}^*$	$u_{i,x}$
Ba	2.8	2.7	2.7	4.2
Ti	6.6	7.6	7.6	8.9
O(1)	-5.3	-2.1	-2.1	-3.4
O(2)	-2.0	-6.0	-2.1	-0.8
O(3)	-2.0	-2.1	-6.0	-0.8