Textures of the polarisation field in ferroelectric nanowires from first principles

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Acknowledgments

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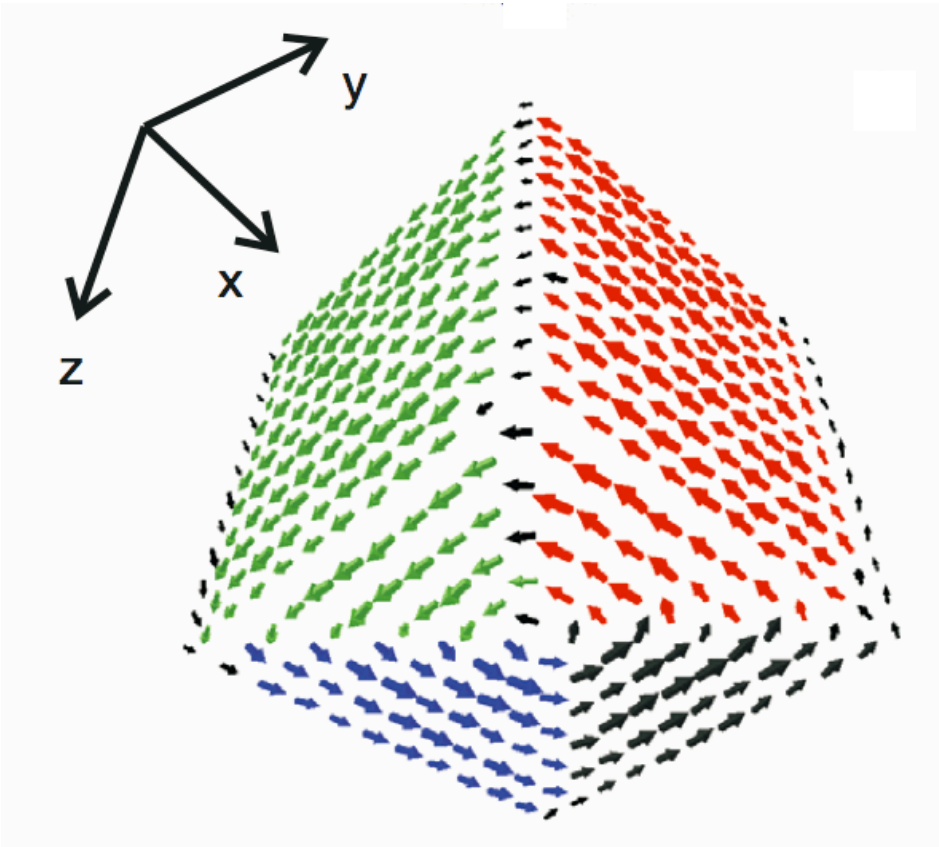
Jim Scott *(U Cambridge)*

Ferroelectric nanostructures
Non-trivial topologies (vortices) proposed



Polarisation field **P**(**r**) *found to be non-homogeneous in disks and rods of PZT (as simulated by local-mode model fitted from DFT)*

S Prosandeev et al, J. Phys.: Condens. Matter **20** (2008) 193201 (Review)

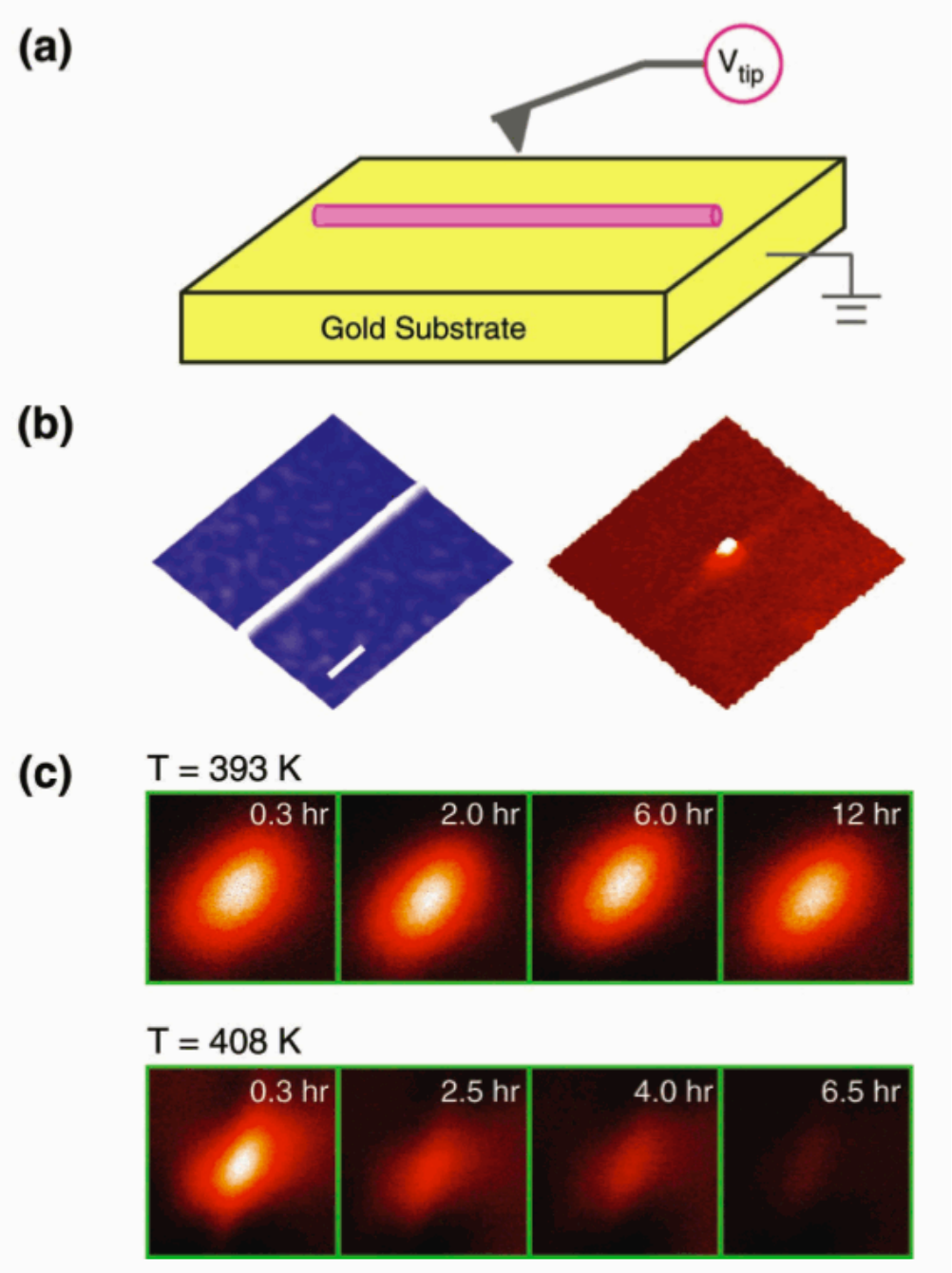
I Naumov, L Bellaiche & H Fu, Nature **432**, 737 (2004) , etc.

Ferroelectric nanowires Experiments

Polarisation in BTO wires of 3nm diameter

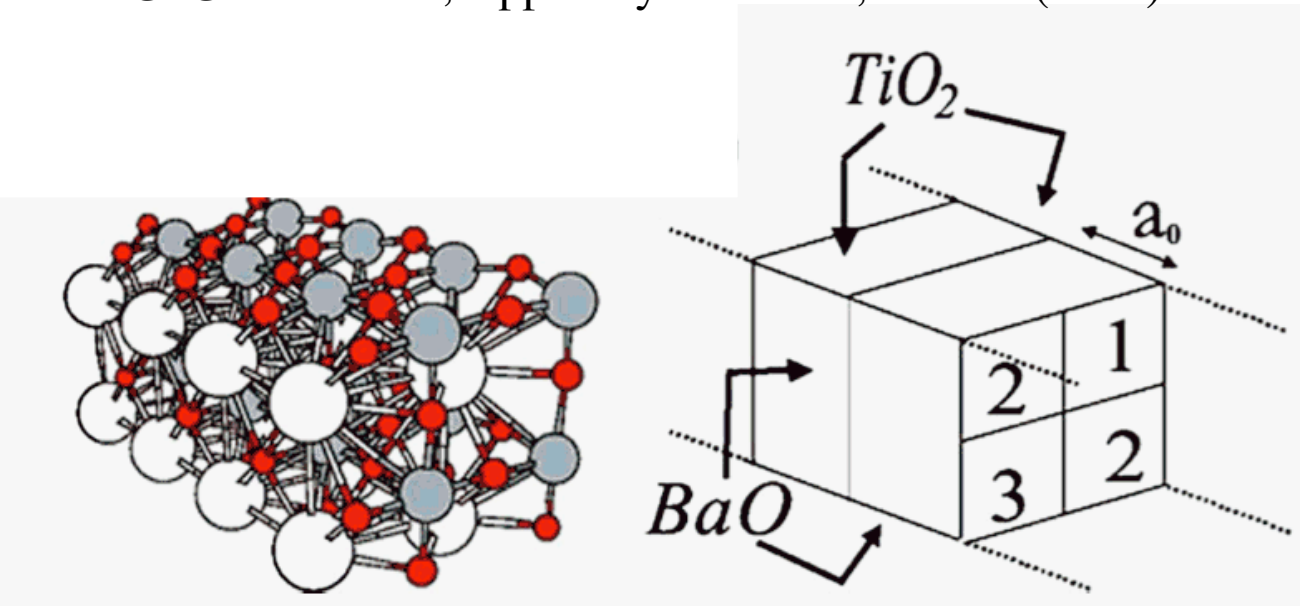
J E Spanier et al,

Nano Lett. **6**, 735 (2006)



First-principles (DFT) simulations of thin wires

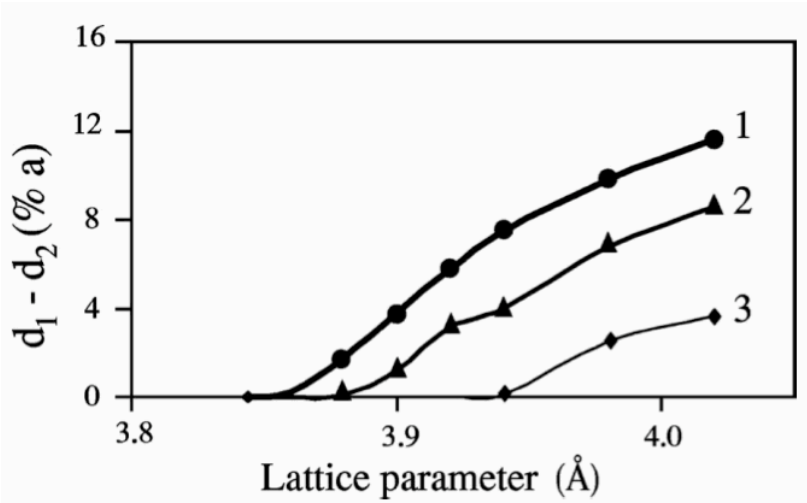
G. Geneste *et al*, Appl. Phys. Lett. **88**, 112906 (2006)



Polarisation field **P**(**r**) *along z*

Stoichiometric wires

Critical thickness (3x3)



The SIESTA method

Linear-scaling DFT based on Numerical Atomic Orbitals

P Ordejon, E Artacho & JM Soler , Phys. Rev. B 53, R10441 (1996)

- *Born-Oppenheimer* *(relaxations, mol. dynamics)*
- *DFT* *(LDA, GGA)*
- *Pseudopotentials* *(norm conserving, factorised)*
- *Numerical atomic orbitals as basis* *(finite range)*
- *Numerical evaluation of matrix elements* *(3D grid)*

*Implemented in the S**IESTA** program*

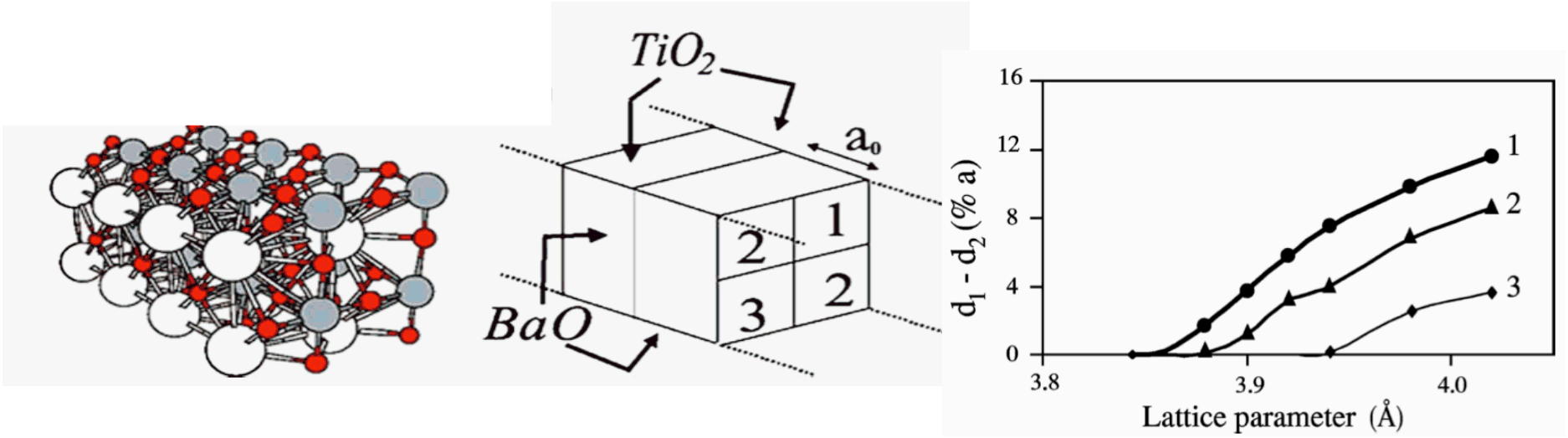
JM Soler, E Artacho, JD Gale, A Garcia, J Junquera, P Ordejon & D Sanchez-Portal,
J. Phys.: Condens. Matter **14**, 2745 (2002)

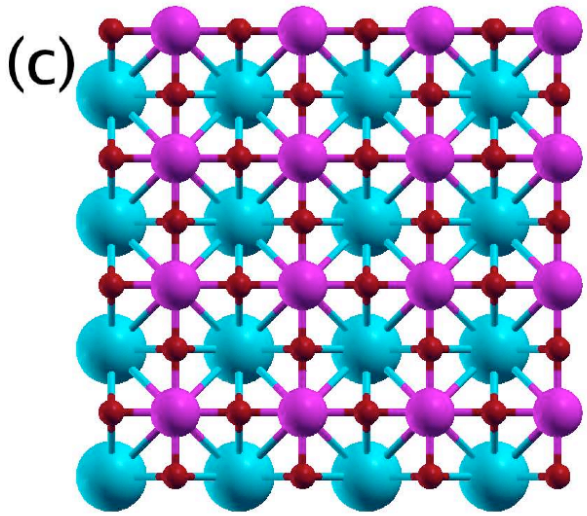
In this work: Structure relaxations from varied starting points

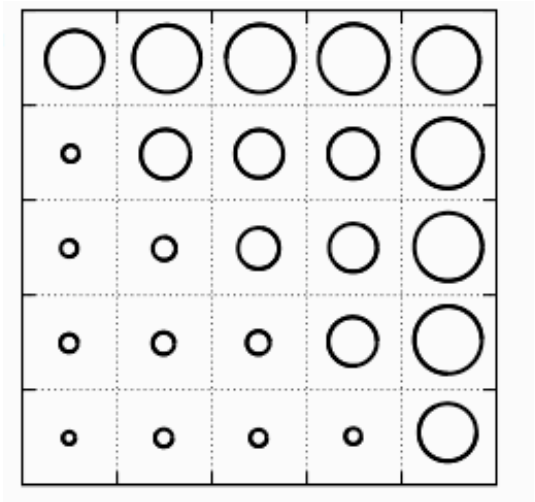
Ti off-centring used as proxy for Polarisation

Reproduced results of Geneste et al

G. Geneste *et al*, Appl. Phys. Lett. **88**, 112906 (2006)





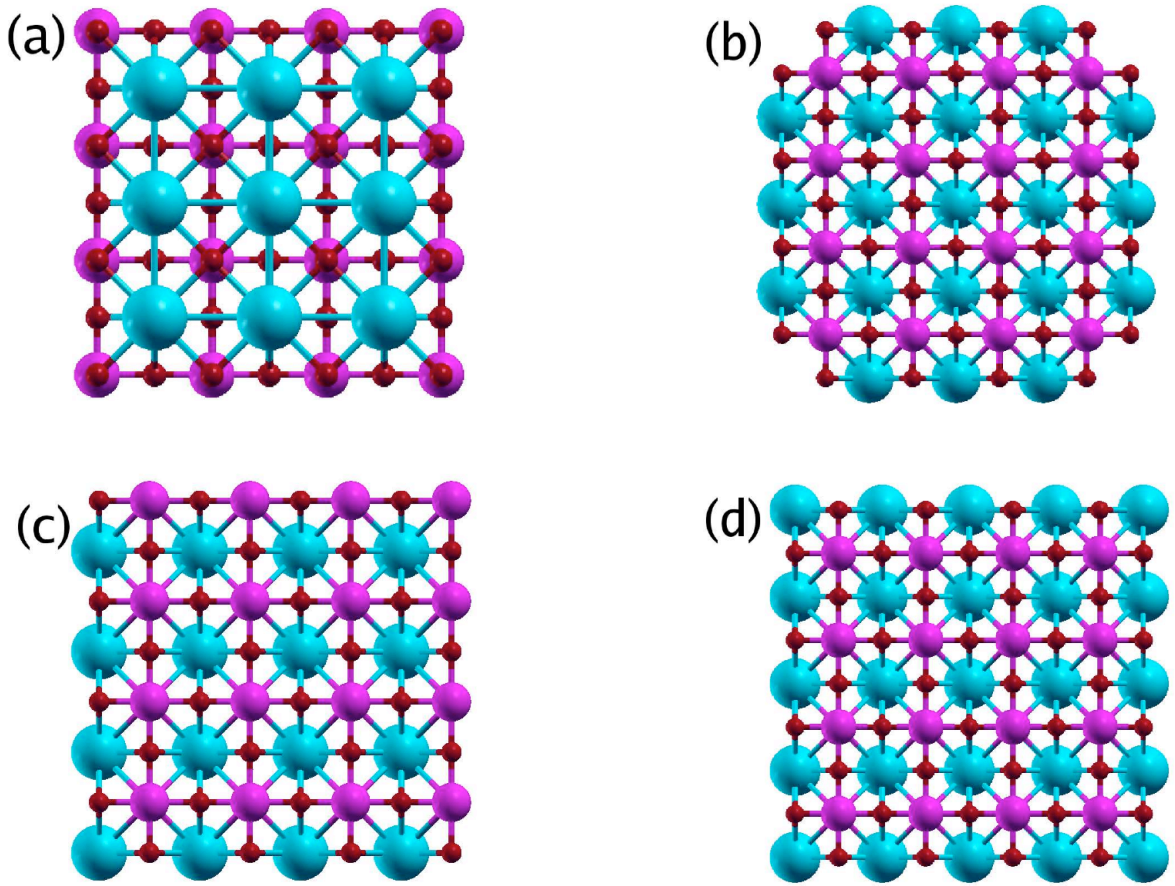


Largest circle for 15 pm

(bulk BTO 13 pm)

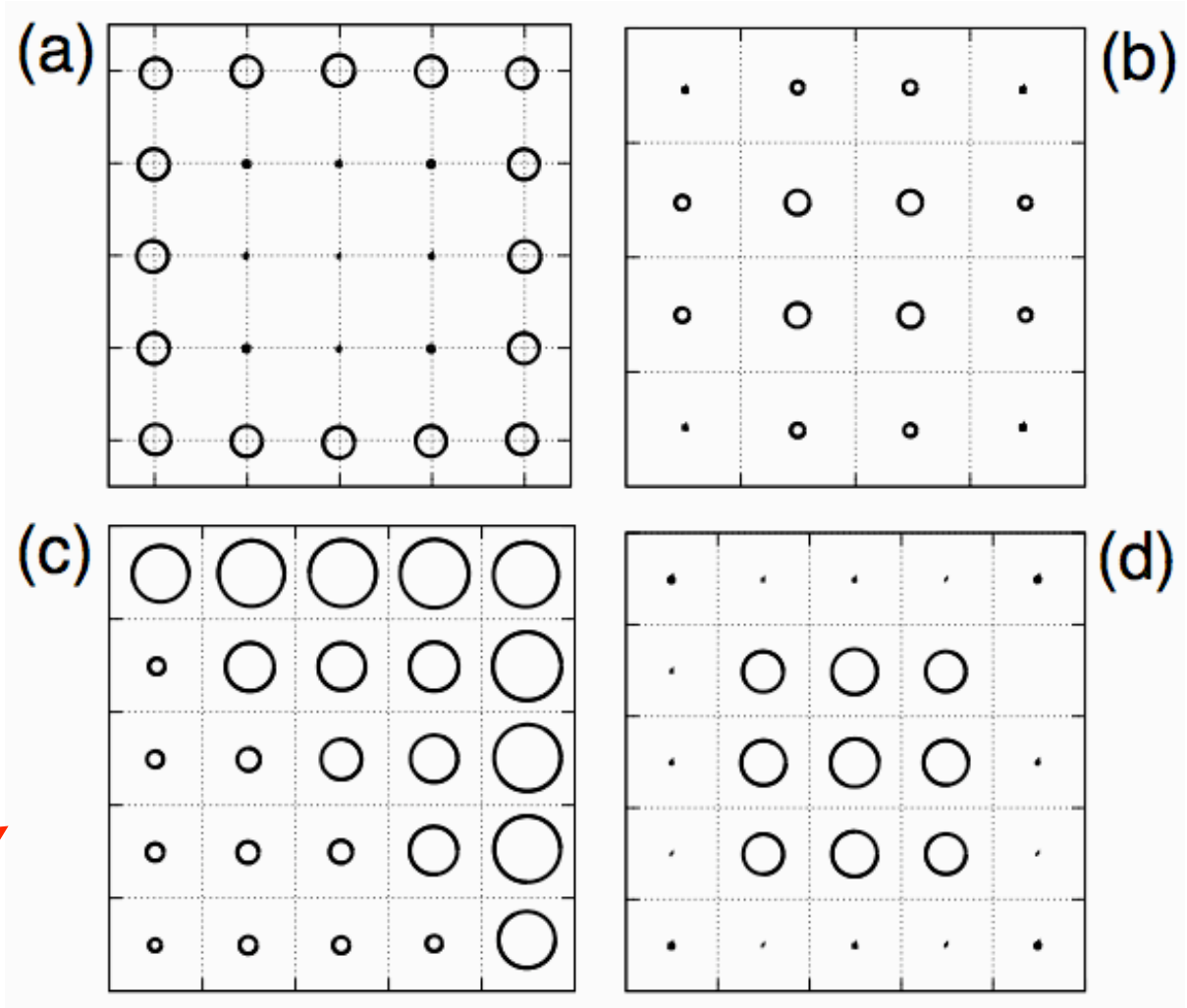
Topology of the polarization field in ferroelectric nanowires

JW Hong, G Catalan, DN Fang, E Artacho & JF Scott (arXiv 2009)



Basal section of the ferroelectric nanowires

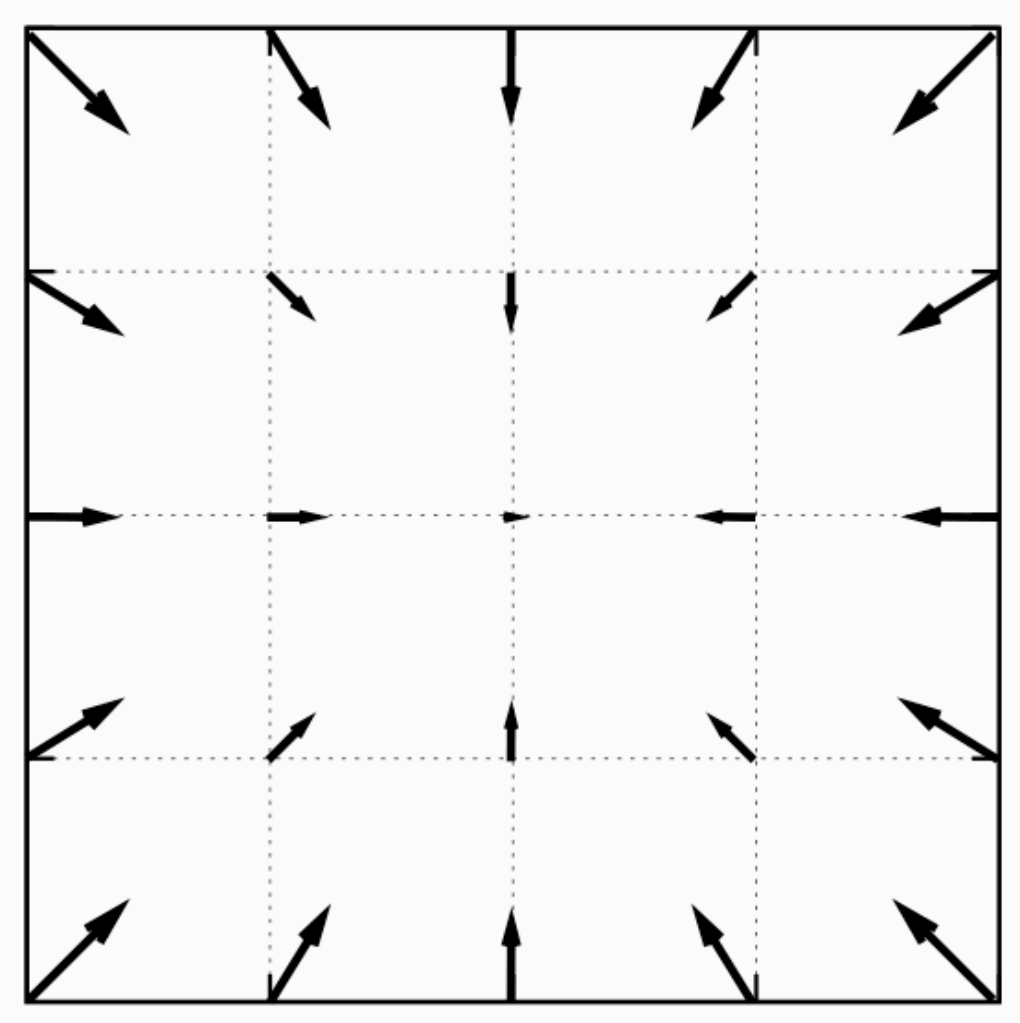
Polarisation along the wire axis (P_z)

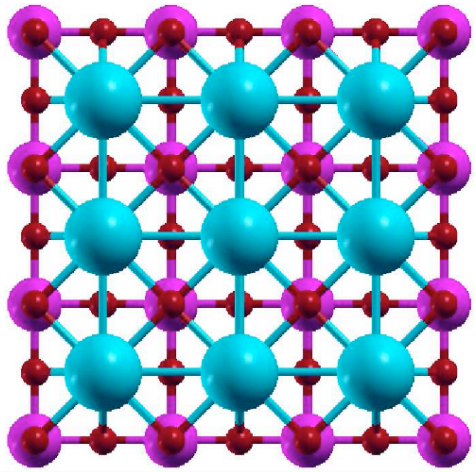


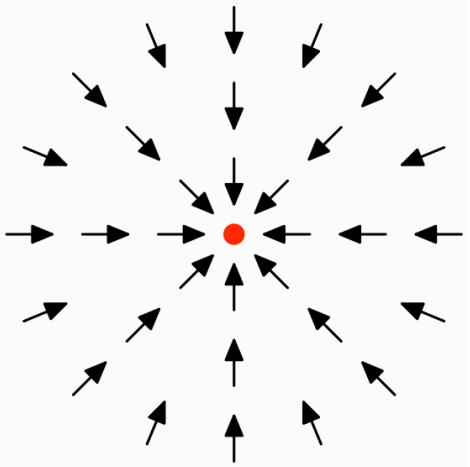
The one shown before (stoichiometric)

Polarization field in the basal plane (P_x,P_y)

TiO_2 terminated







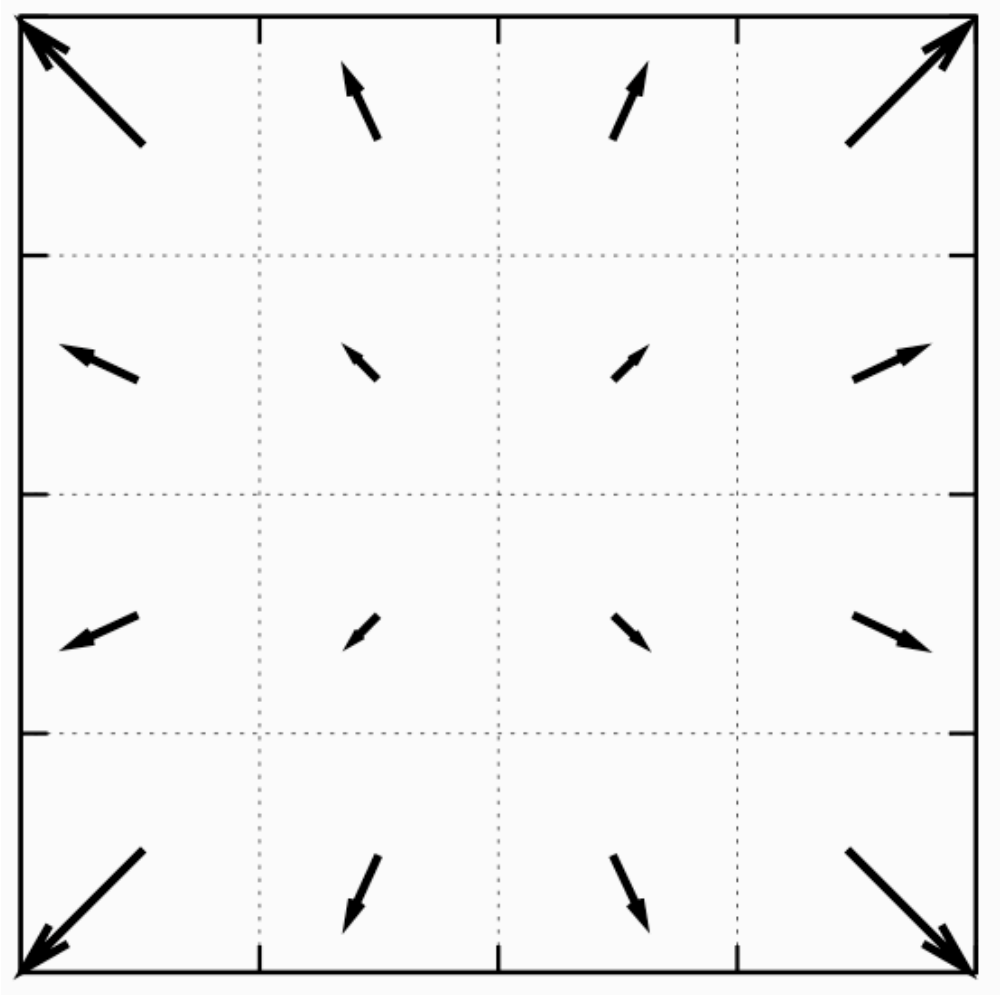
Discretisation of polarisation field

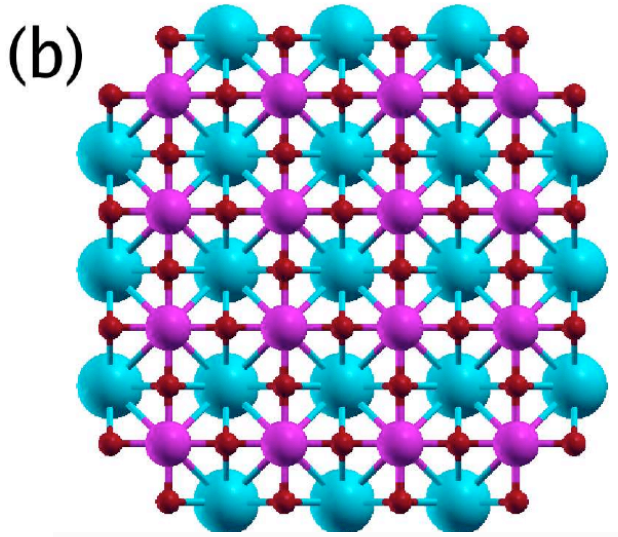
Surface & edge driven (both push in here)

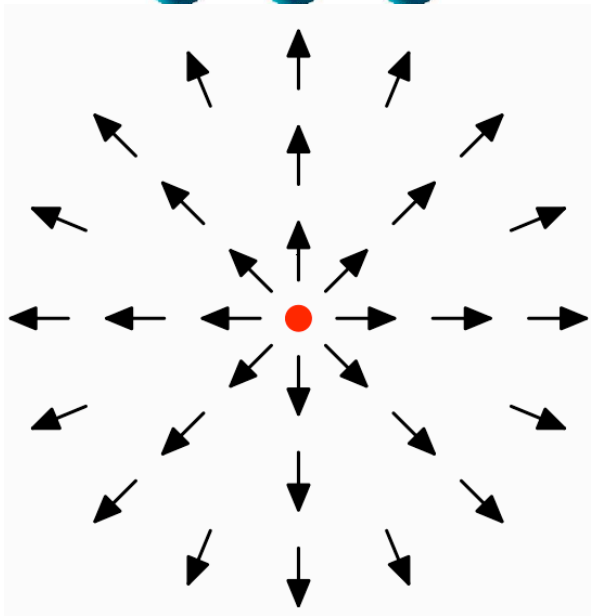
(largest 21 pm)

Different termination

BaO terminated removing corners



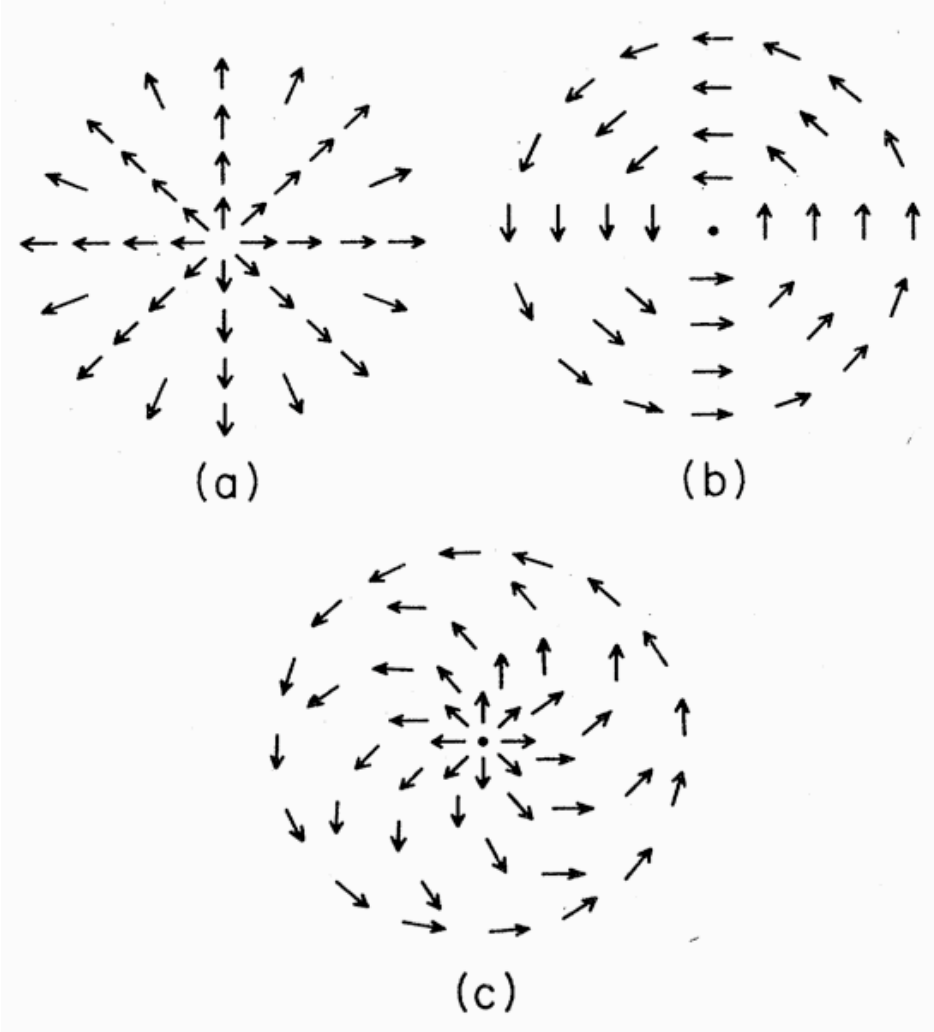




Surface and edge pull out.

This and previous homotopical to vortex

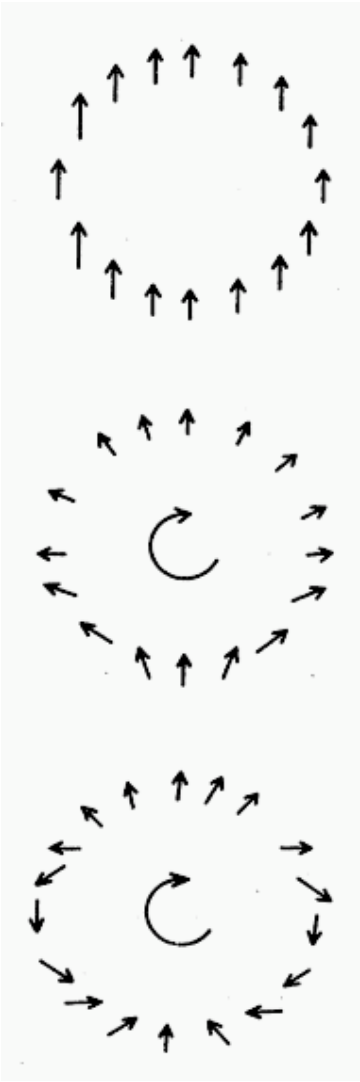
Smooth connection of homotopical textures



Both previous and vortex, homotopical: Same topology
no disruption needed to transform from one to the other

ND Mermin, Rev. Mod. Phys. **51**, 591 (1979)

Topological defects



*characterised by **winding number***

*or **topological charge***

Number of times the field makes a full turn when going around in a closed circuit

For a continuum field, n is integer

(half-integer if non-directional field: disclinations in liquid crystals)

Sign: positive if field turns in same direction as circuit

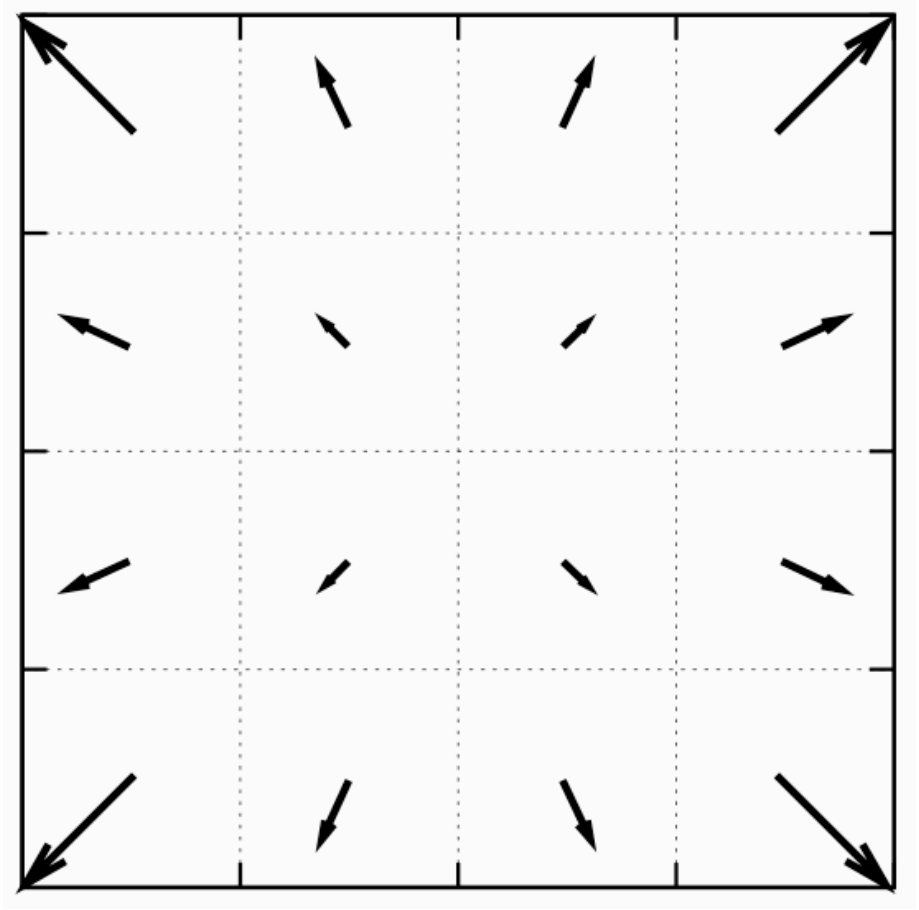
They are difficult to get rid of (need general disruption)

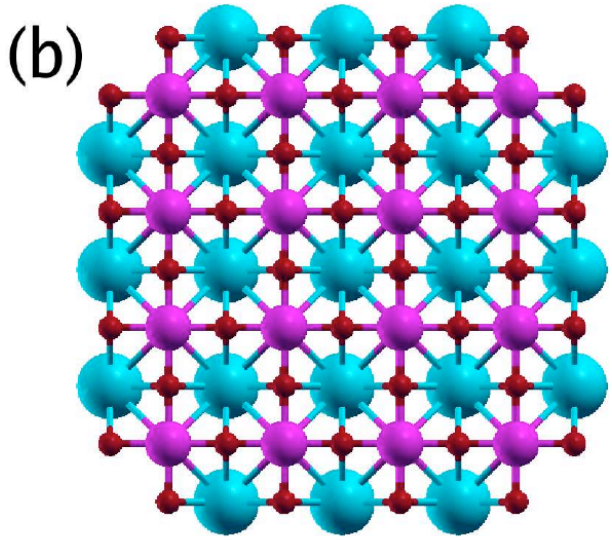
⇒Stable (at least metastable)

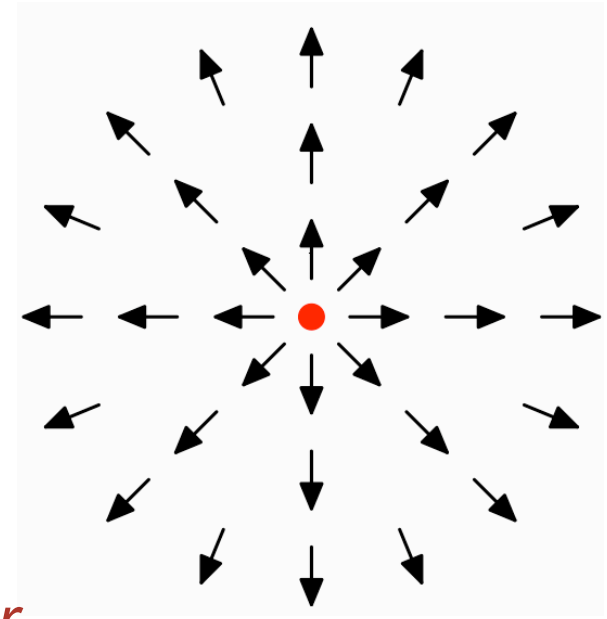
(as solitons in 1D)

Naumov et al: nano phase transition

Back to radial pattern

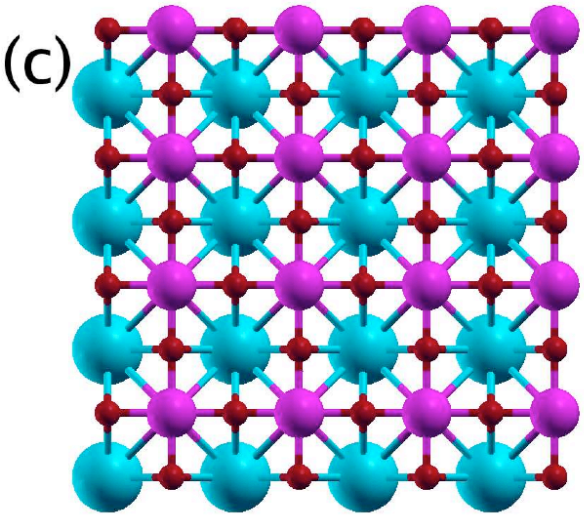


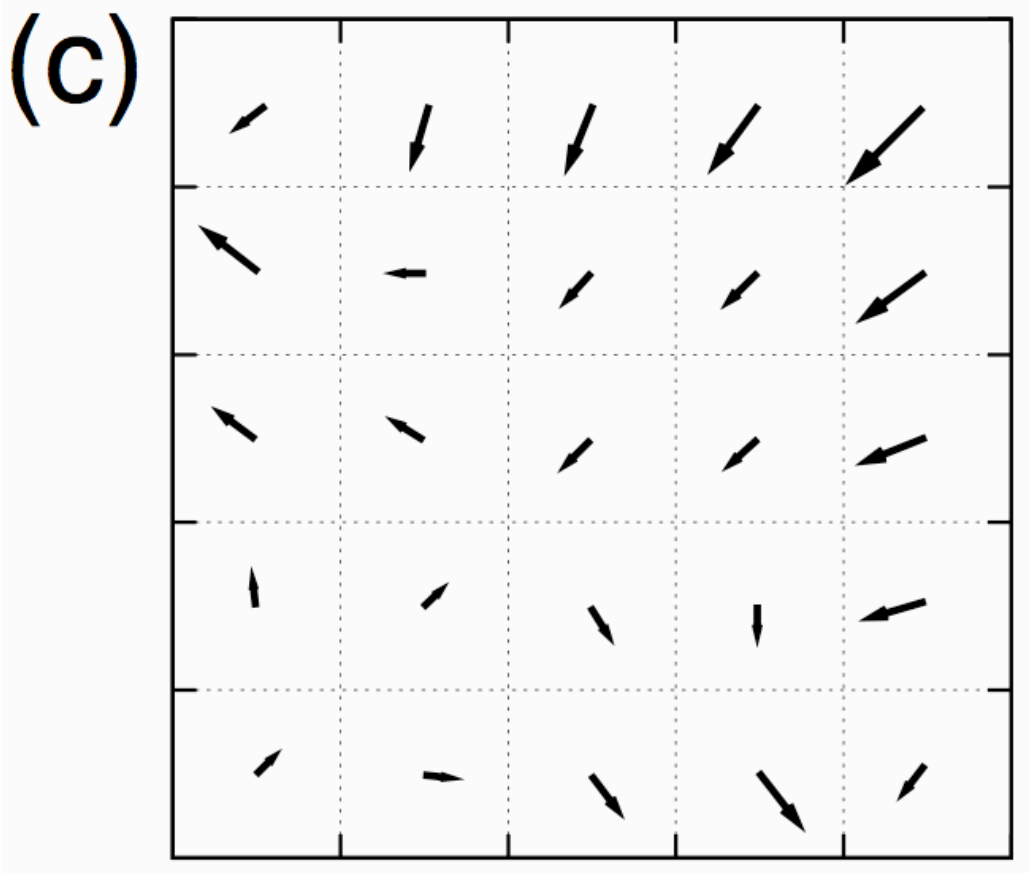


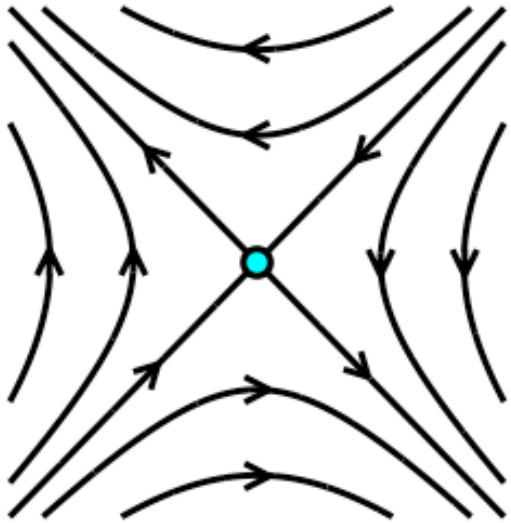


Topological defect with winding number
n = +1 (homotopical to vortex)

Change termination:
Stoichiometric wires

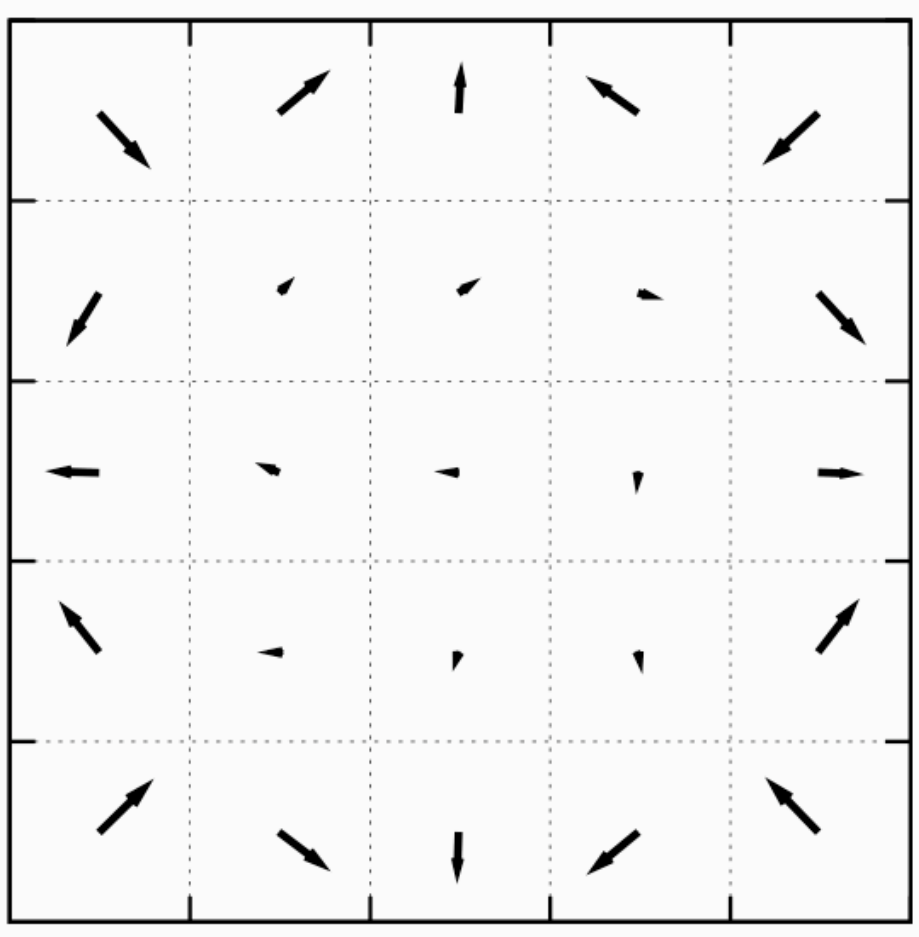


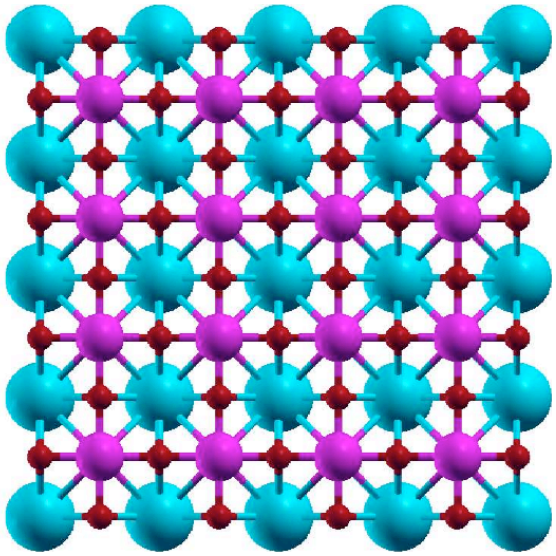


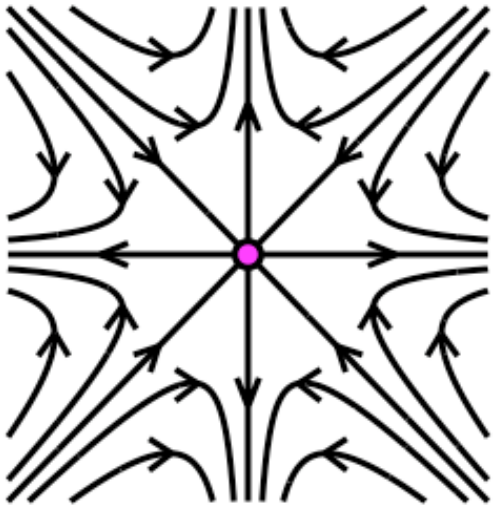


Topological defect with winding number n = -1

BaO terminated



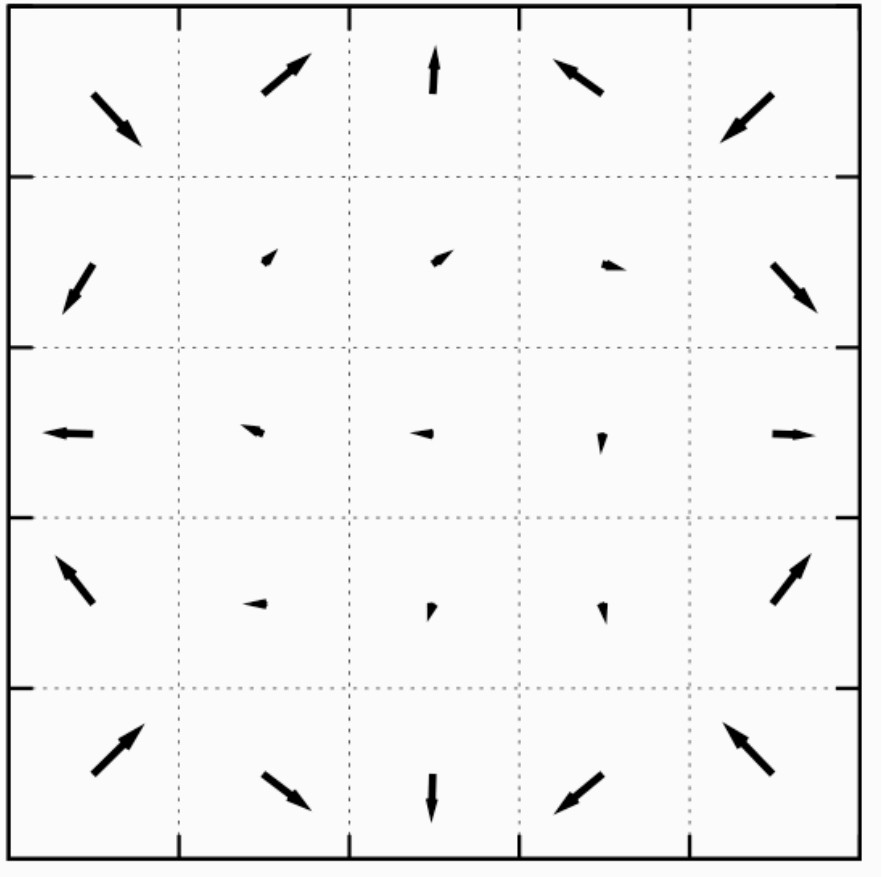


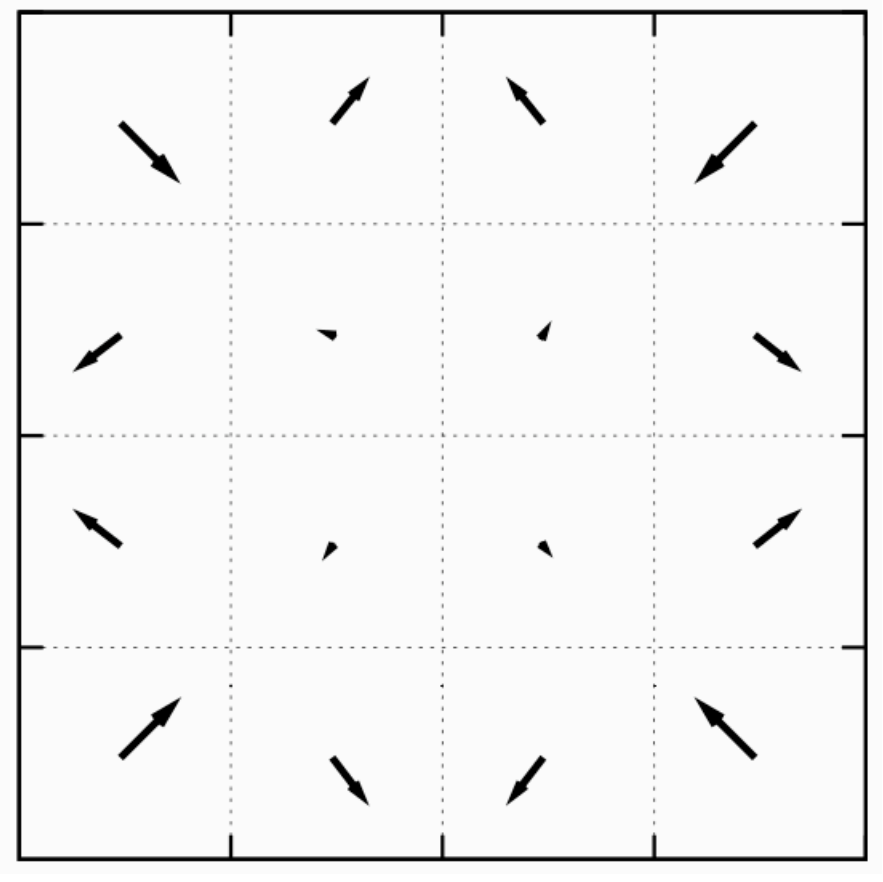


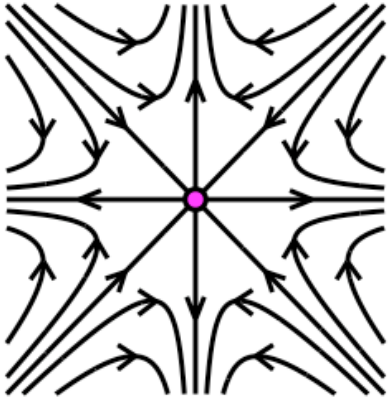
Topological defect with winding number n = -3

Ba edge pushes, Ba surface pulls *(largest 7 pm)*

BaO terminated (different sizes)



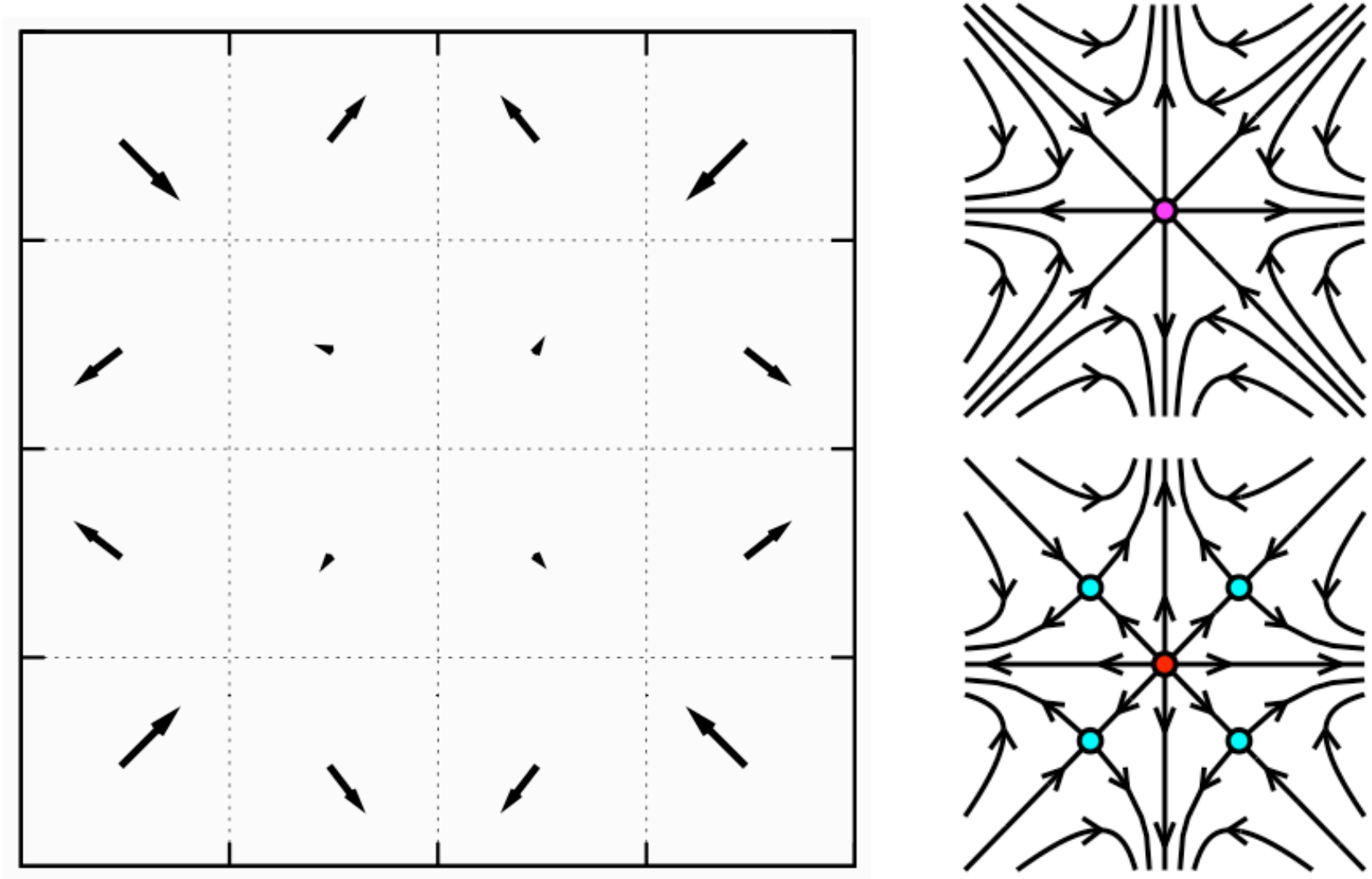




- *Both same outer-loop behaviour*
- *5x5: no clear inner*
- *4x4: inner: outwards (not n=-3)*

BaO terminated (4x4)

Topological charge = Sum of charges of the topological point defects within



Topological defect with winding number n = -3

But now decomposed in 5 defects: 4 x (n = -1) + 1 x (n = +1)

Back to the Ferroelectric nanowires Experiments

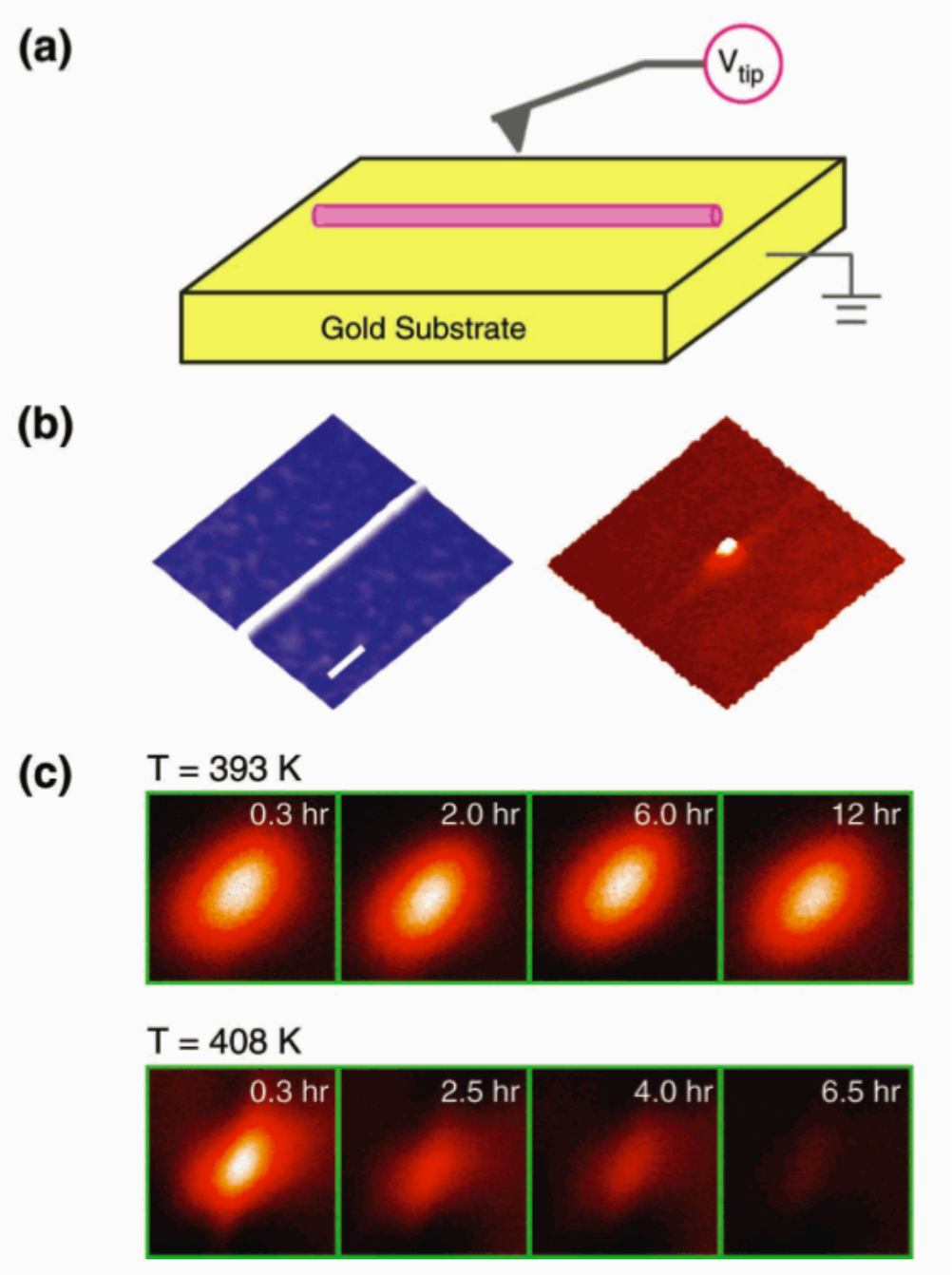
Polarisation in BTO wires of 3nm diameter

J E Spanier et al,
Nano Lett. **6**, 735 (2006)

Transverse (homogeneous) net polarization => n = 0

Ground state n<>0
P ~ 0

Both states separate by energy barrier



Summary

- *Ferroelectric nanowires: topological defects*
- *Rich textures*
- *Experiments may be reflecting this*
- *Depend on surface chemistry*
- *Other terminations (e.g. hydroxilated) may be different again*
- *Possible base for ternary memory (-1, 0, +1)*