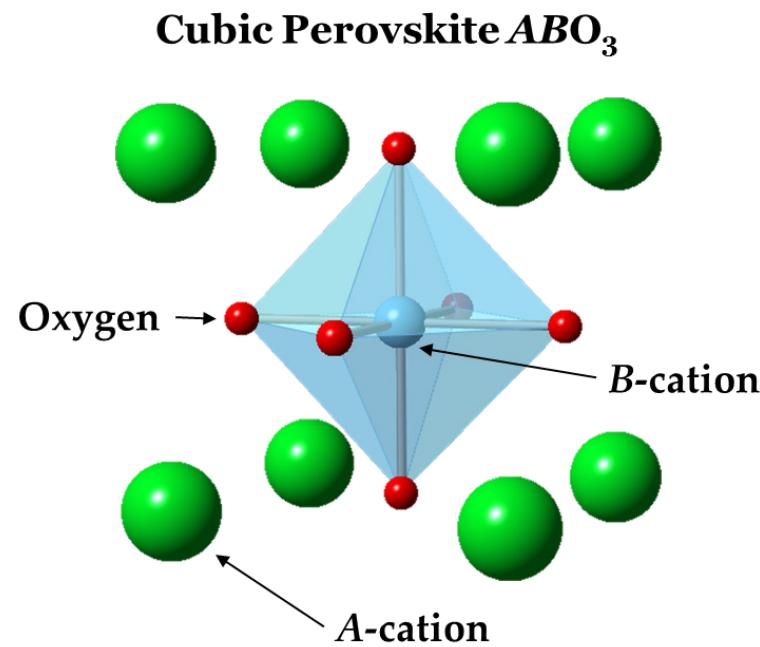
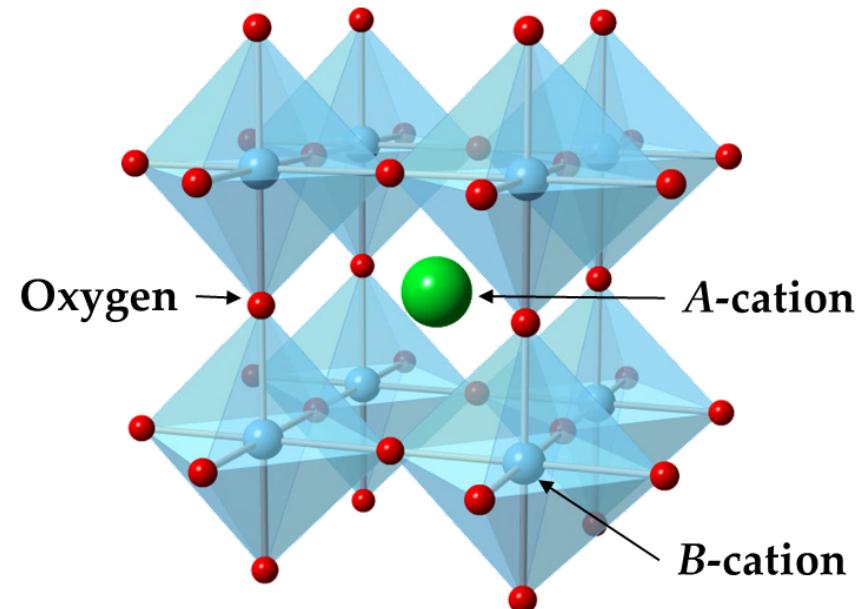


Cubic Perovskite



Cubic Perovskite ABO_3



Distortions occurring in perovskites:

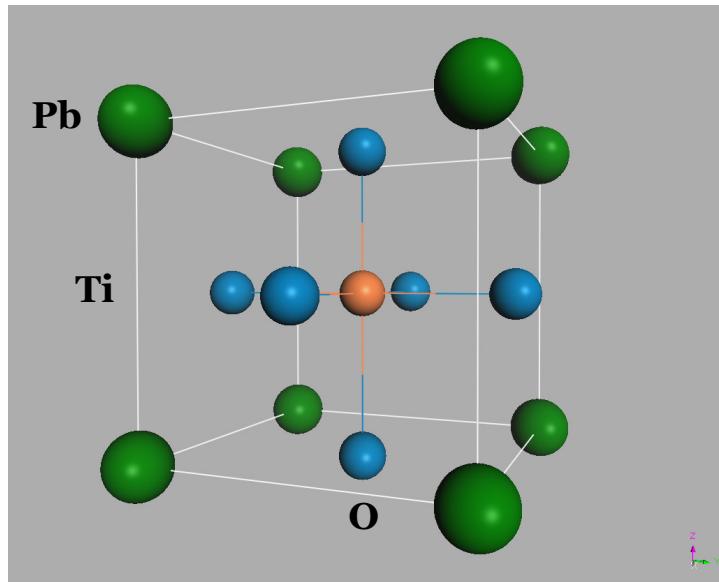
- Tilting of the octahedra
- Cation displacements
- Jahn-Teller distortions

Electronic, magnetic and dielectric properties depend on the details of such distortions

Ferroelectric ABO_3 oxides

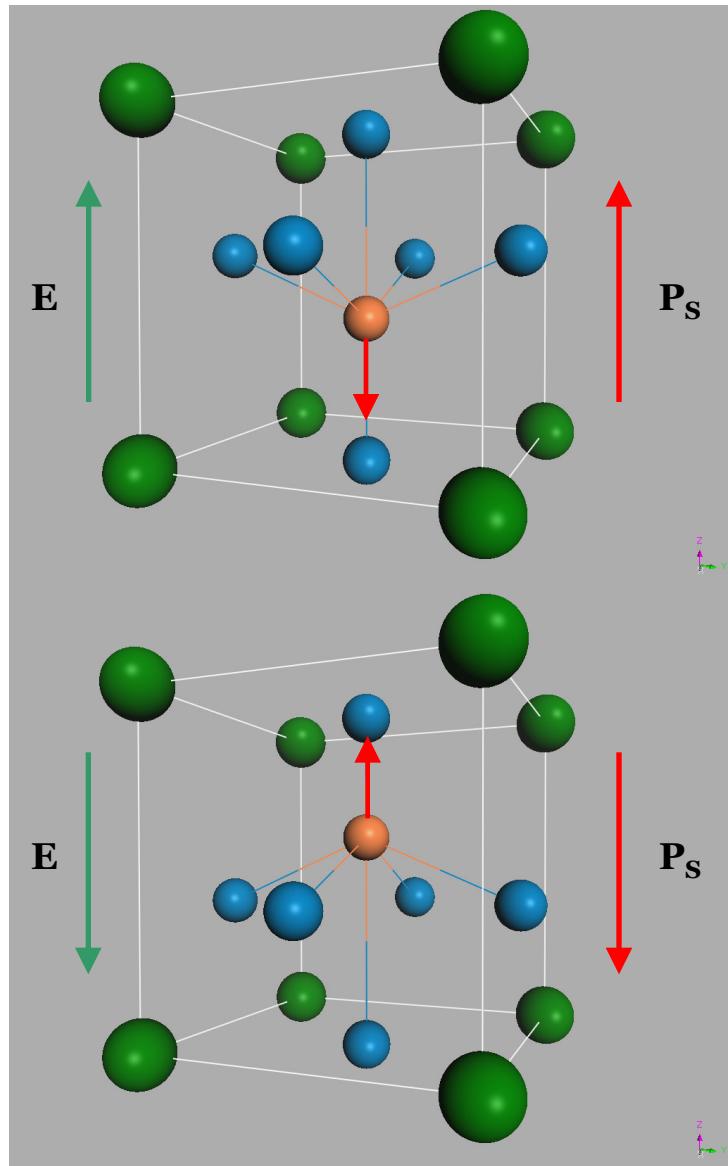
PbTiO₃

Cubic Paraelectric Phase



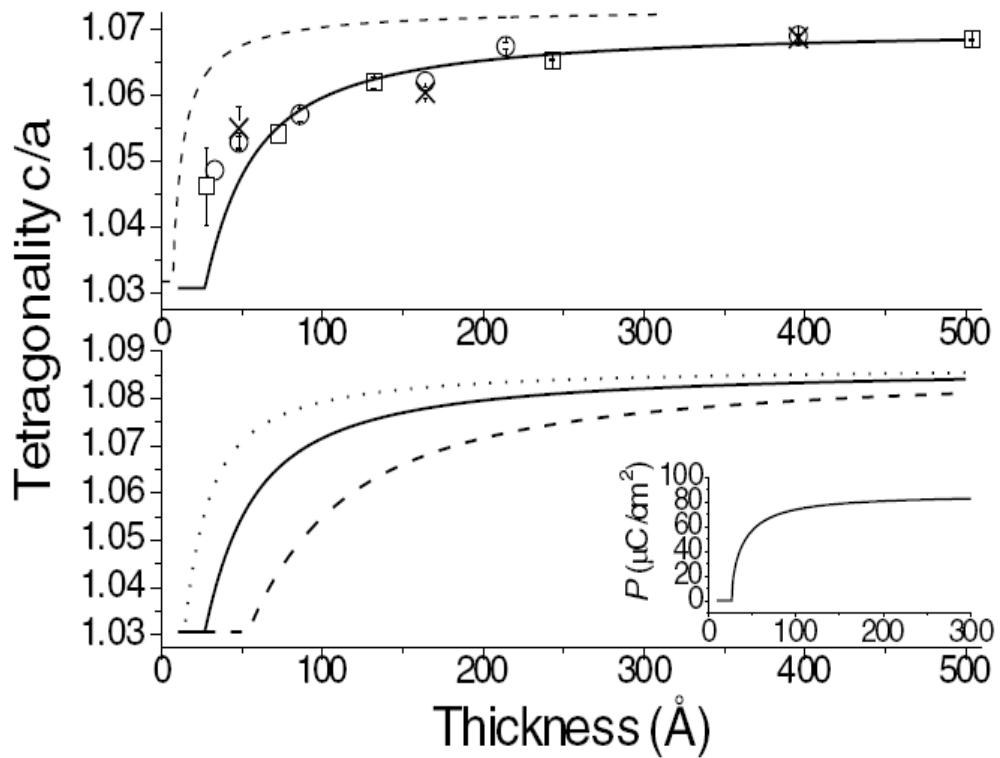
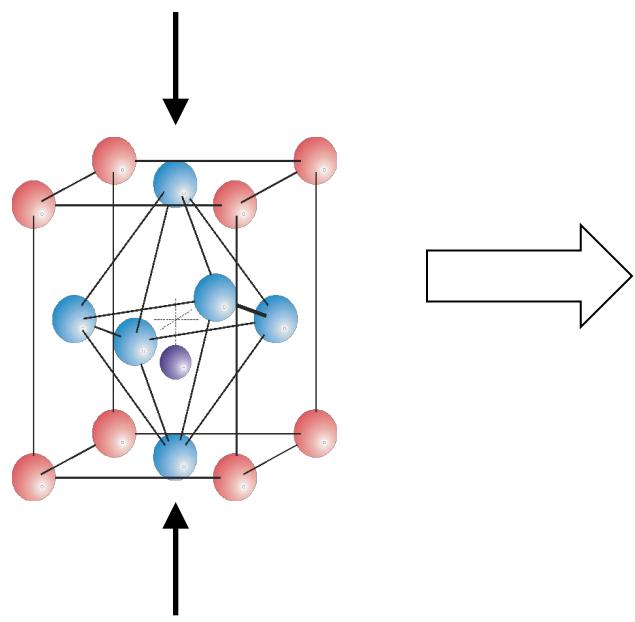
Ferroelectric materials exhibit electric dipole in the absence of electric field

Tetragonal Ferroelectric Phase



Indirect measurement of polarization

Reduction of tetragonality



- Reduction of polarization for film thicknesses $< 20 \text{ nm}$

XRD Results

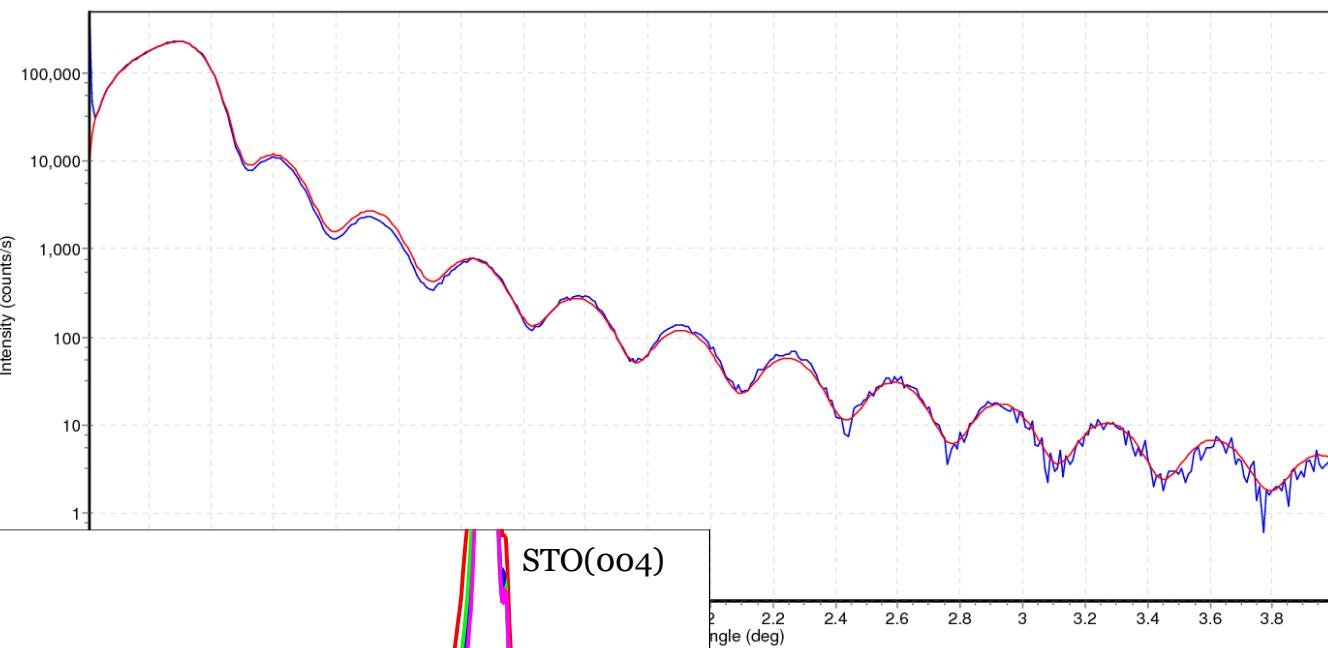
Layer	Layer Description	Density	(Min.)	(Max.)	Thickness	(Min.)	(Max.)	Roughness	(Min.)	Max.)
Substrate	DensityOnly, SrTiO ₃	5.118	(-)	(-)	600000	(-)	(-)	0.05	(-)	(-)
1, 0	DensityOnly, PbTiO ₃	7.97	(-)	(-)	12.893	(-)	(-)	0.186	(-)	(-)

Best fit value: 5.66

Best background: 1 counts/s

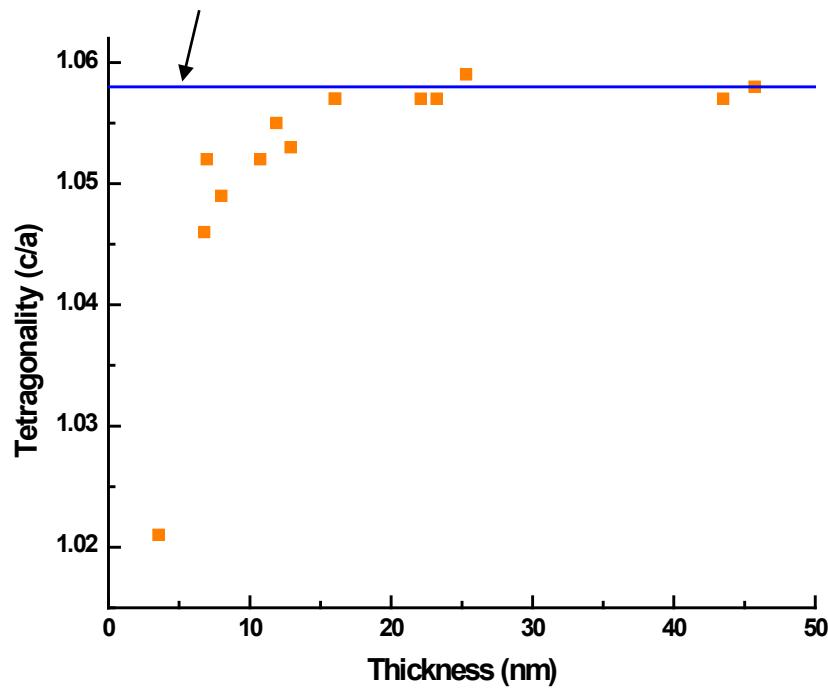
Best divergence: 0.0016 deg

Best intensity: 989760 counts/s



Page #1

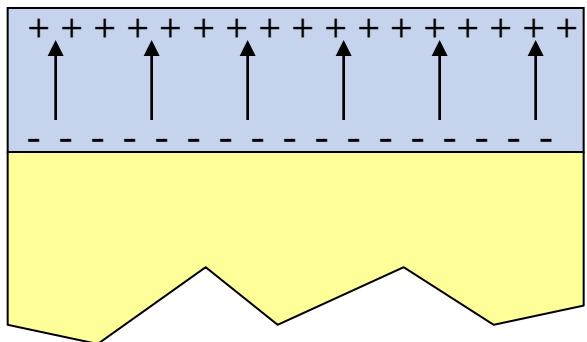
Tetragonality of bulk PTO



Direct measurement of polarization

PbTiO₃ on insulating STO substrate

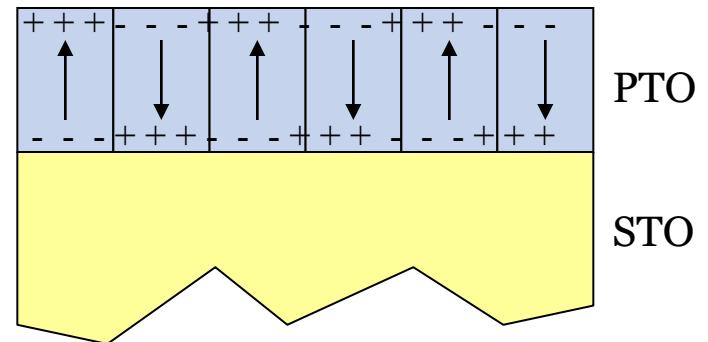
Mono-domain state



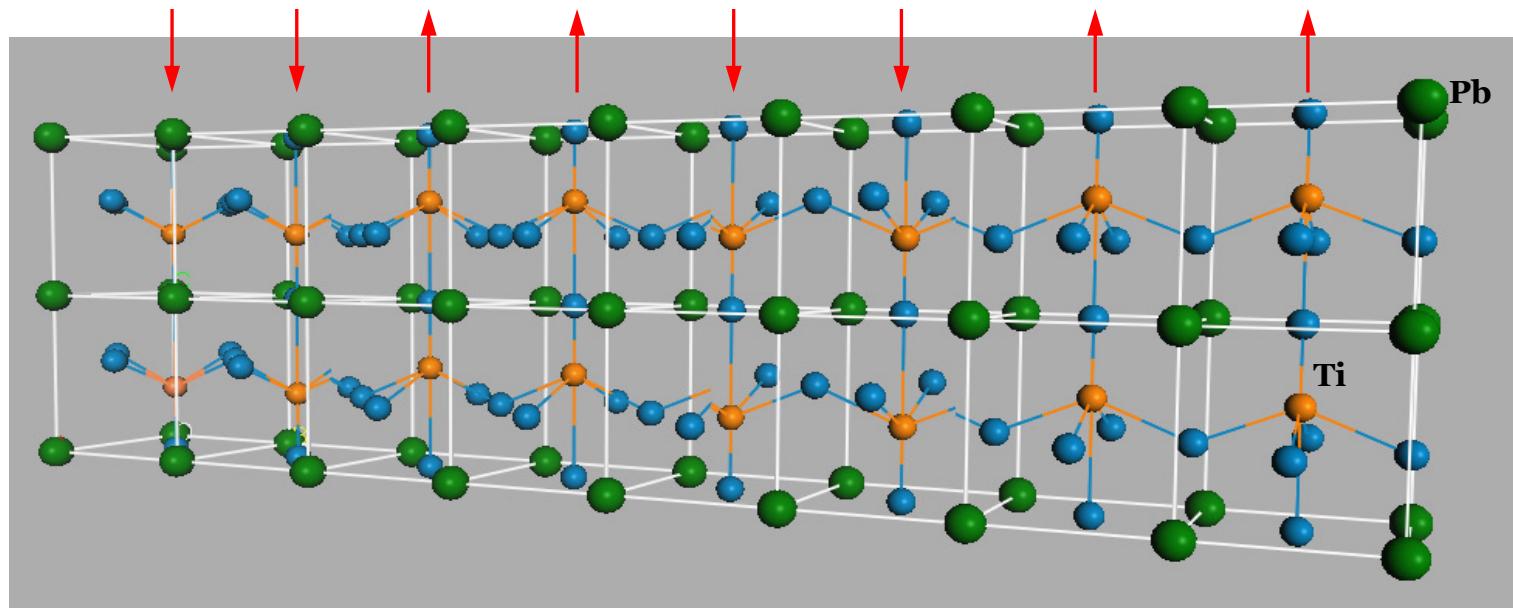
PTO
STO

- Reduce electrostatic energy by formation of domains
- Domains provide direct evidence of ferroelectricity

Poly-domain state



PTO
STO

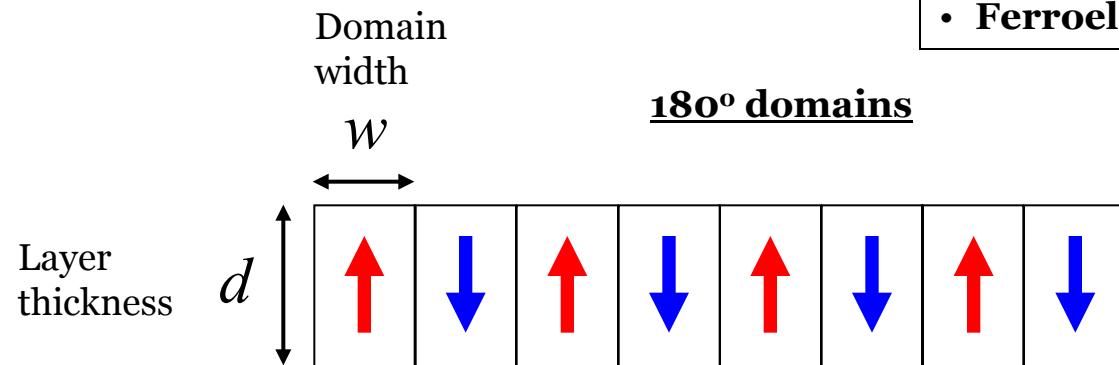


X-ray diffraction intensities are sensitive to relative Ti and Pb positions

Basic physics for domain periodicities

General property of ferroic domains of any kind:

- Ferromagnetic Kittel, 1946
- Ferroelectric Mitsui and Furuichi, 1953
- Ferroelastic Roytburd, 1976



$$F = Uw + \gamma \frac{d}{w}$$

Electrostatic energy of a free surface

Domain wall energy

Under equilibrium conditions:

$$\frac{\partial F}{\partial w} = 0 = U - \gamma \frac{d}{w^2}$$

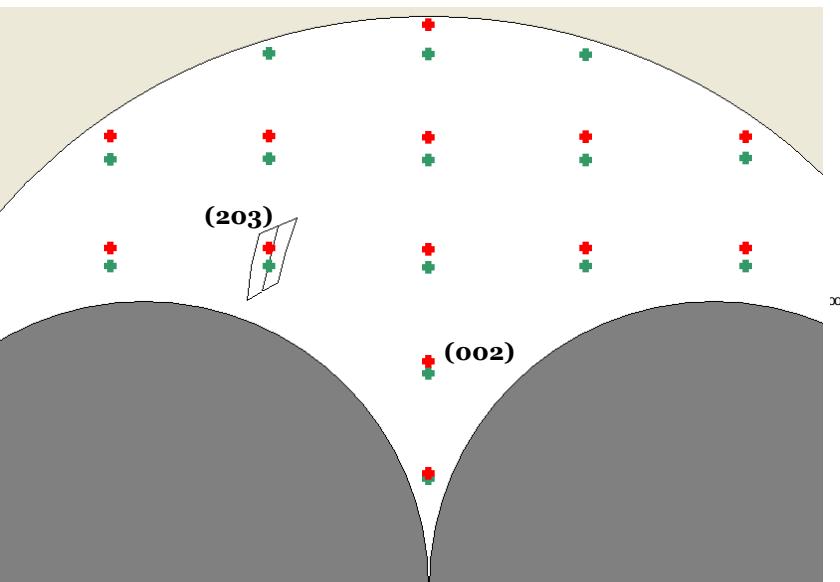


$$w^2 = \gamma \frac{d}{U}$$



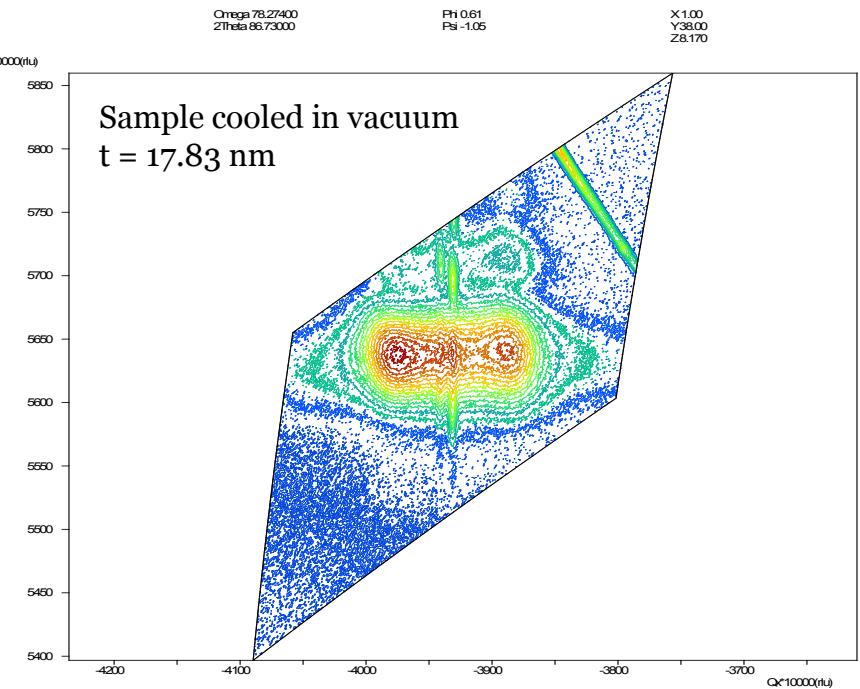
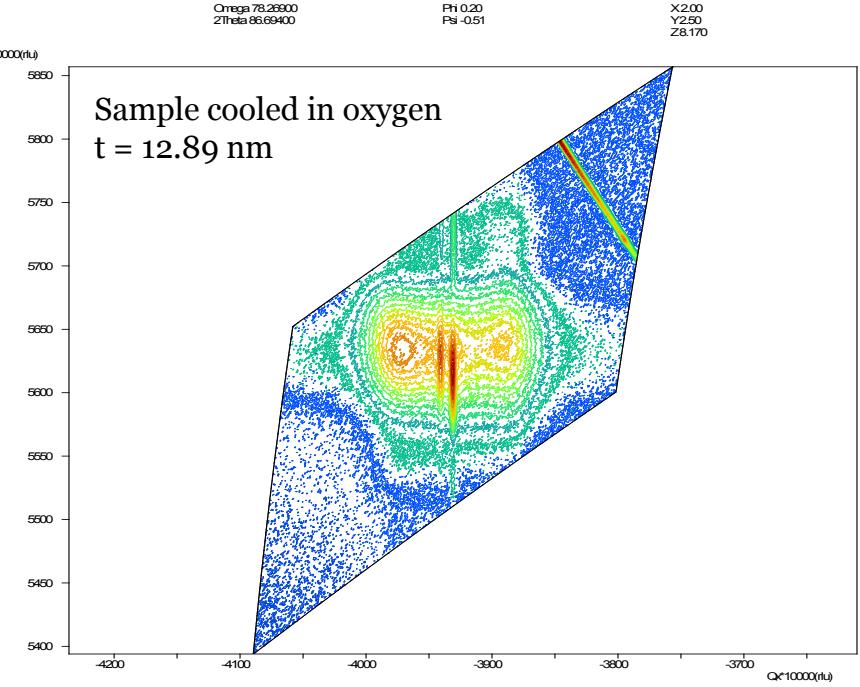
$$w \propto d^{1/2}$$

Reciprocal space maps PTO(203)

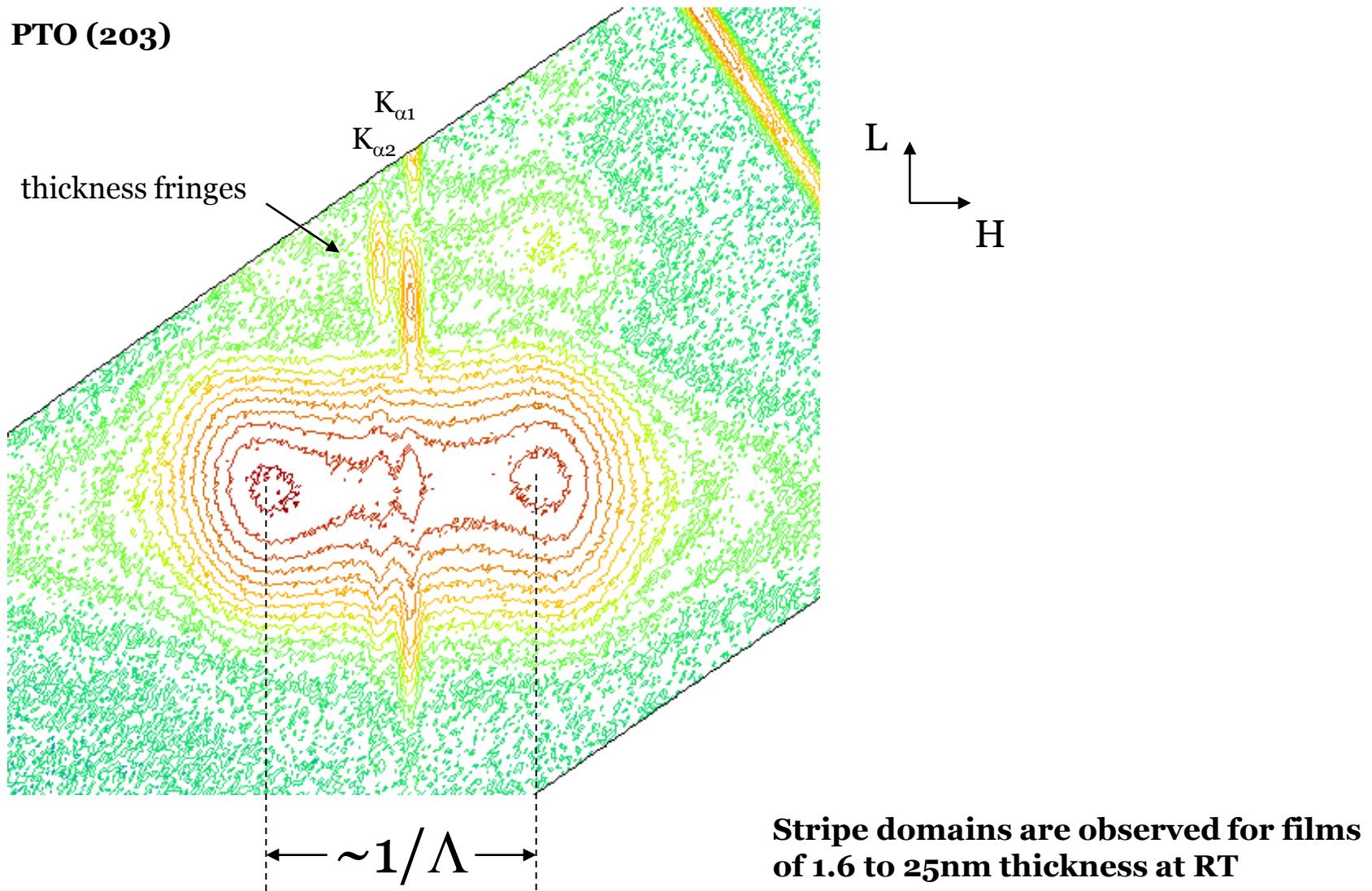


STO

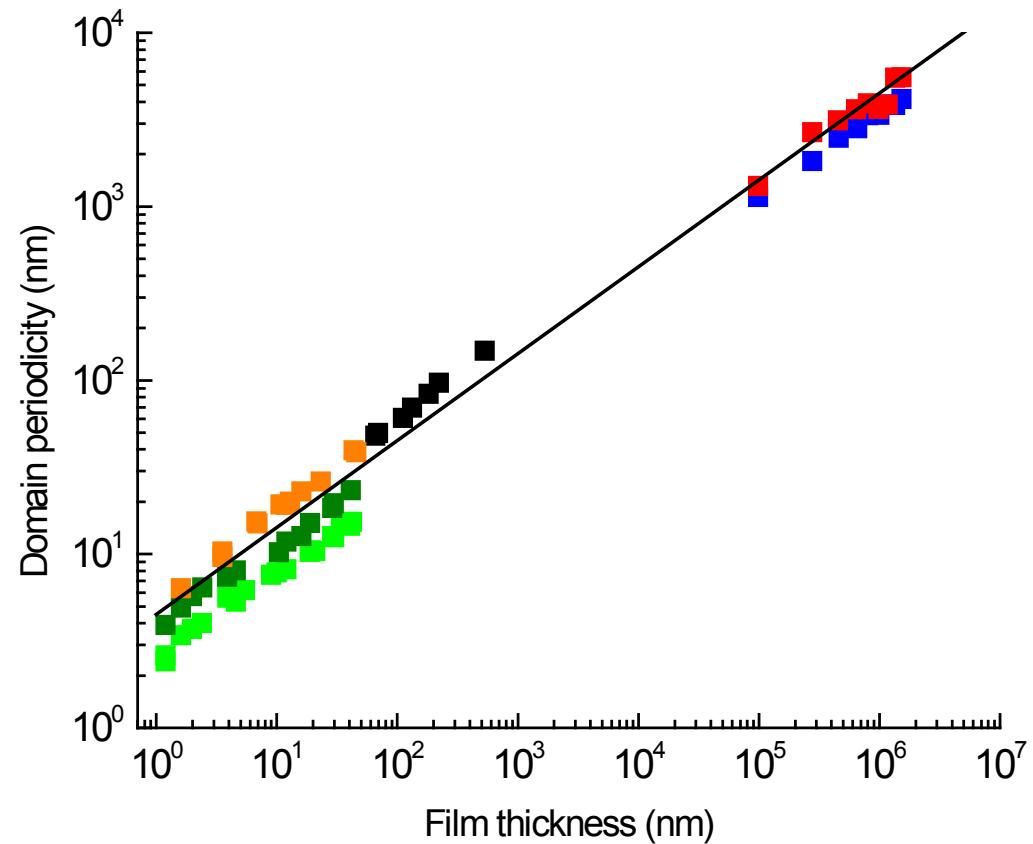
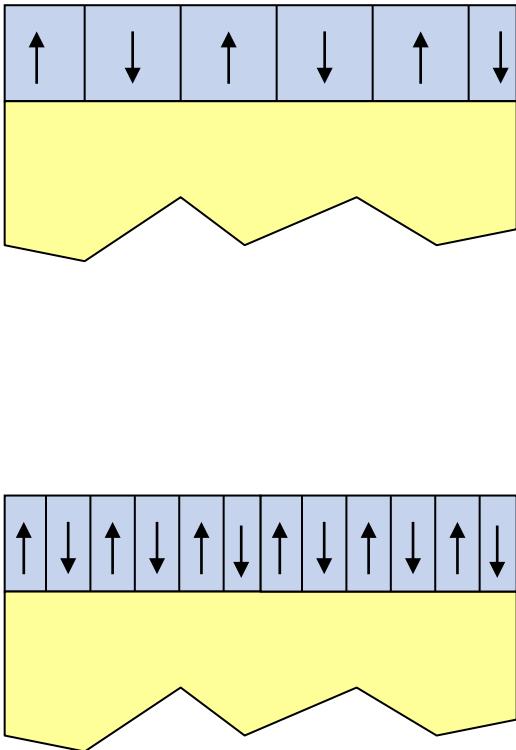
PTO



Stripe Domain Observation at Room Temperature



Domains in Ferroelectrics



- A. Schilling *et al.*, Phys. Rev. B **74**, 024115 (2006)
- S.K. Streiffer *et al.*, Science **304**, 1650 (2004)
- T. Mitsui *et al.*, Physical Review **90**, 193 (1953)
- R. Meyer *et al.*, submitted to Phys. Rev. B

