

# Avalanche statistics, nonlinear dynamics, and self-affine roughening of ferroelectric domain walls during polarisation switching



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[ferro.unige.ch](http://ferro.unige.ch)

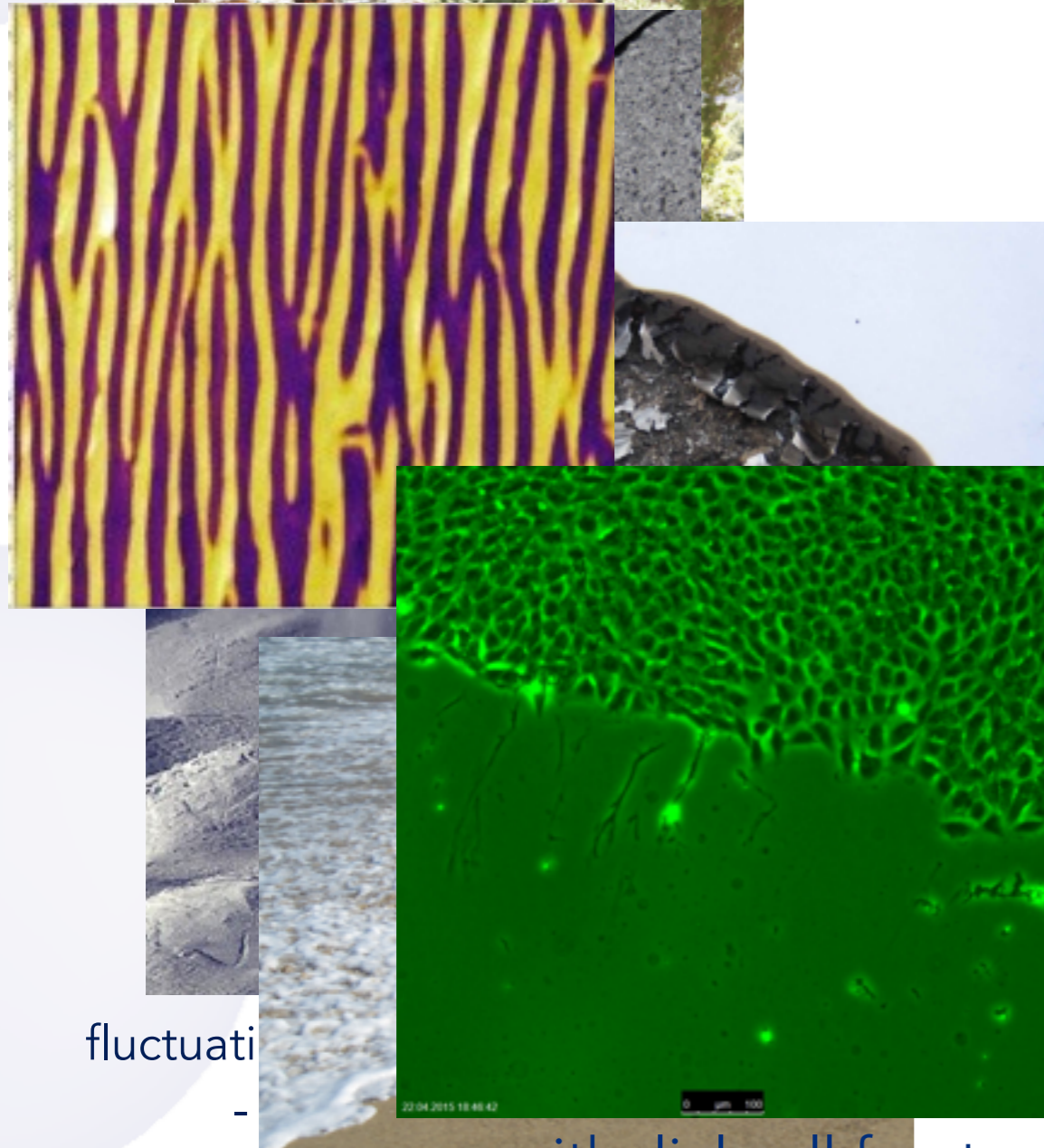


**UNIVERSITÉ  
DE GENÈVE**

**FACULTÉ DES SCIENCES**  
Département de physique  
de la matière quantique

# Elasticity + disorder : simple ingredients...

ferroelectric domain walls



many metastable states, glassy behaviour

statics: self-similarity, scaling laws

dynamics: universality, scaling laws, nonlinear

out-of-equilibrium, ageing, thermal effects

... of complex physics

fluctuati

-

epithelial cell fronts

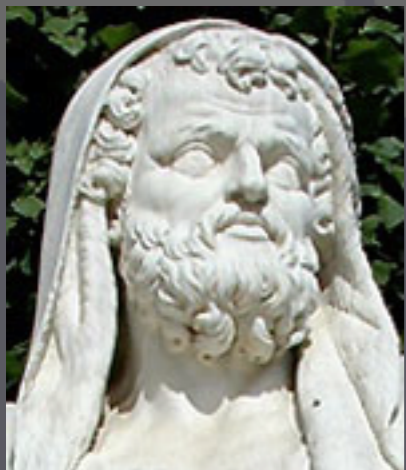
interfaces separate regions with different properties

diverse interfaces show common dynamics and geometric properties

# Ferroelectrics - late to the party



"dawn of humanity"  
Louis Néel 1948  
Ferromagnetism



Theophrastus 314 BC  
Carl Linnaeus 1747  
Pyroelectricity  
heat - electricity



Pierre Seignette 1675, La Rochelle



Pierre Curie 1880s

Piezoelectricity  
strain - electricity



Joseph Valasek 1920

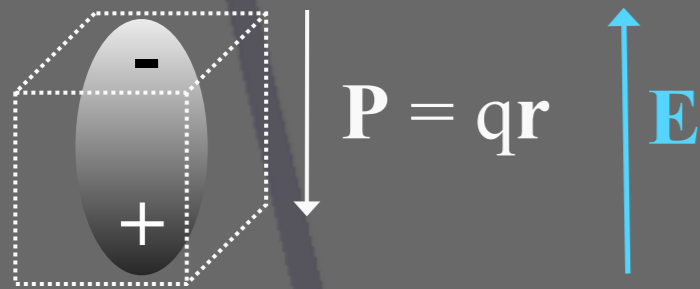
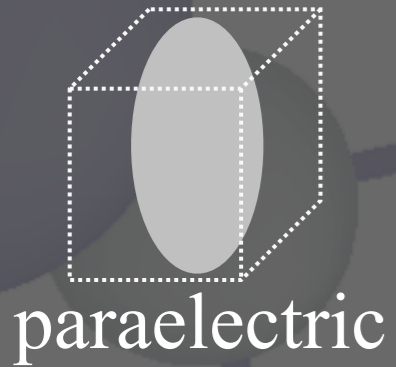
Ferroelectricity

spontaneous  
switchable  
electric polarization

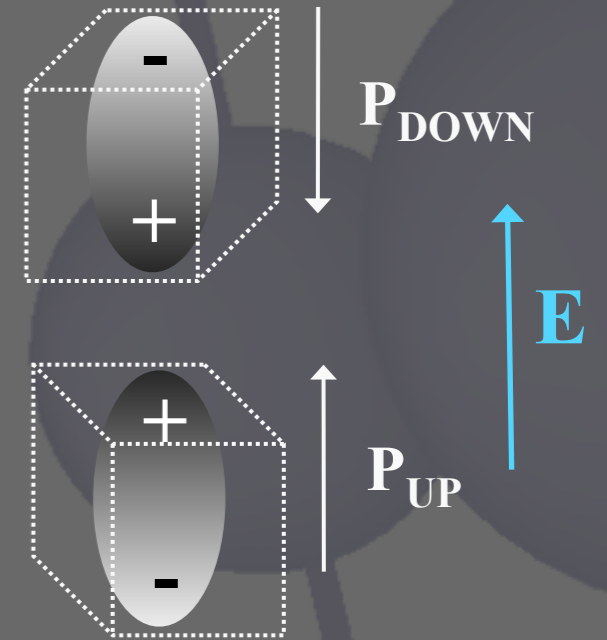
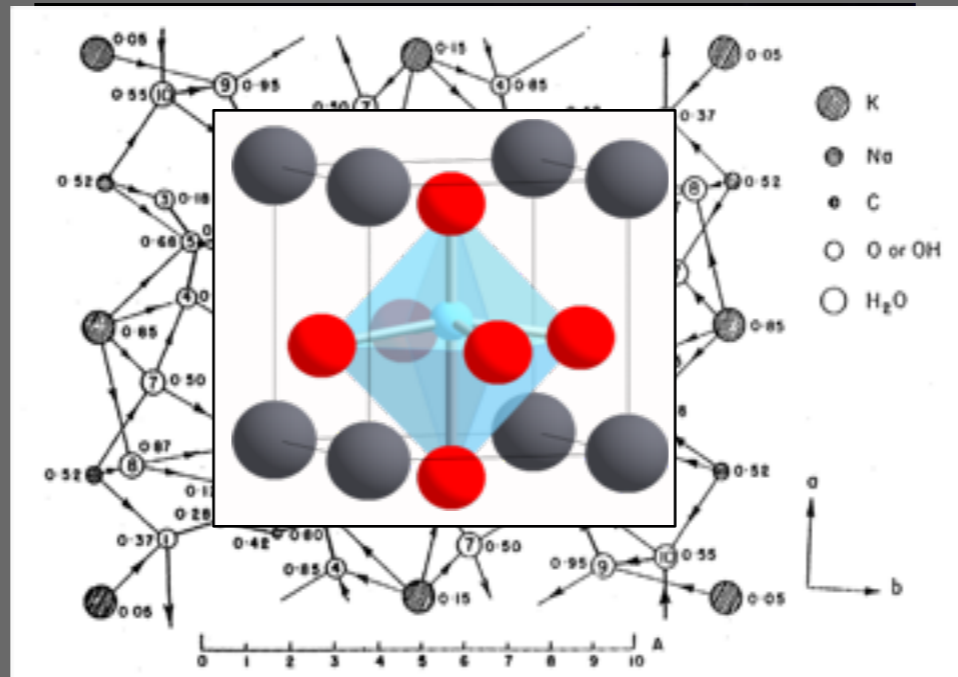
# Ferroelectrics - late to the party



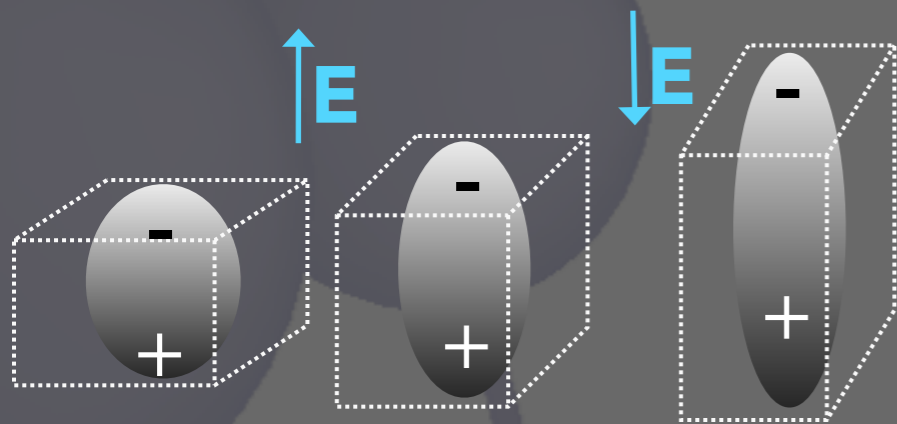
$P = 10 \mu\text{C}/\text{cm}^2 = 6.2 \times 10^{13} \text{ charges}/\text{cm}^2$



Pyroelectricity  
heat - electricity



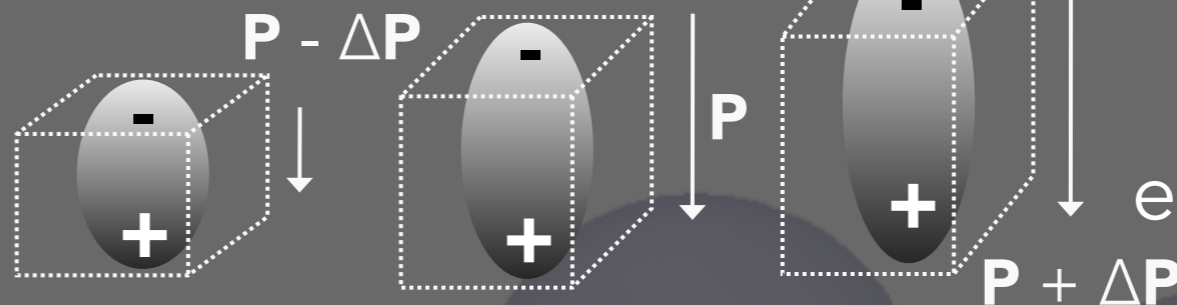
Ferroelectricity



$\Delta X_j = d_{ij}^t E_i$

Piezoelectricity  
strain - electricity

compression



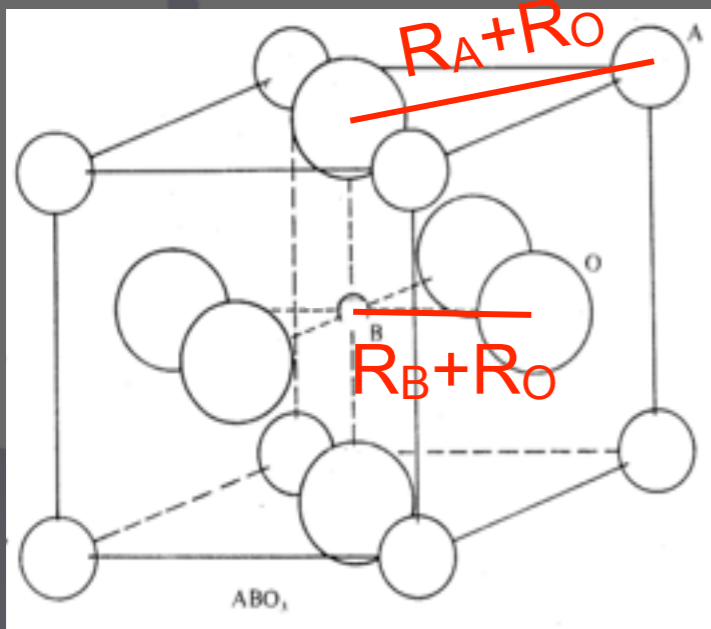
$\Delta P_j = d_{ij} T_i$

tension

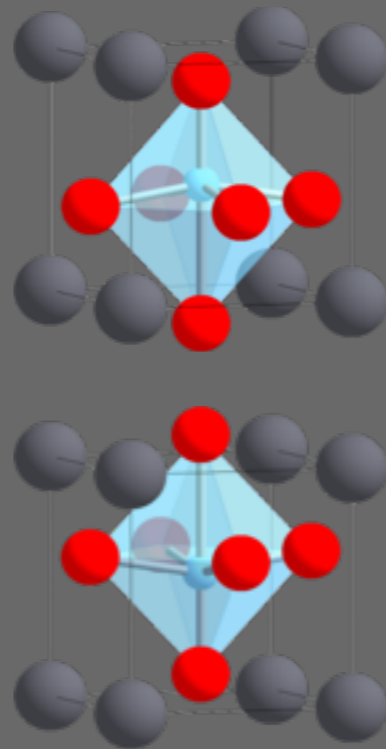
spontaneous  
switchable  
electric polarization

# Instabilities in $ABO_3$ perovskites

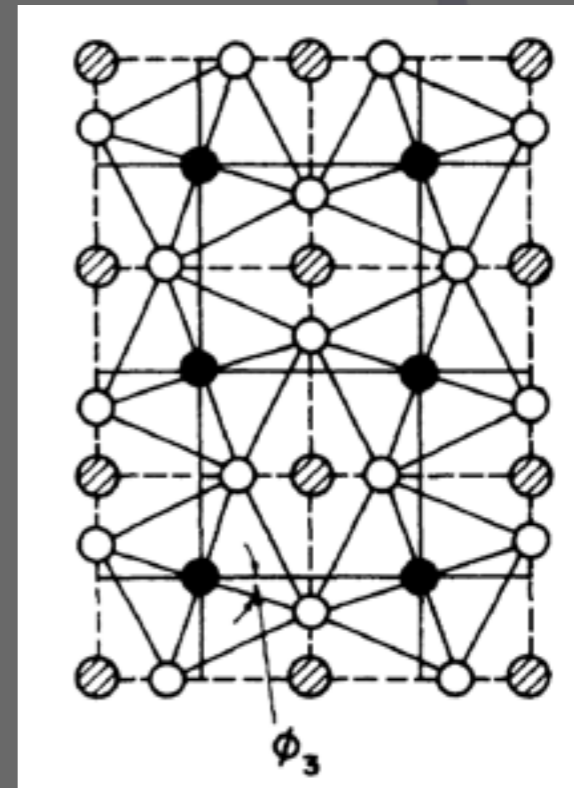
$$R_A + R_O = \sqrt{2}(R_B + R_O)$$



ideal perovskite structure  
 $t = 1$



$t > 1$   
 $BaTiO_3$



$t < 1$   
 $CaTiO_3$

Goldsmith's  
criterium

tolerance factor  $t = \frac{R_A + R_O}{\sqrt{2}(R_B + R_O)}$

# Origin of the ferroelectric instability

Cochran's model:

Competition between SR and LR forces

$$\langle \eta | \mathbf{D} | \eta \rangle = \langle \eta | \mathbf{D}^{\text{SR}} | \eta \rangle + \langle \eta | \mathbf{D}^{\text{LR}} | \eta \rangle$$

$$\omega^2 \qquad \omega_{\text{SR}}^2 \qquad \omega_{\text{LR}}^2$$

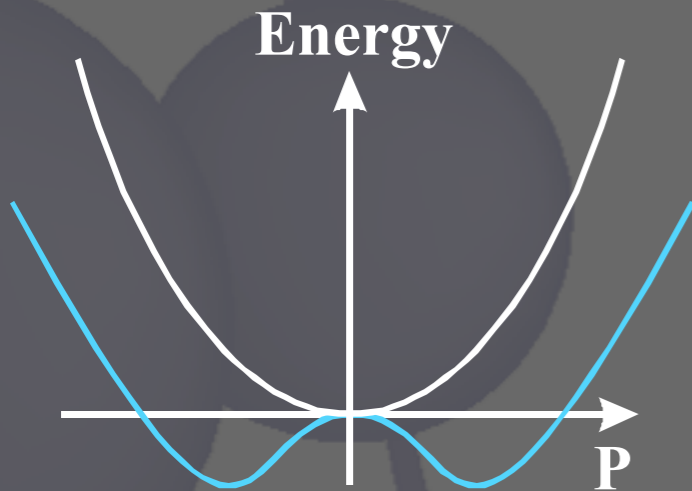
$$< 0 \qquad >> 0 \qquad <<< 0$$

SR interactions  
Function of the  
Chemical bond  
Pauli repulsion  
...

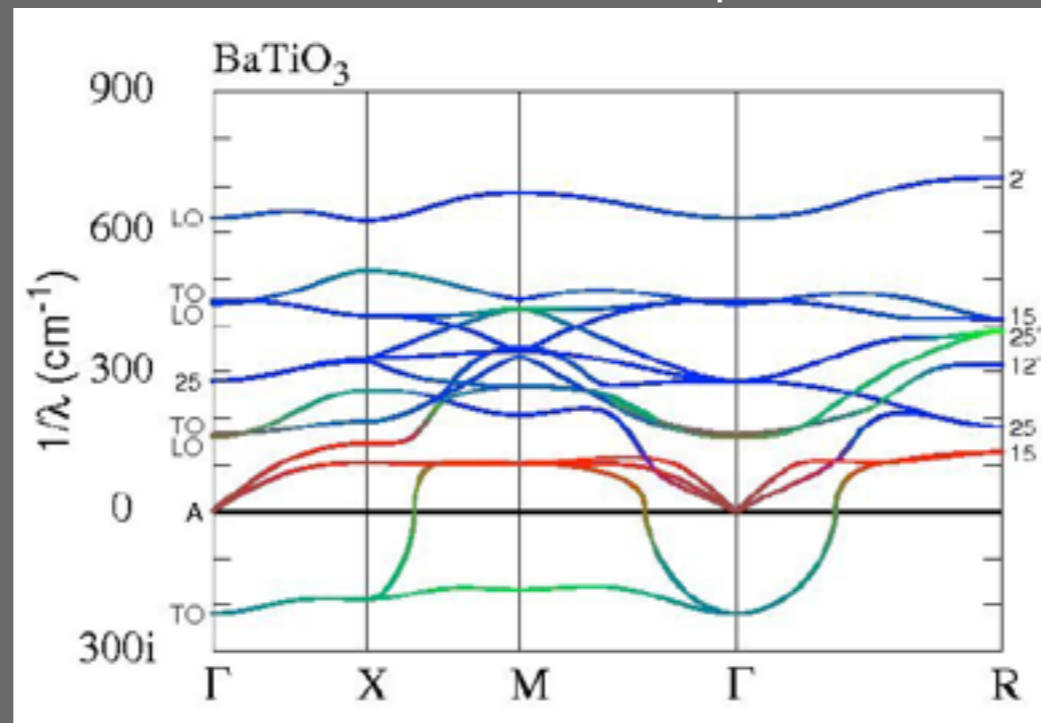
LR Coulomb forces  
Dipole-dipole  
interaction

DFT calculations of BaTiO<sub>3</sub> phonon modes

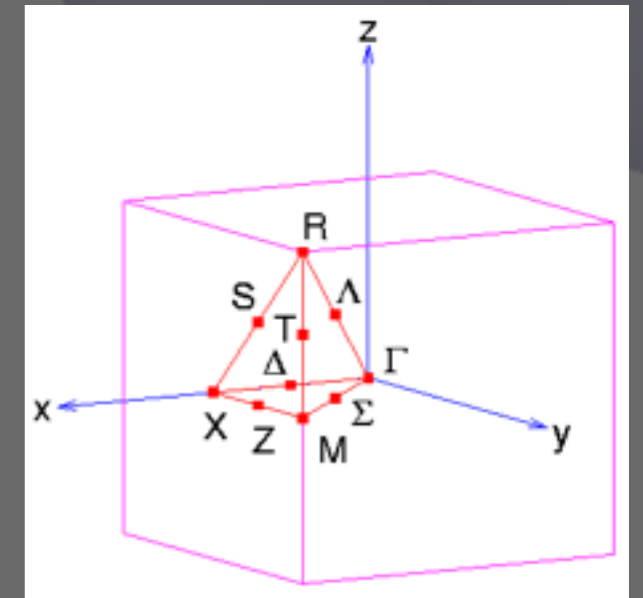
positive curvature  $\omega^2 > 0$



negative curvature  $\omega^2 < 0$



Ghosez et al, PRB 60 836 (1999)

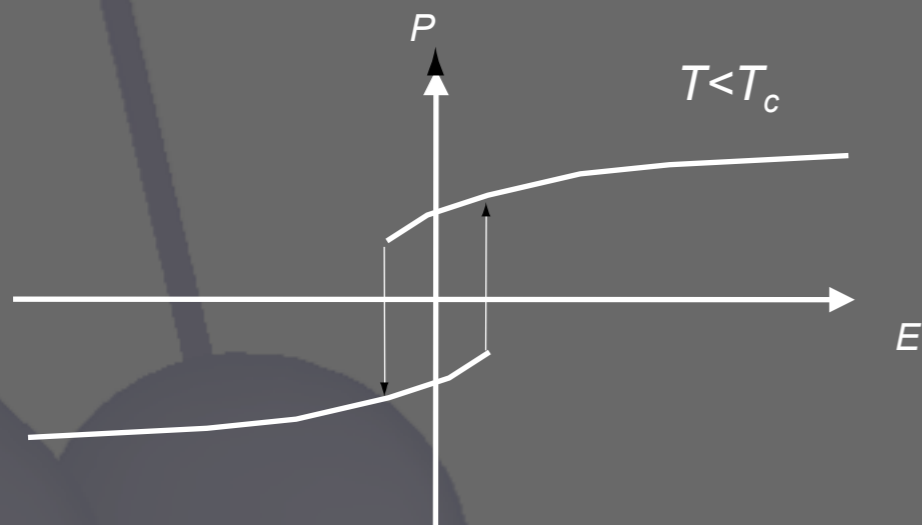


Pattern of lattice distortion associated with instability (soft phonon mode) freezes in at T<sub>C</sub>

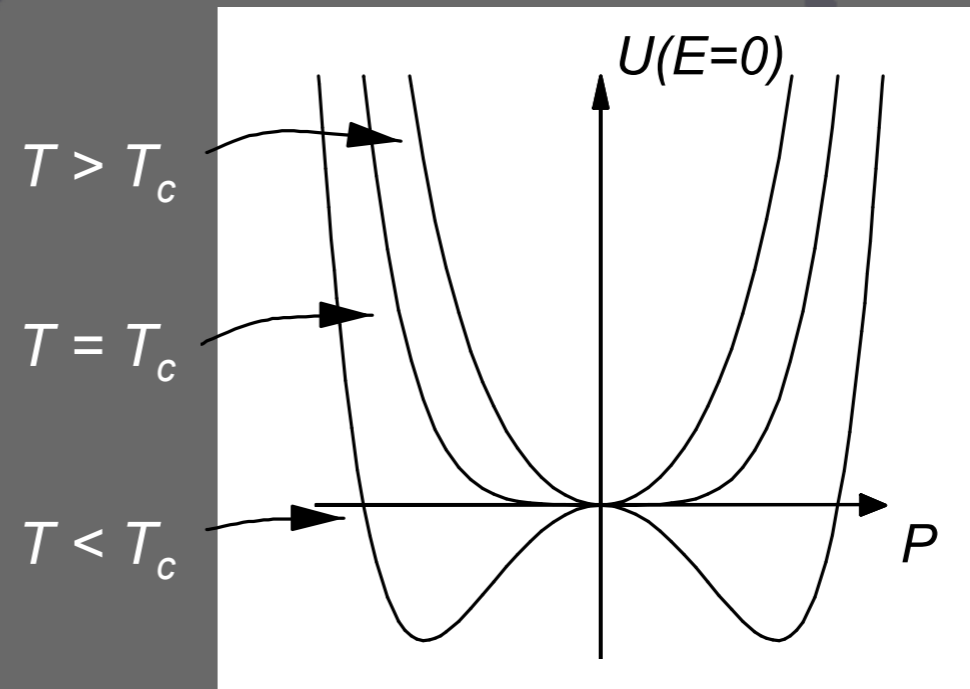
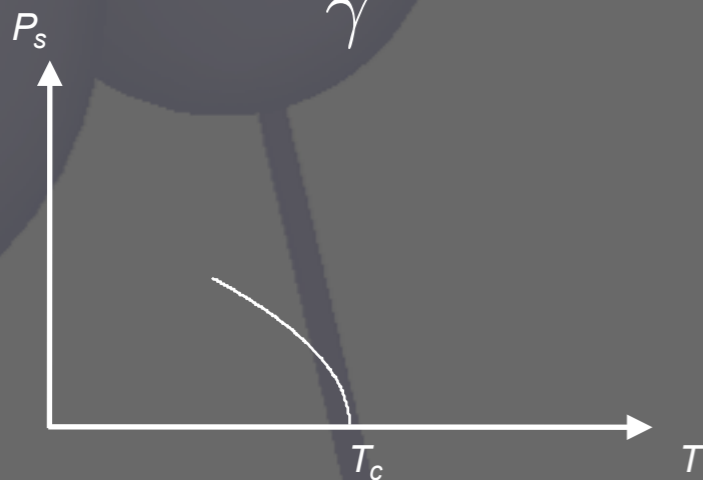
# Landau-Ginzburg-Devonshire

$$U = \frac{\alpha}{2}P^2 + \frac{\gamma}{4}P^4 + \frac{\delta}{6}P^6 - EP$$

$$\alpha = \beta(T - T_c)$$

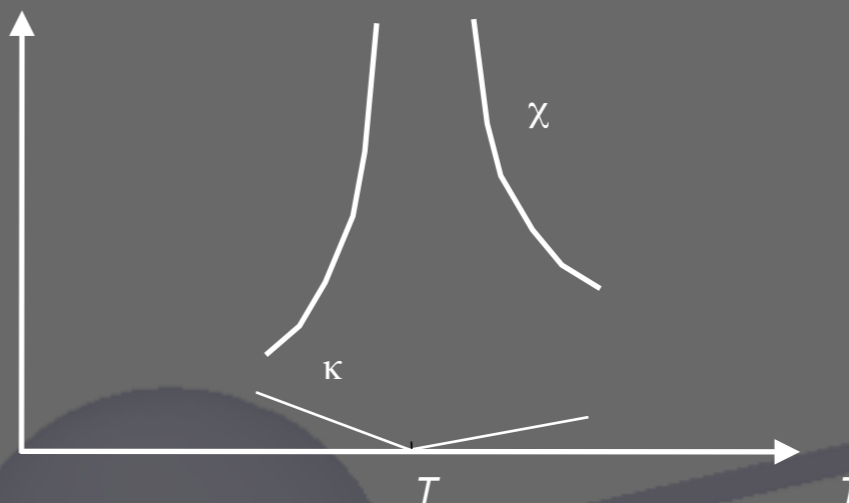


$$P_S^2 = \frac{\beta}{\gamma}(T_c - T)$$



$$\kappa^{X,T} = \beta(T - T_c), T > T_c$$

$$\kappa^{X,T} = 2\beta(T_c - T), T < T_c$$



Phenomenological theory of ferroelectricity

# Ferroelectricity vs Ferromagnetism

## Similarities

Order parameter decreases with  $T$  until transition to para- state  
Coupling between strain and order parameter  $\rightarrow$  piezo- effects  
Large susceptibilities to applied fields (electric/magnetic)  
Order parameter - Field hysteresis useful for storage applications

## Differences

FE: off-center ionic displacements caused by long range interactions  $\rightarrow$  space inversion symmetry breaking

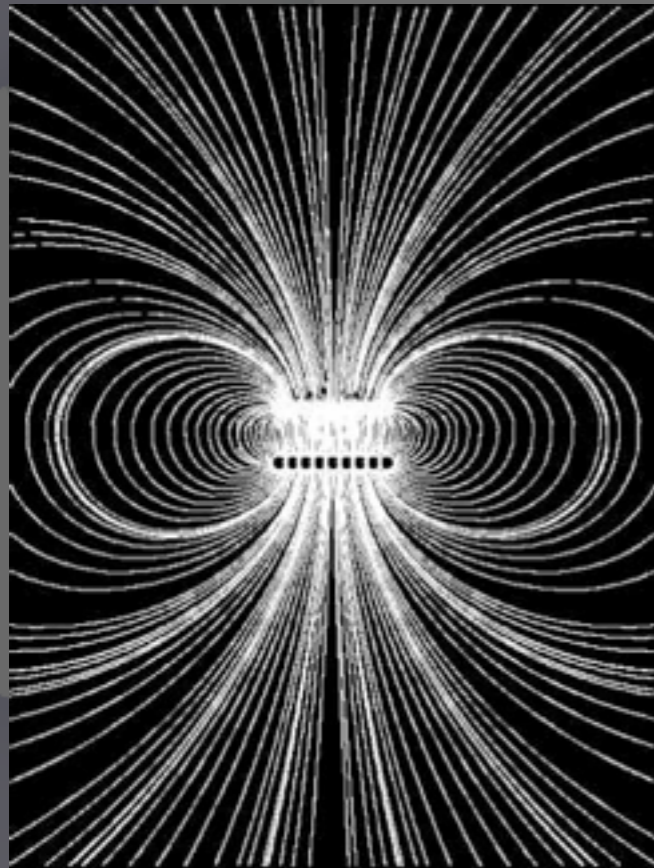
FM: net electronic angular momentum due to spin-spin exchange energy  $\rightarrow$  time inversion symmetry breaking

electric monopoles : screening / electric boundary conditions

collective phenomenon : size, lattice, strain effects



# Energy considerations in domain formation

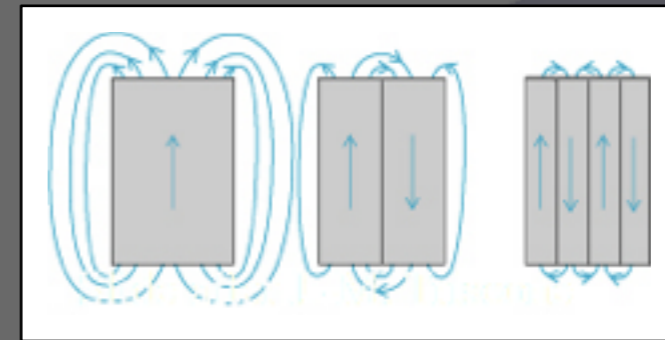


Boundary conditions: screening, dead layers, symmetry

⇒ depolarising field

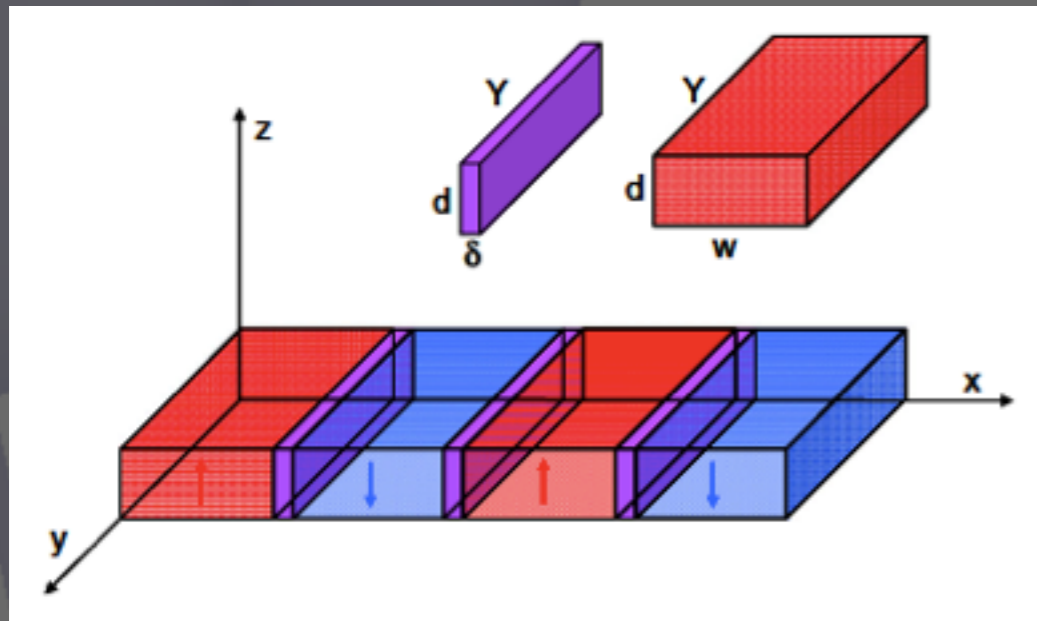
$$\mathbf{E} = -\mathbf{P}/\epsilon$$

⇒ domains



Energy densities per unit area of film  $U_{domain} \sim \sigma_{DPW}$

$$U_{DW} \sim \sigma_{DW}Nd \sim \sigma_{DW}d/w$$



Minimising total energy

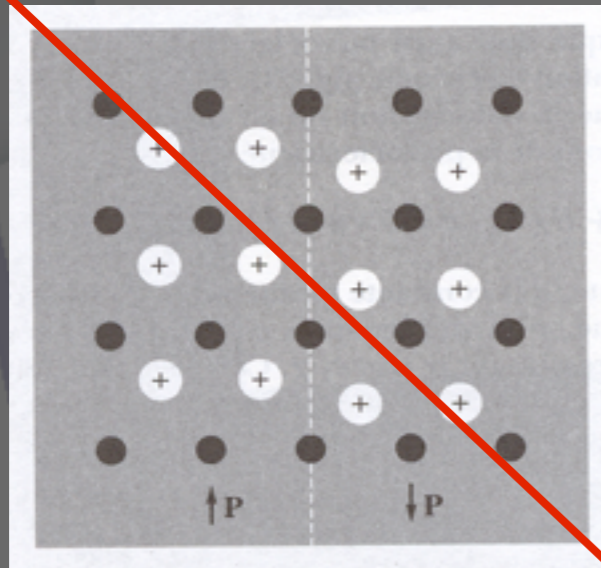
$$w = \left( \frac{\sigma_{DW}}{\sigma_{DP}} d \right)^{1/2}$$

Landau-Lifshitz-Kittel scaling

Landau and Lifshitz, Phys. Zeits. Sowjetunion **8**, 153 (1935)

Kittel, Phys. Rev., **70**, 965 (1946)

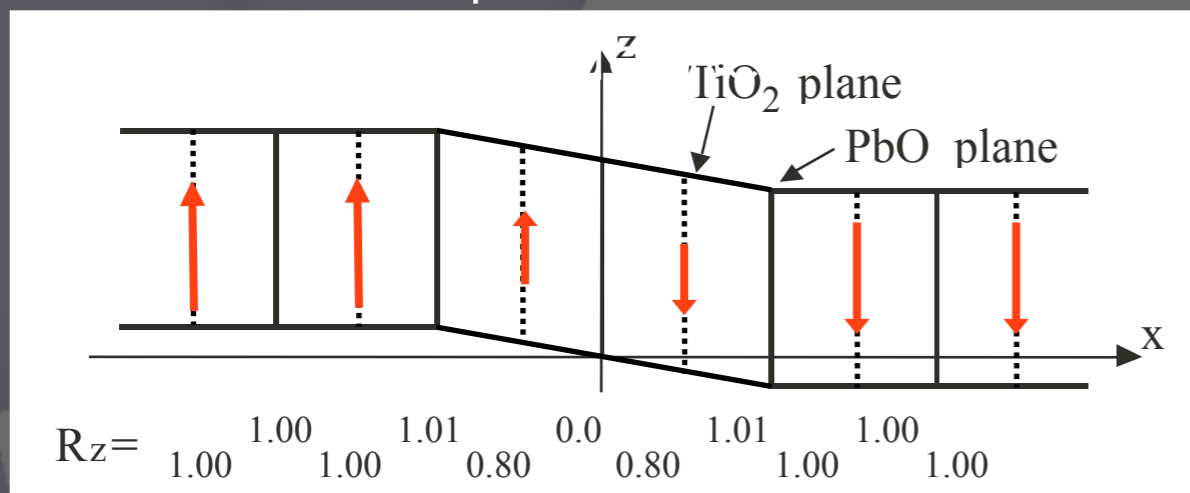
# Domain walls in ferroic materials



Actual physical objects with a finite (very small) width

FE DWs

atomic displacements in lattice

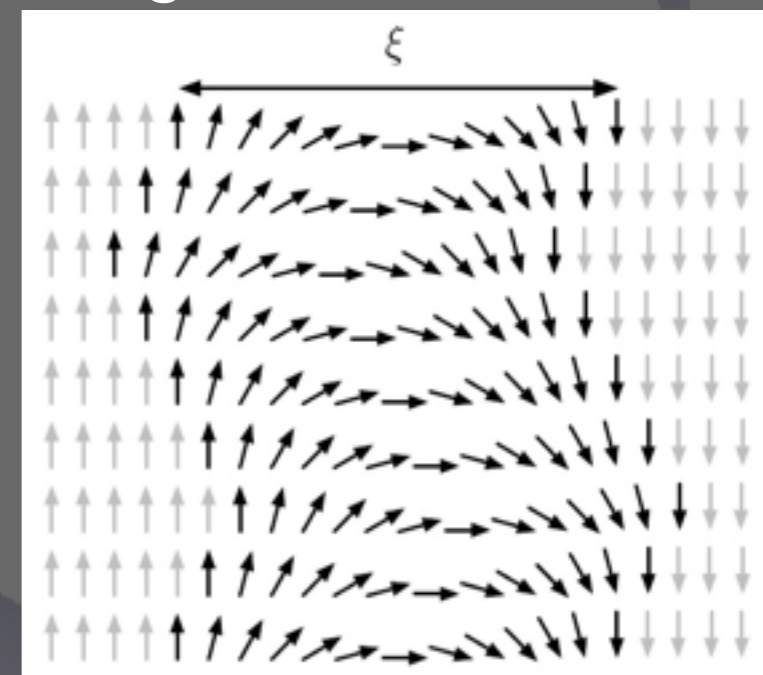


Meyer and Vanderbilt PRB 65, 104111 (2002)

(O) 1 nm

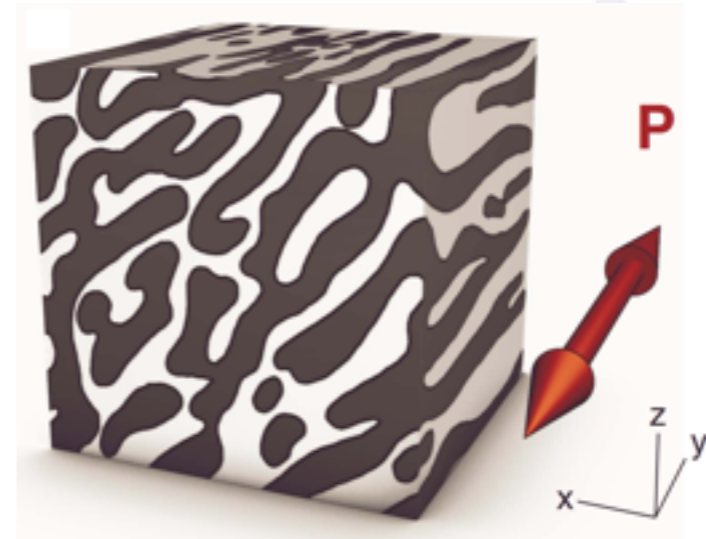
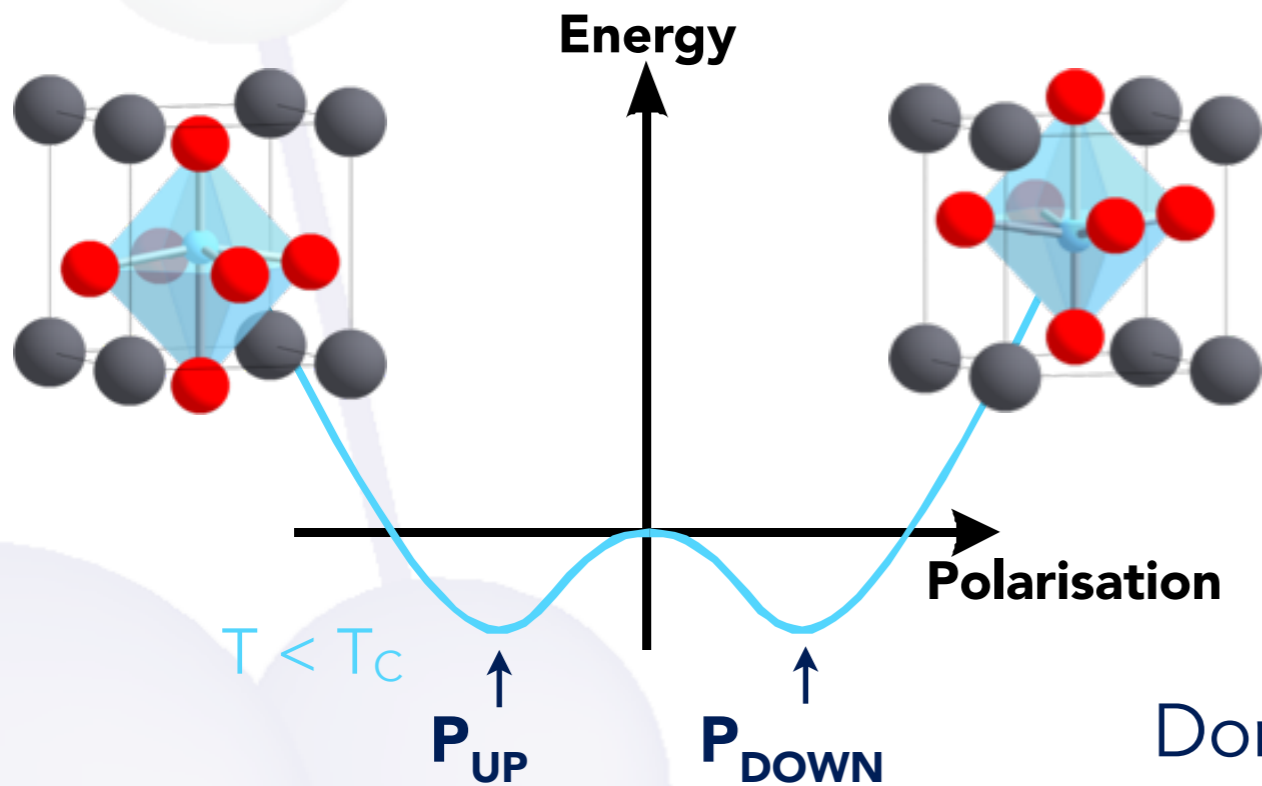
FM DWs

Bloch or Néel walls  
magnetization rotation



(O) 10-100 nm

# Domain walls in ferroelectric materials



Domain walls separate regions with different polarisation orientation  
- and can alter or enhance material properties

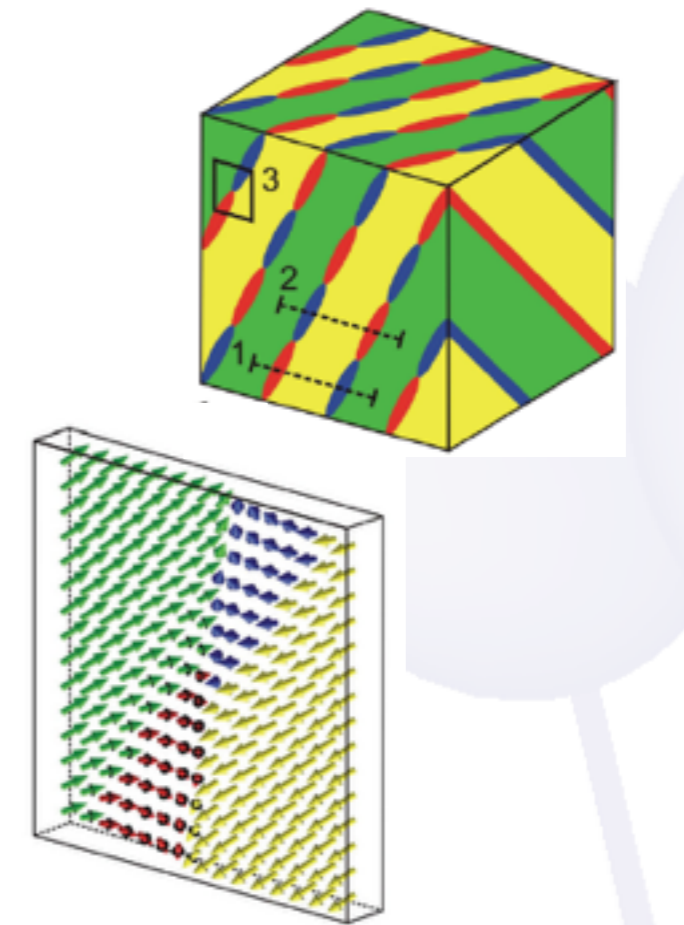
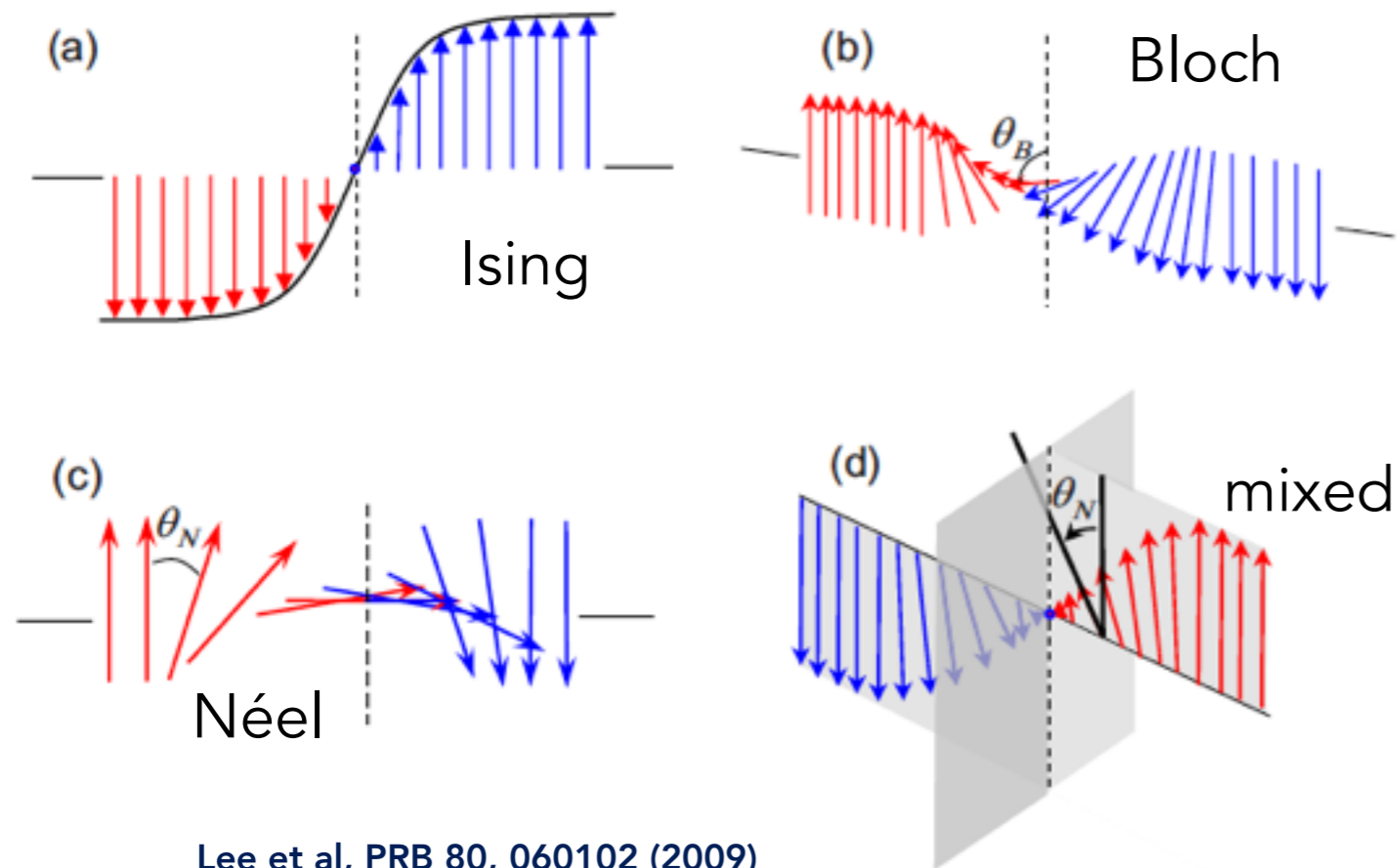
Catalan et al. Rev. Mod. Phys., 84, 119 (2012)  
D. Damjanovic: Ferroelectric Domain Walls

As samples get thinner, more domain walls can be expected

Landau, Lifshitz, Phys. Zeits. Sowjetunion 8, 153 (1935)  
Kittel, Phys. Rev., 70, 965 (1946)

$$w = \left( \frac{\sigma_{DW}}{\sigma_{DP}} d \right)^{1/2}$$

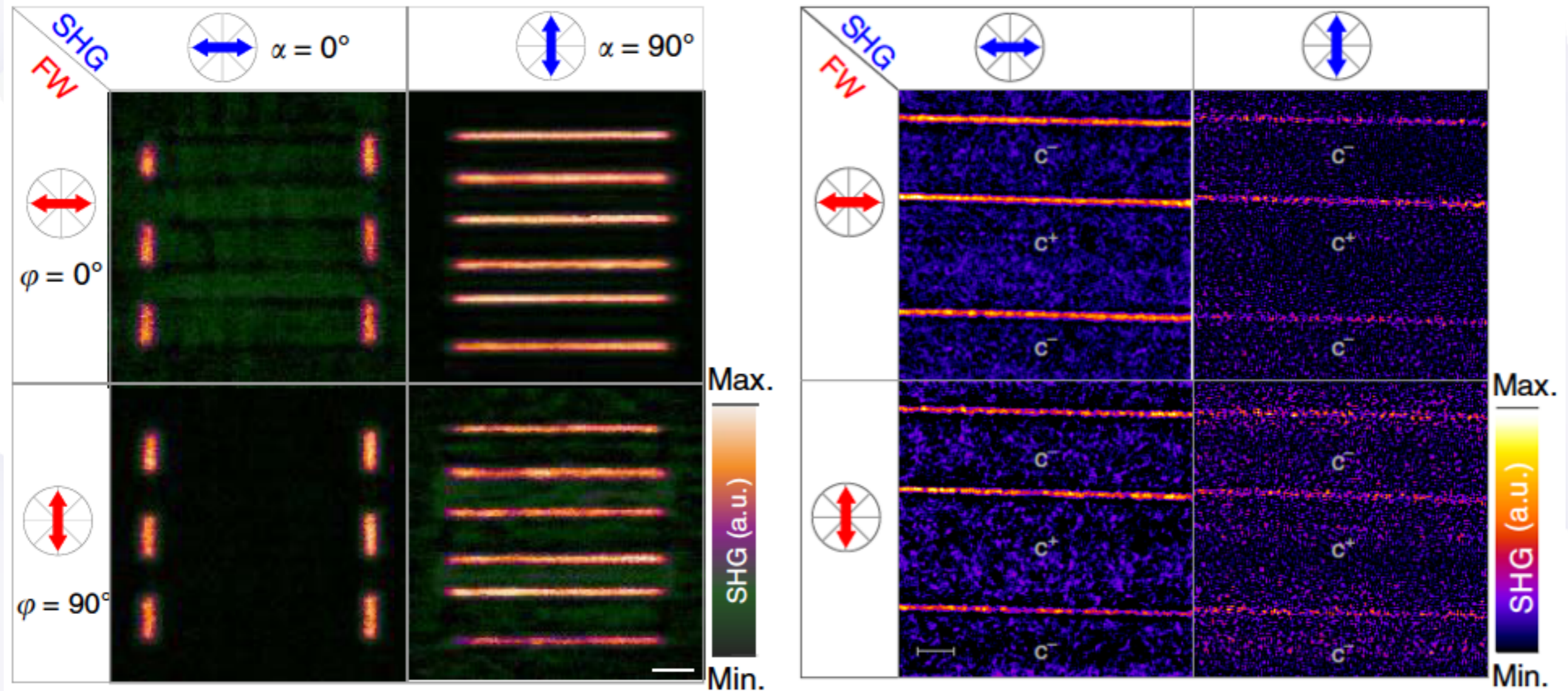
# Complex polarisation textures at domain walls



Predictions of Néel, Bloch and mixed structures in different ferroelectrics

Lajzerowicz and Niez, J. Phys. Lett. 40, 165 (1979)  
Stepkova et al, JPCM 24, 212201 (2012)  
Eliseev et al, PRB 85, 045312 (2012)  
Morozovska, Ferro 438, 3 (2012)  
Wojdel et al, PRL 112, 247603 (2014)

# Complex polarisation textures at domain walls



Néel polarisation at  $180^\circ$  domain walls in PZT

mixed Bloch-Néel polarisation with chirality reversal possible at  $180^\circ$  domain walls in LiTaO<sub>3</sub>

Cherifi et al. Nat. Comm. 8, 15768 (2017)

Wei et al, Nat. Comm. 7, 12385 (2016)

De Luca et al, Adv. Mat. 29, 1605145 (2017)

# Domain walls present novel, highly localised functional properties

Domain walls can show quite different physics from the parent phase

Ferrielectric domain walls in  $\text{CaTiO}_3$

Goncalves-Ferreira et al. PRL (2008)

Conducting domain walls in  $\text{BiFeO}_3$

Seidel, et al. Nat. Mat. 8, 229 (2009)

Photovoltaic domain walls in  $\text{BiFeO}_3$

Yang et al. Nat. Nanotech. (2010)

Magnetism at domain walls (?)

Bartels. et. al J. P. Cond. Mat 15, 957-962 (2003)

Přívratká, Janovec, Ferroelectrics 222, 23 (1999)

Daraktchiev et al. PRB 81, 224118 (2010)

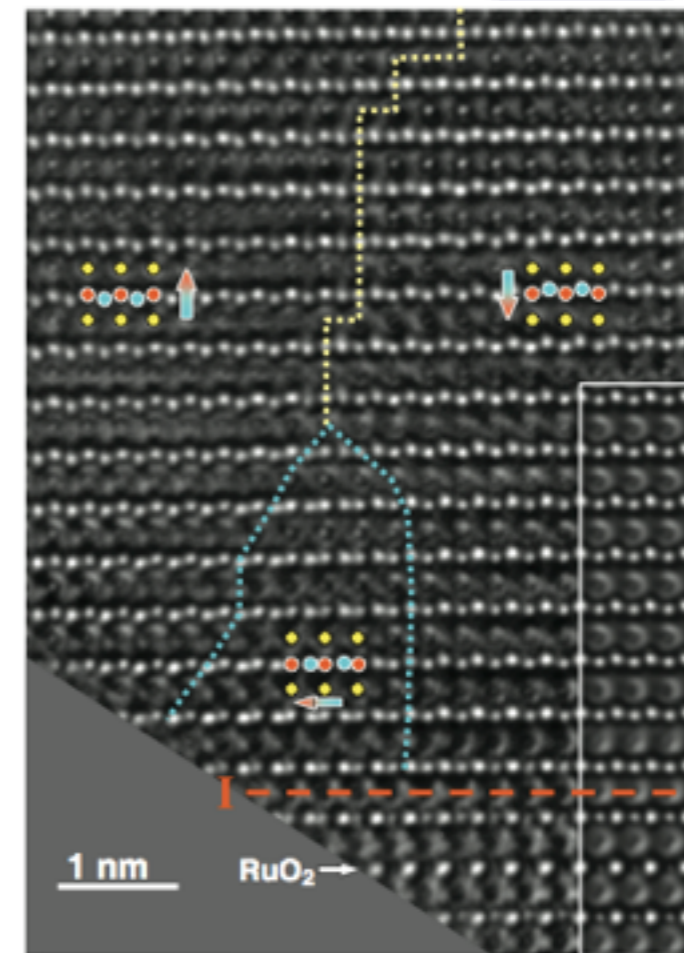
Different polar/structural order

Aguado-Puente and Junquera. PRL 100, 177601 (2008)

Polar domain walls in  $\text{SrTiO}_3$

Zubko. et al. PRL 99, 167601 (2007)

Domain walls are extremely small

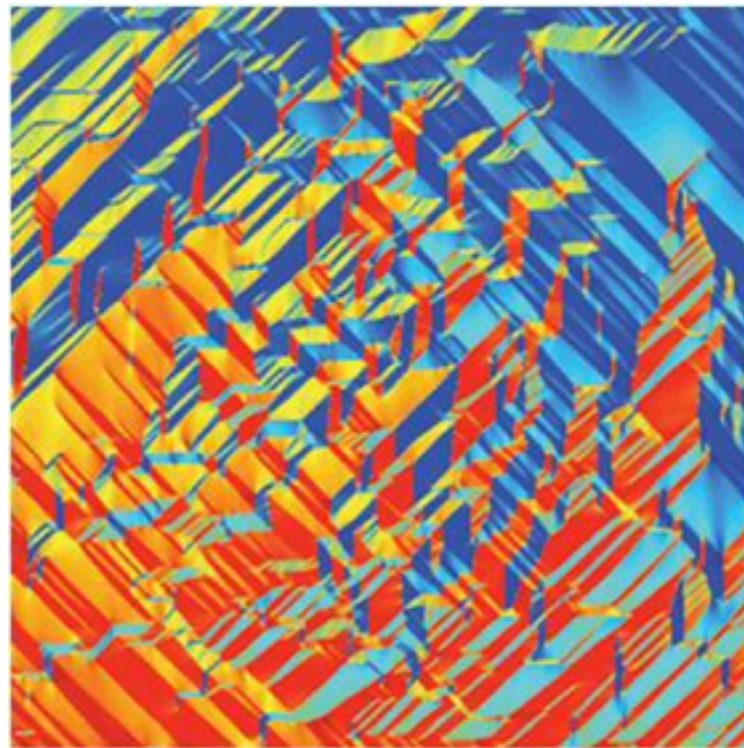


Jia et al. Science 331, 1420 (2011)

Lee et al. PRB 80, 060102 (2009)

# Towards domain wall nanoelectronics

Domain walls can show quite different physics from the parent phase



thanks to J. M. Gregg

Domain walls are extremely small

Parkin et al. *Science* 320, 190 (2008)  
Béa, Paruch. *Nat. Mat.* 8, 168 (2009)  
Salje, *ChemPhysChem* 11, 940 (2010)  
Yang et al. *Nat. Nanotech.* (2010)  
Catalan et al., *Rev. Mod. Phys.* 84, 119 (2012)  
Whyte and Gregg, *Nat. Comm.* 6, 7361 (2015)  
Meier and Selbach, *Nat. Rev. Mater* 7, 157 (2021)

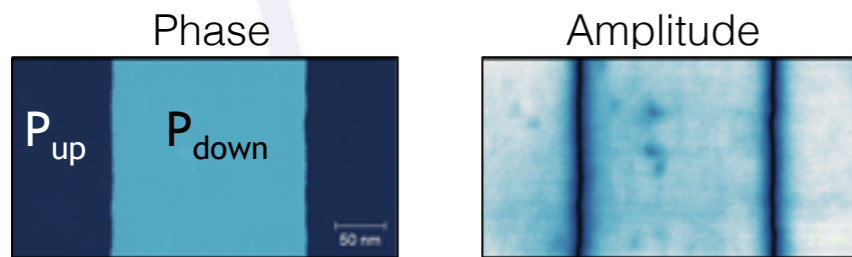
Can we use ferroelectric domain walls as active device components?

Need nanoscale access to probe/control their properties

Need to understand their fundamental behaviour

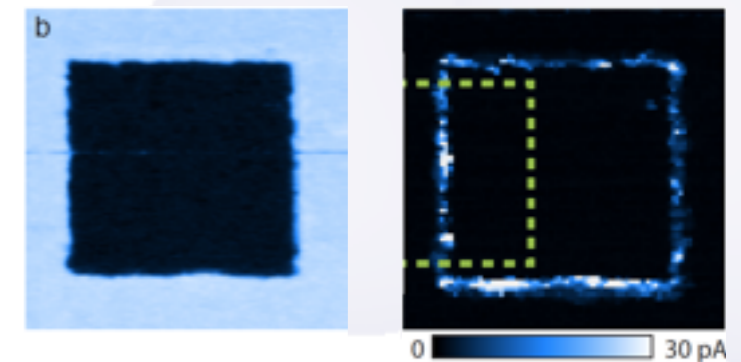
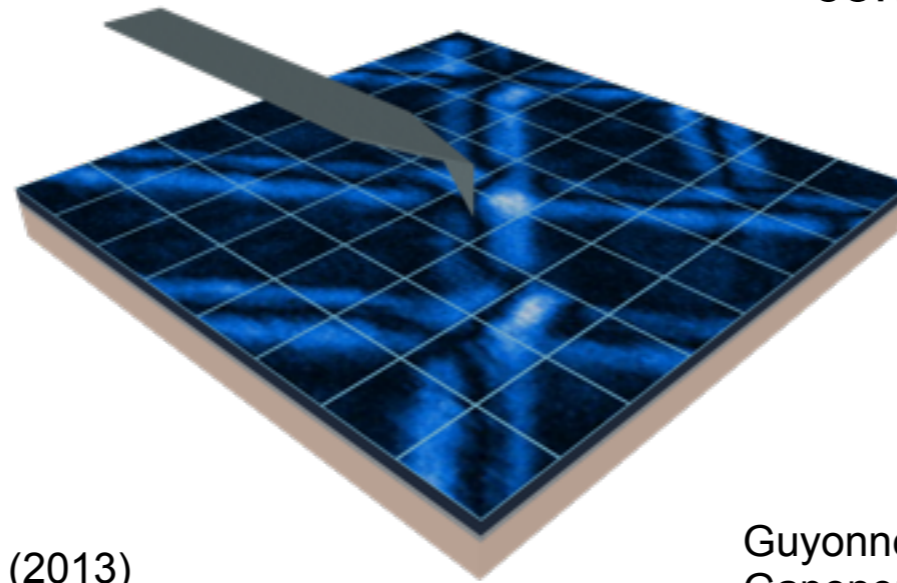
# Mapping polarisation and functional properties with scanning probe microscopy

## piezoresponse force microscopy PFM



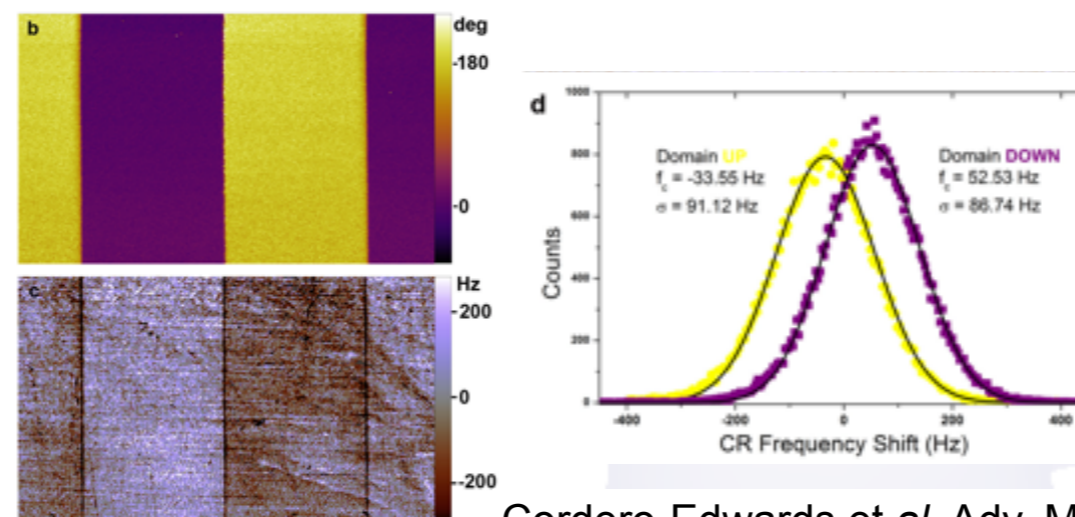
Tuckmantel et al, PRL 126, 117601 (2021)  
Guyonnet et al. APL 95, 132902 (2009)  
Guyonnet et al. PRL 109, 147601 (2012)  
Ziegler et al. PRL 111, 247604 (2013)  
Paruch, Guyonnet, C.R.A.S. Physique 14, 667 (2013)

## conductive atomic force microscopy CAFM



Guyonnet, Gaponenko et al, Adv. Mat. 23, 5377 (2011)  
Gaponenko et al. APL 106, 162902 (2015)

## contact resonance frequency microscopy CRFM

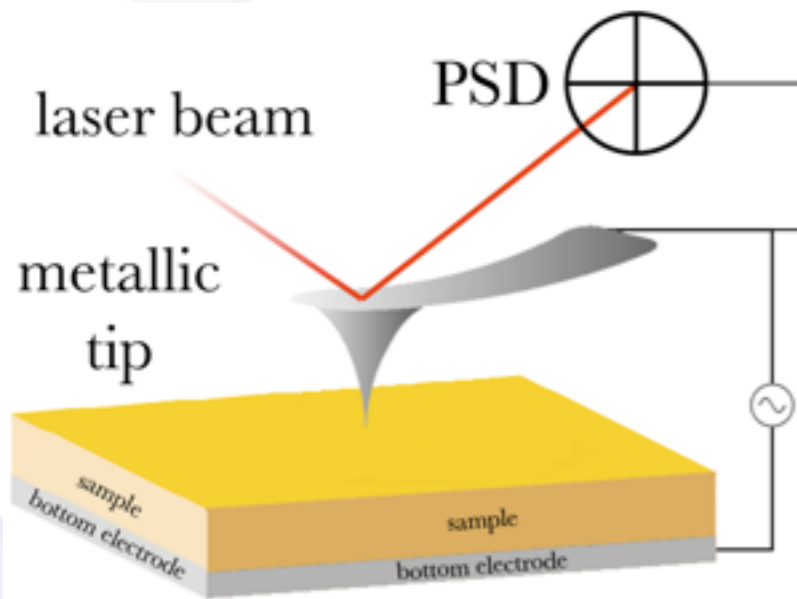


Cordero-Edwards et al. Adv. Mat. 29, 1702210 (2017)  
Stefani et al. PRX 10, 041001 (2020)



# Imaging domains and domain walls : PFM

## Piezoresponse Force Microscopy

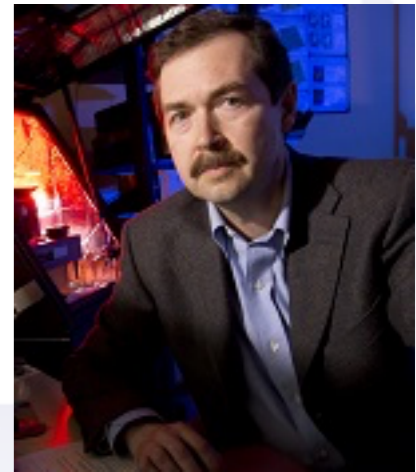


**Piezoresponse** : first harmonic component of tip deflection

lock-in amplifier —  $A = A_0 + A_{1\omega} \cos(\omega t + \varphi)$

induced by  $V_{tip} = V_{dc} + V_{ac} \cos(\omega t)$

Deformation is given by the piezoelectric tensor :  $X_j = d_{ij} E_i$



Alexei Gruverman

ruverman et al. APL 69, 3191 (1996)

Eng et al. APL 74, 233 (1999)

Tybell et al. APL 75, 856 (1999)

Eng et al. APL 74, 233 (1999)

Hong et al. JAP 89, 1377 (2001)

Kalinin et al. PRB 63, 125411 (2001)

Harnagea et al. APL 83, 338 (2003)

Jesse et al. RSI 77, 073702 (2006)

Jesse et al. Nanotech. 18, 435503 (2007)

Morozovska et al. PRB 80, 214110 (2009)

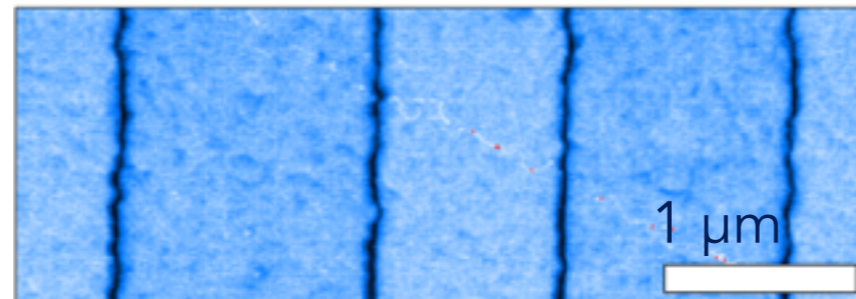
Johann et al. PRB 81, 094109 (2010)

Balke et al. ACS Nano 8, 10229 (2014)

PFM phase



PFM amplitude



PFM has become a key tool for nanoscale studies of ferroelectrics

# Outline

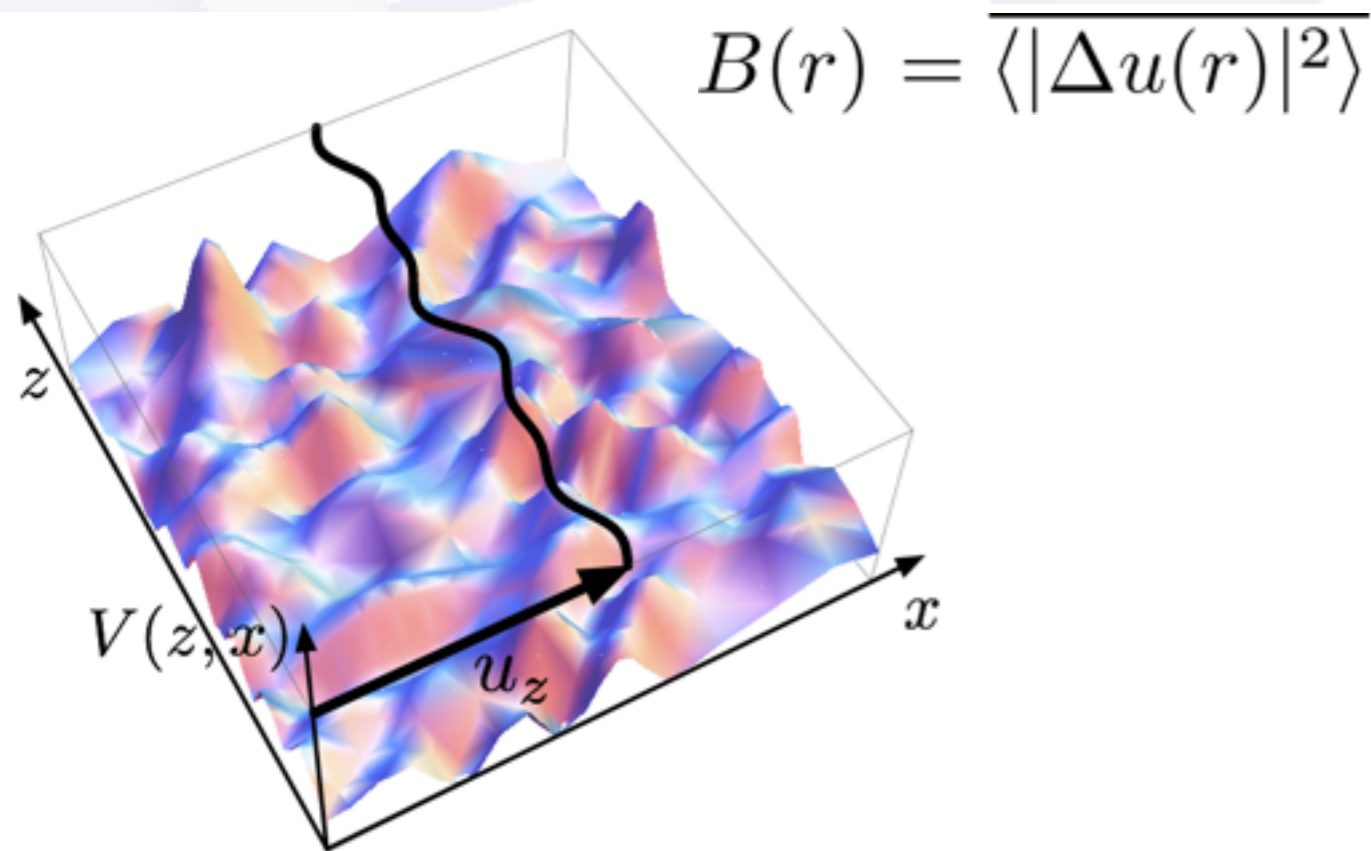
Ferroelectric domain walls as a disordered elastic system  
untangling the effects of defects and surface adsorbates

(Roughness and dynamics of epithelial cell fronts)  
different regimes to identify characteristic lengthscales

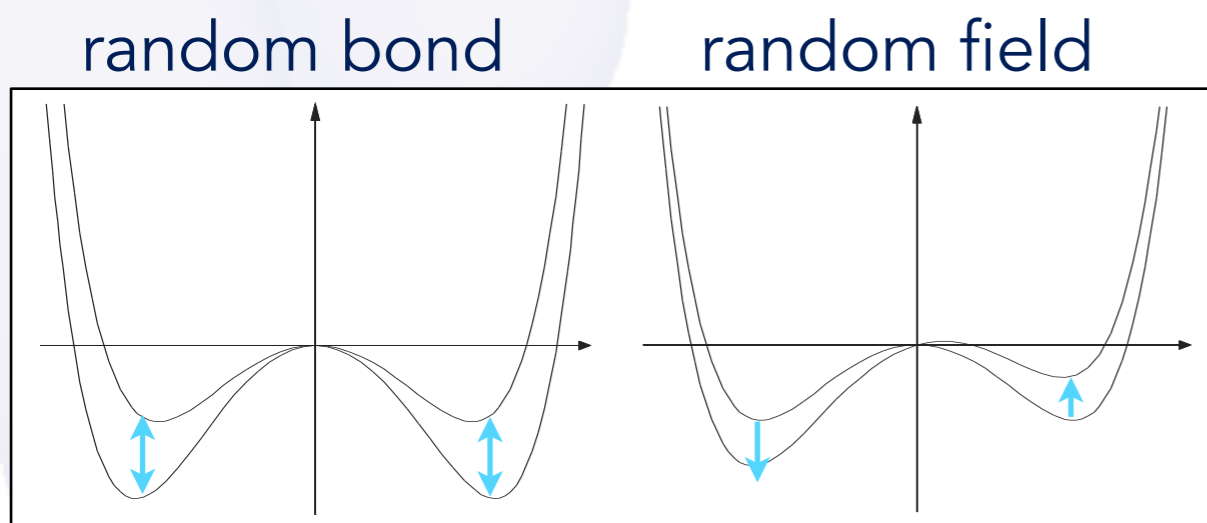
*Every wall is a door*

Emerson

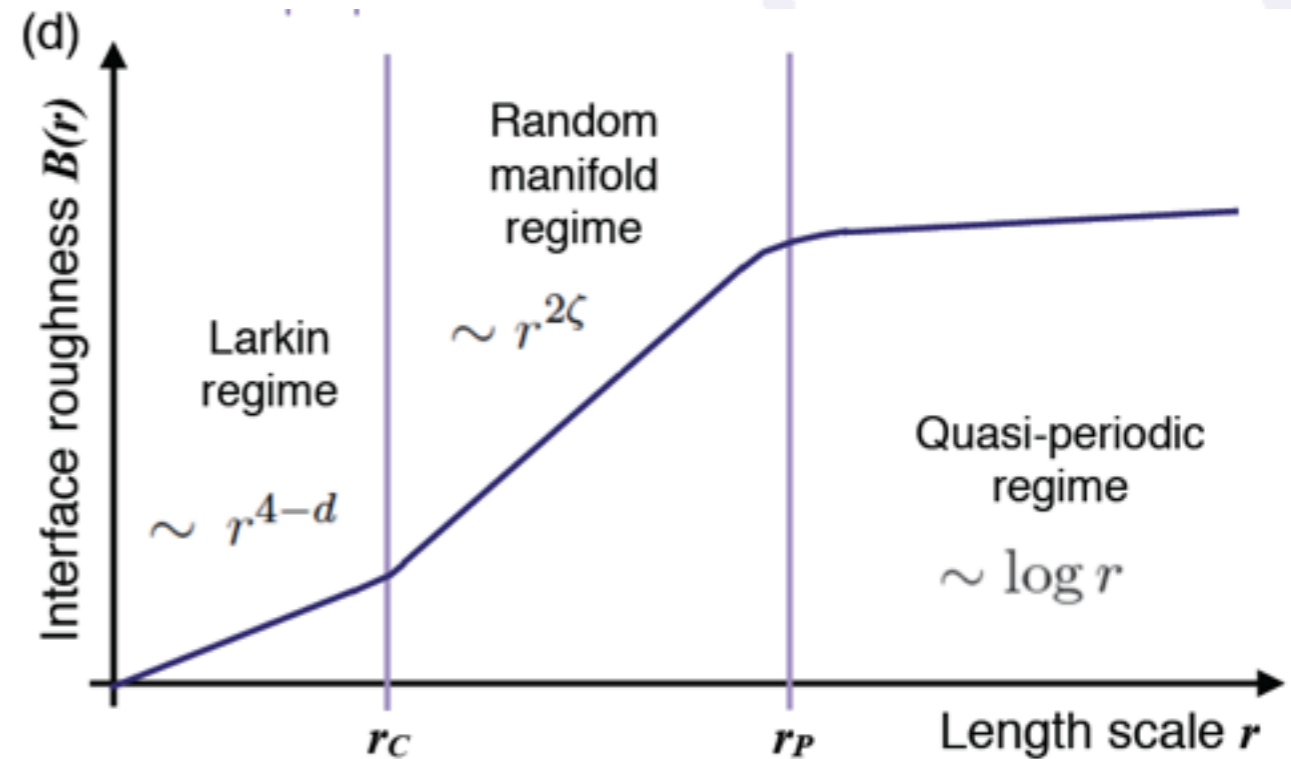
# Characteristic self-affine roughening of interface



Agoritsas, Phys. B 407, 1725 (2012)



Paruch, Guyonnet, C.R.A.S. Physique 14, 667 (2013)



$$\zeta_{TH} = 1/2 \quad (d = 1)$$

$$\zeta_{RB} = 2/3 \quad (d = 1)$$

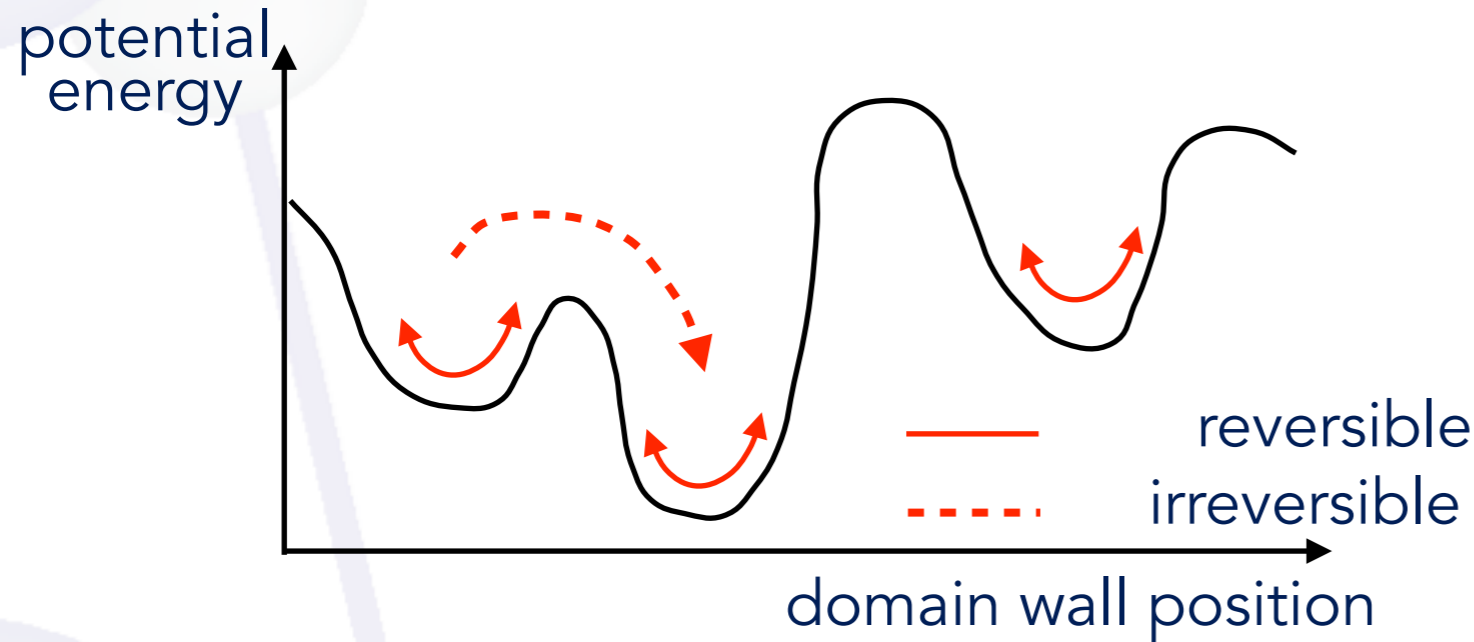
$$\zeta_{RB} \sim 0.2084 \quad (4 - d_{eff})$$

$$\zeta_{RF} = (4 - d_{eff}) / 3$$

Dimensionality and disorder determine roughness scaling

# Complex dynamic response of interface

Paruch, Guyonnet, C.R.A.S. Physique 14, 667 (2013)

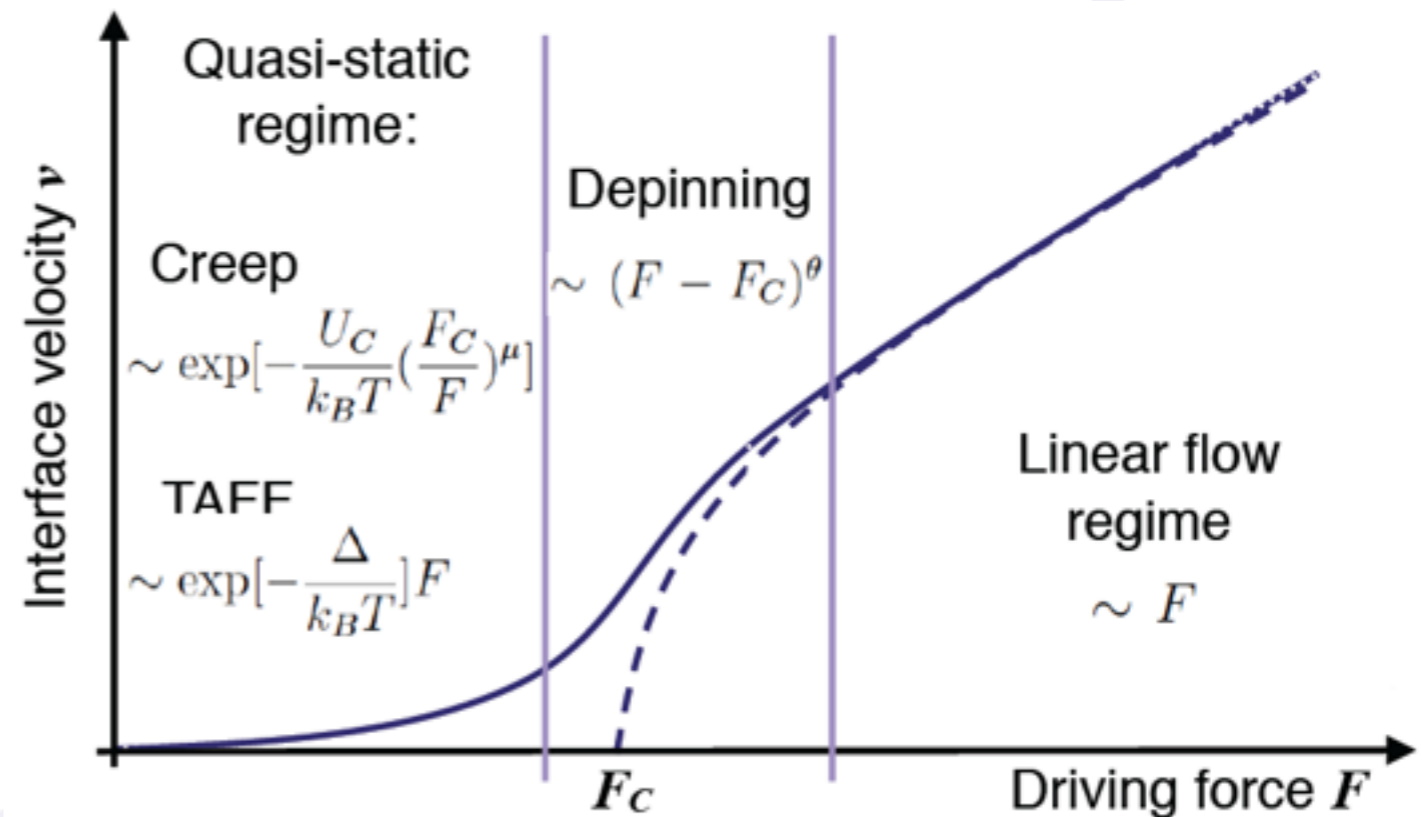


Damjanovic, Rep. Prog. Phys. 61, 1267 (1998)

Interface has to move through fluctuations in potential energy landscape

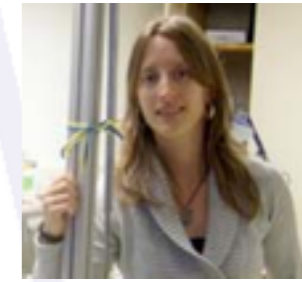
Dimensionality and disorder determine creep response

$$\mu = \frac{d_{\text{eff}} - 2 + 2\zeta}{2 - \zeta}$$



# Measuring domain wall roughness and dynamics

Paruch, Guyonnet, C.R. Physique 14, 667 (2013)

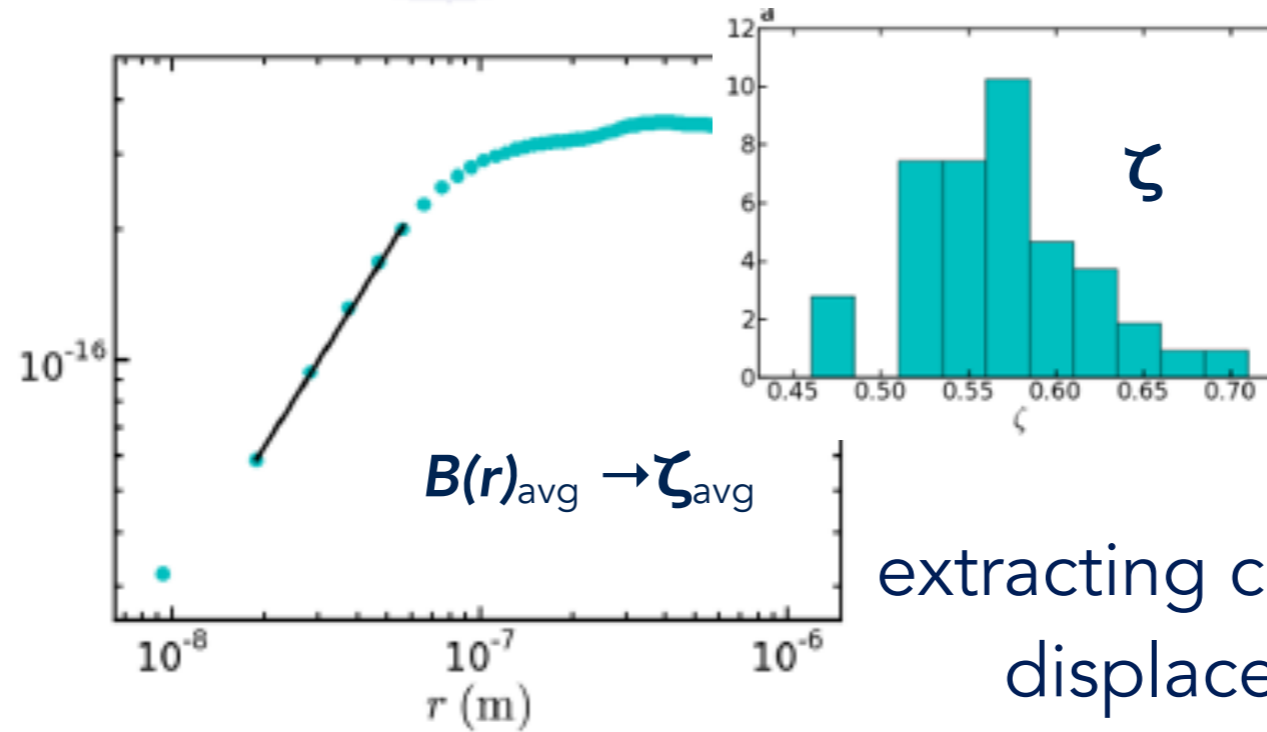
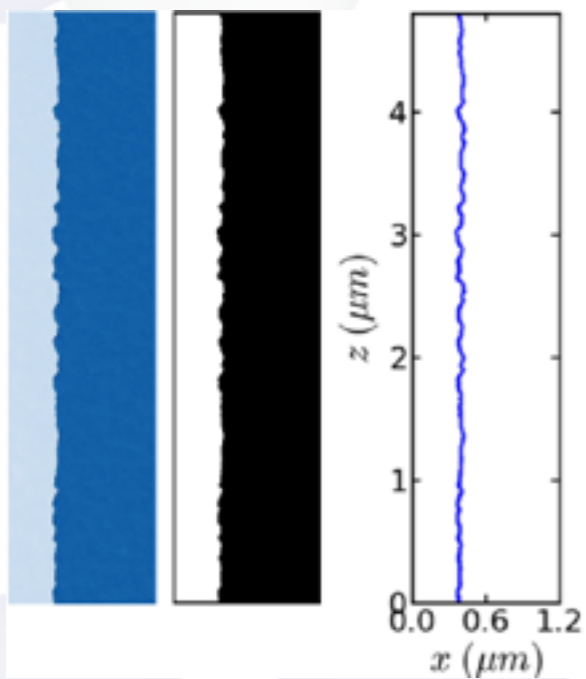


Jill Guyonnet

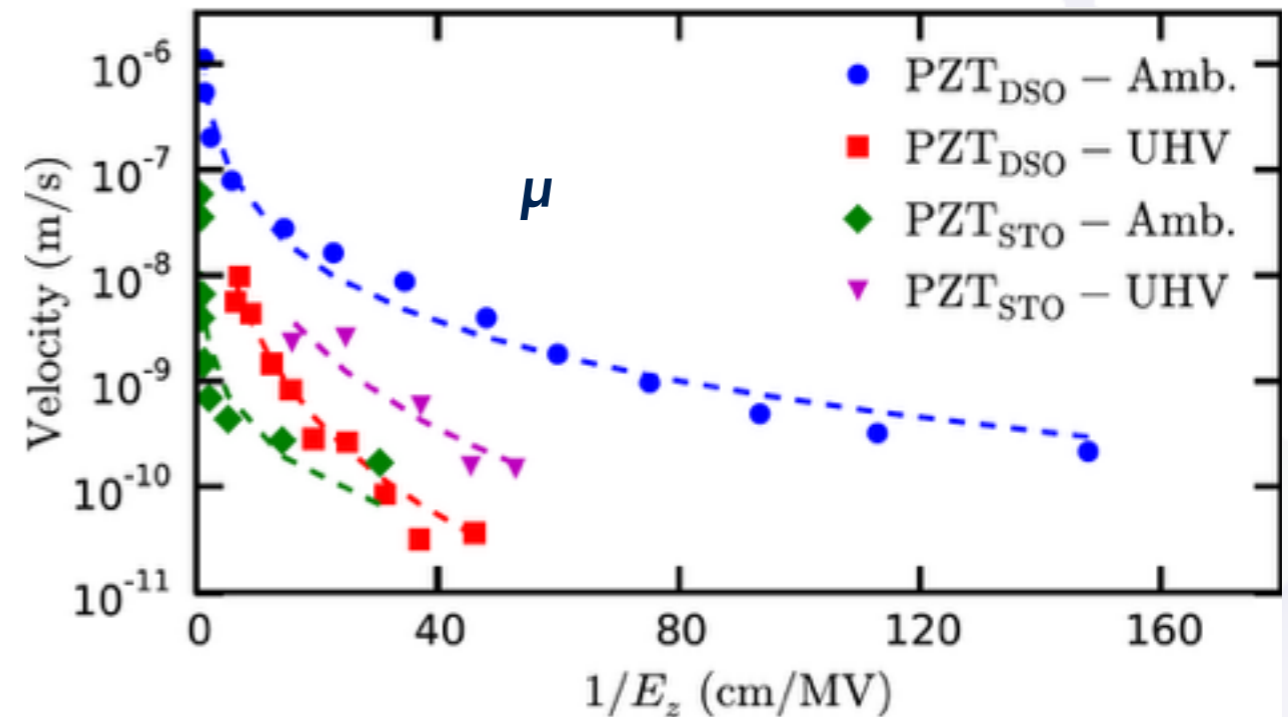
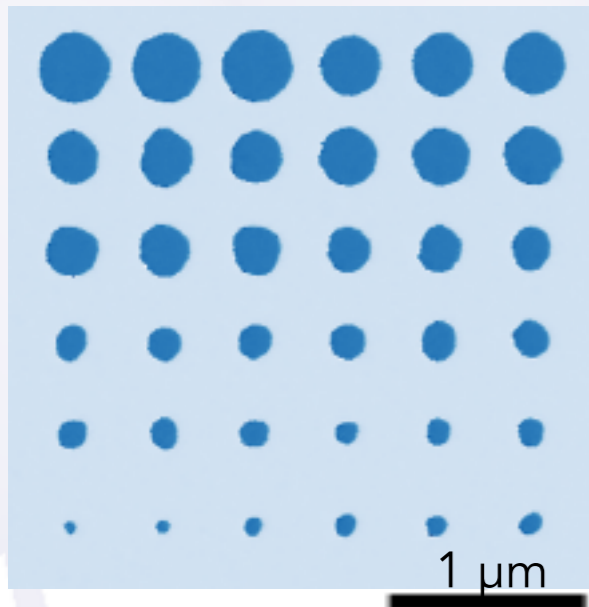


Benedikt Ziegler

mapping DW position



extracting correlations of relative displacements along DW

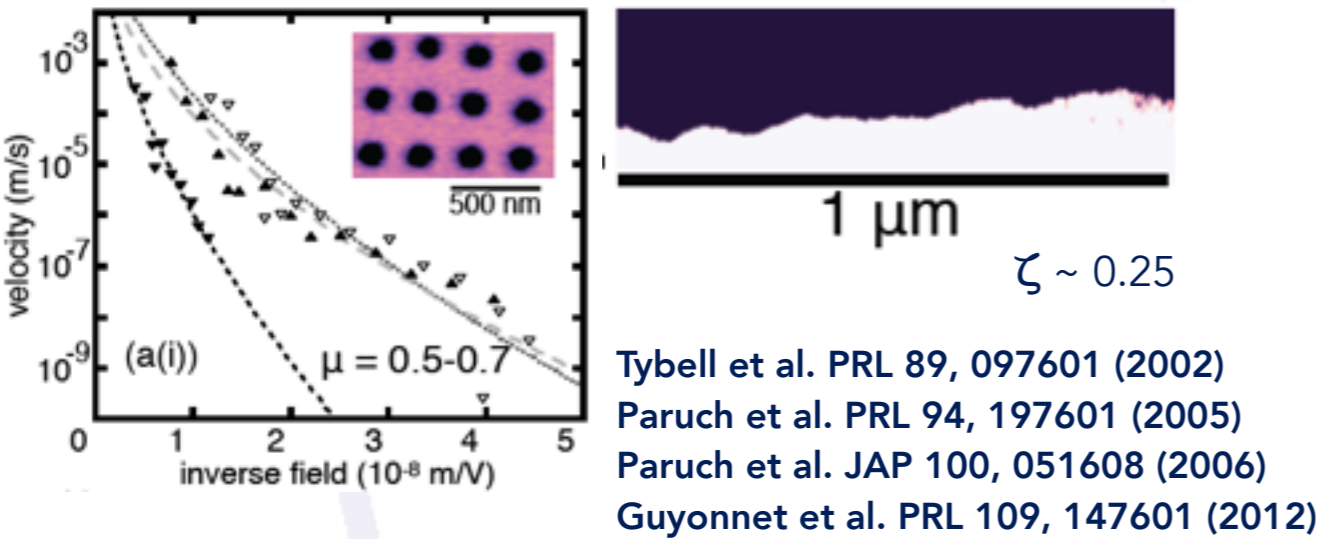


extracting electric field driven DW dynamics

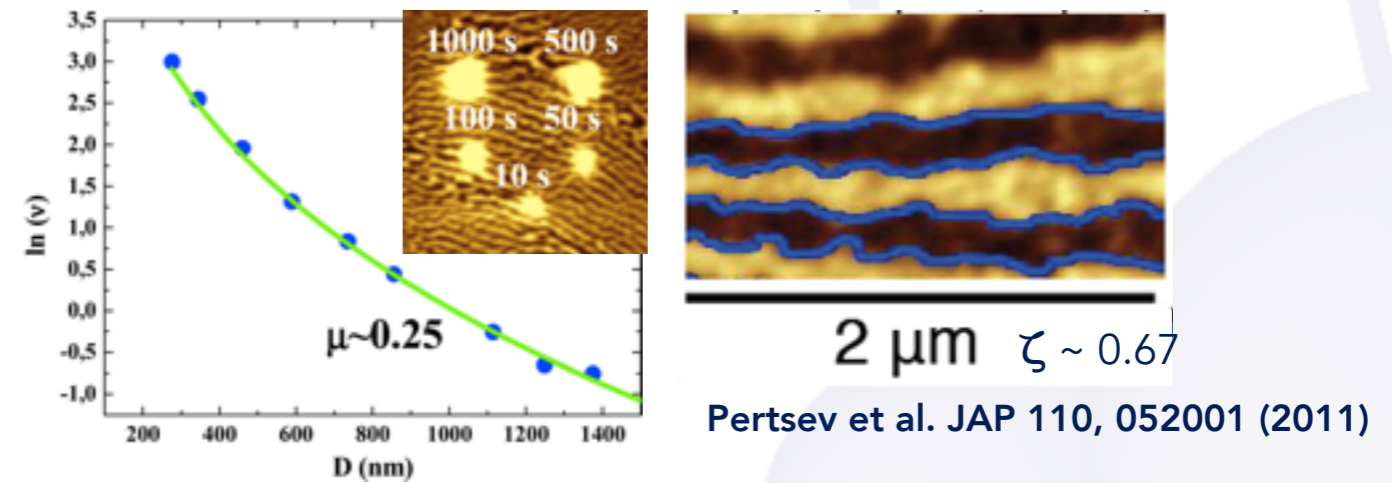
$$v(r) = \frac{r_{n+1} - r_n}{t_{n+1} - t_n} \quad \text{vs.} \quad E_z(r)$$

# A universal behaviour in ferroelectrics

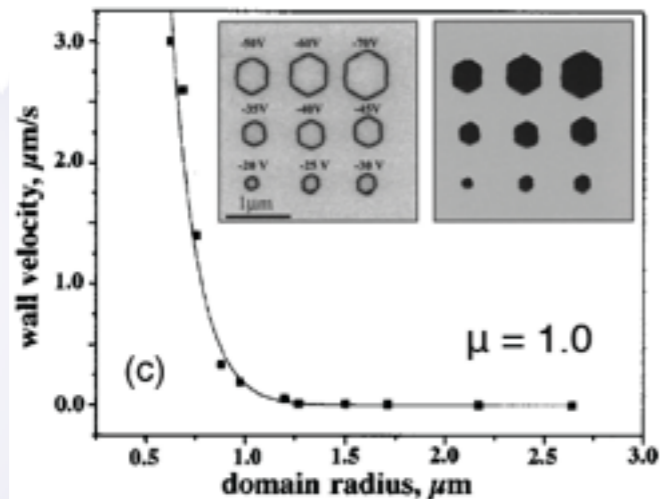
## written domain walls



## intrinsic domain walls

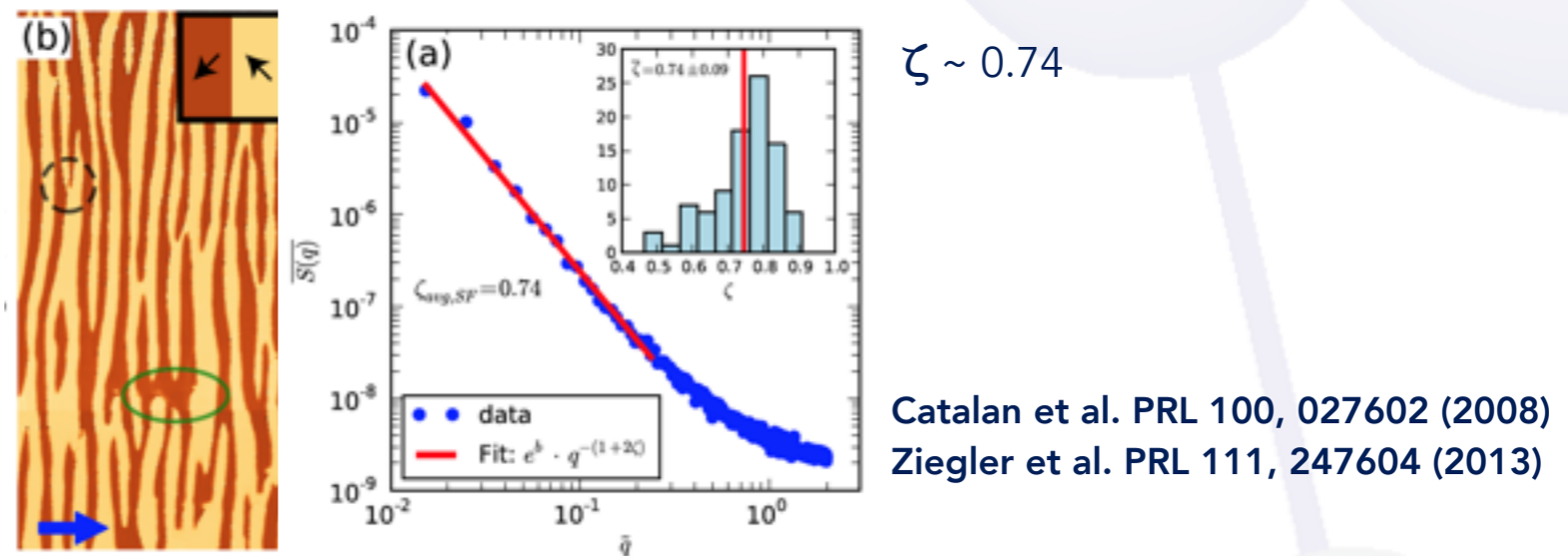


## domain walls in single crystals



Rodriguez et al. APL 86, 012906 (2005)

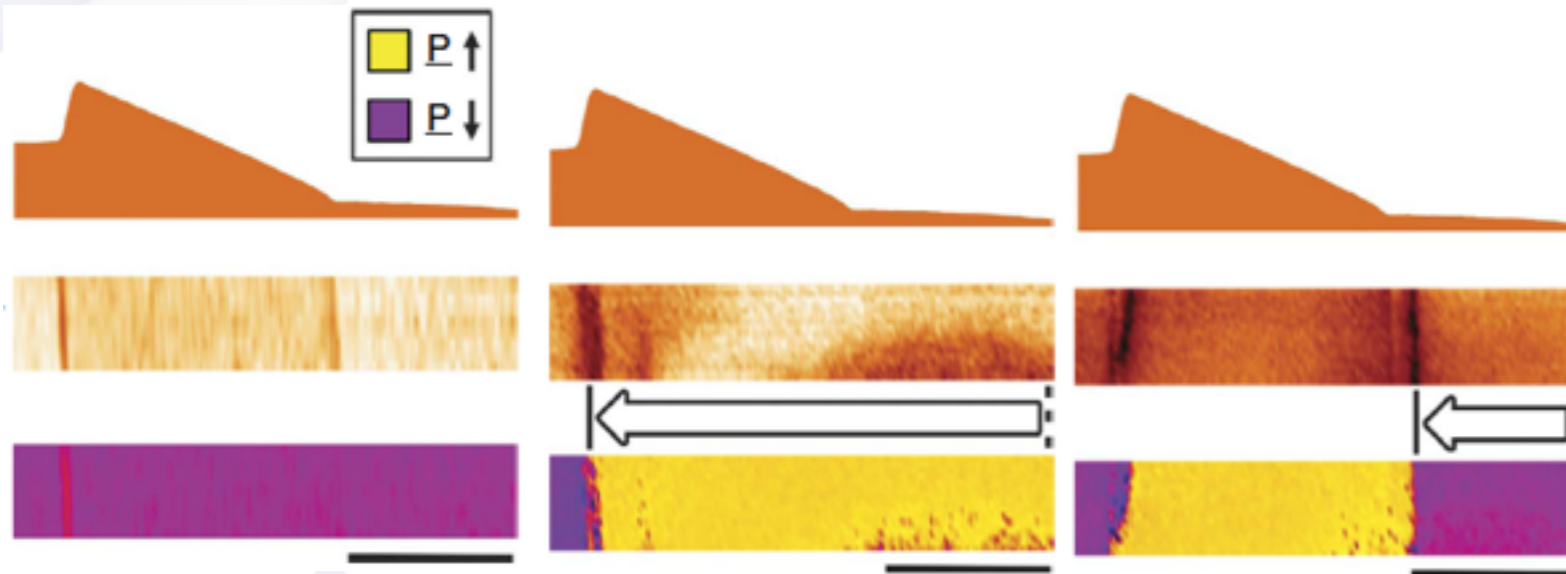
## multiferroic domain walls



Scaling behaviour with characteristic roughness exponent  $\zeta$

Highly nonlinear dynamic response with creep exponent  $\mu$

# Artificial pinning sites and engineering motion

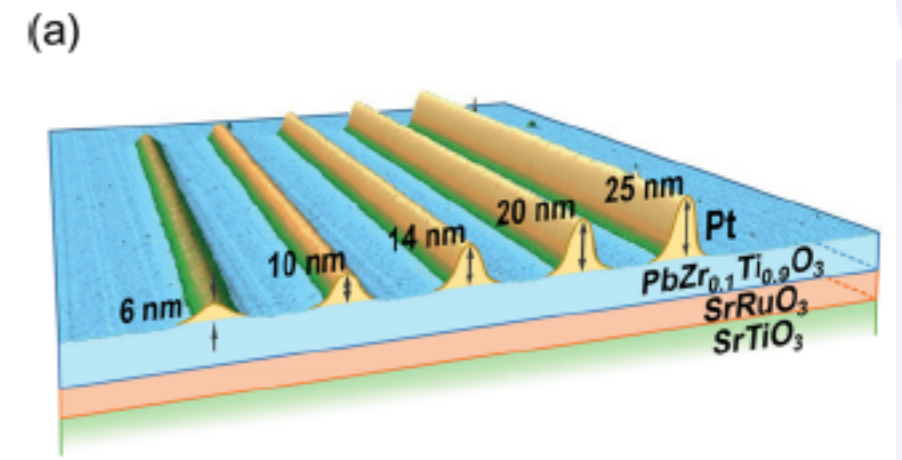
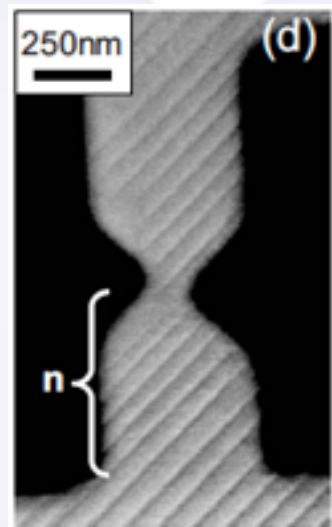


Whyte and Gregg. Nat. Comm. 6, 7361 (2015)

(anti)notches and sawtooth diodes  
to control DW pinning in  
nanofabricated BaTiO<sub>3</sub> lamellae

McMillan et al. APL 96, 042904 (2010)

McQuaid et al. NL 10, 3566 (2010)



McGilly et al, Nano Lett 16, 68 (2016)

McGilly et al, Nat. Nanotech 10, 145 (2015)

mobility control via  
electrode conductance

Towards domain wall nanoelectronics

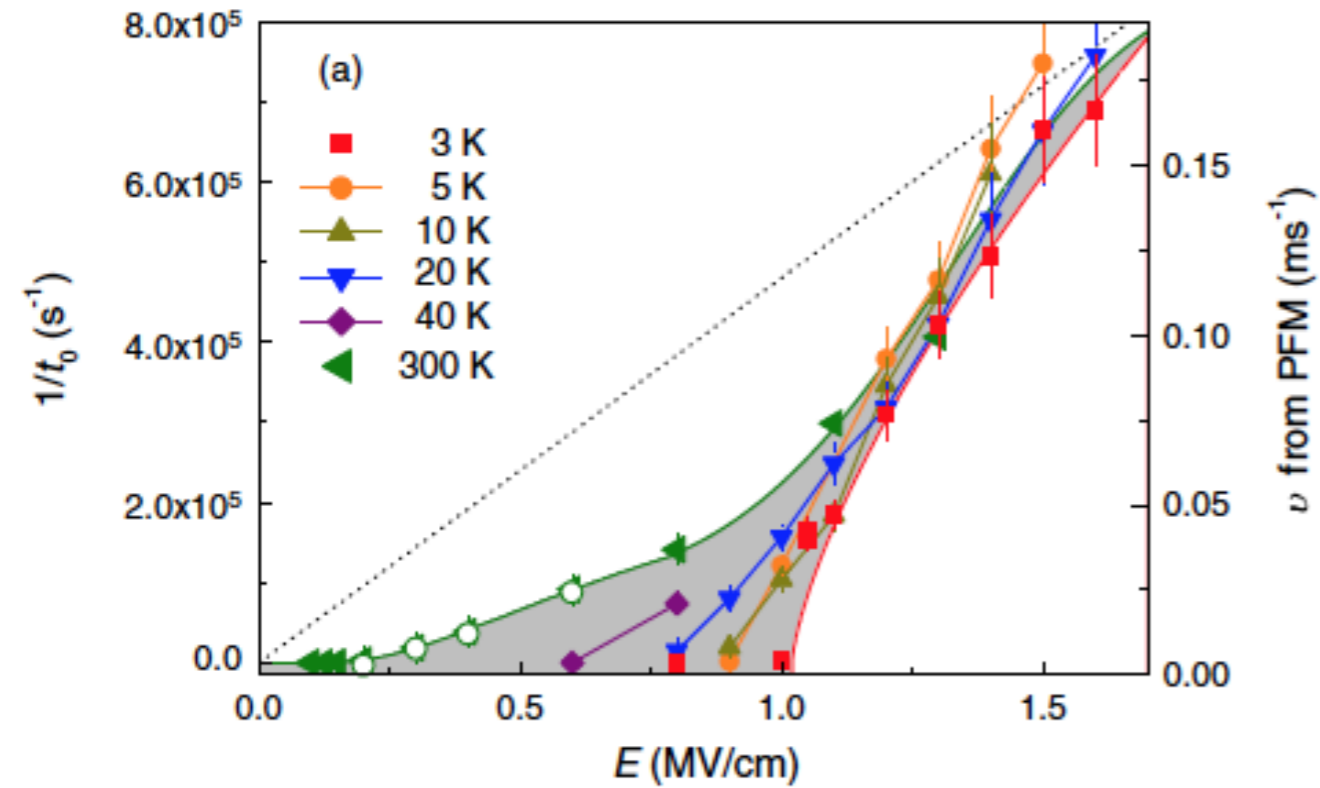
Béa and Paruch Nat. Mat. 8, 168 (2009)

Salje ChemPhysChem 11, 940 (2010)

Yang et al. Nat. Nanotech. (2010)

Catalan et al. Rev. Mod. Phys. 84, 119 (2012)

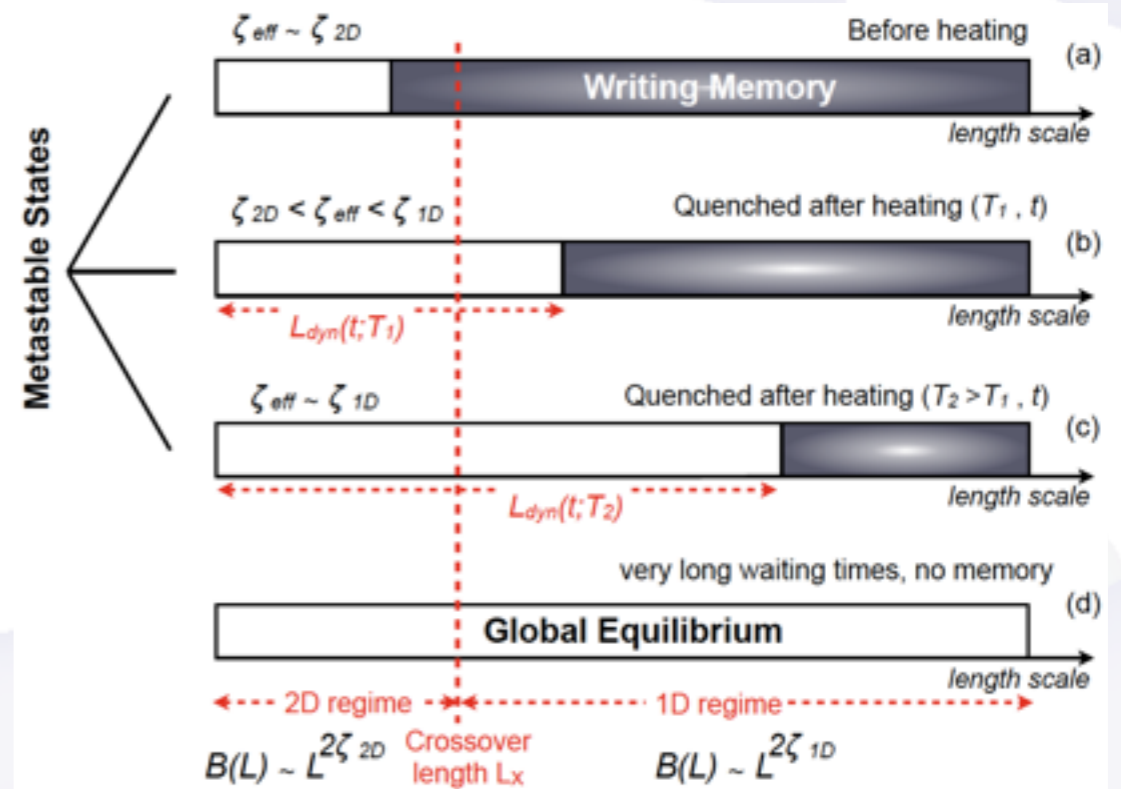
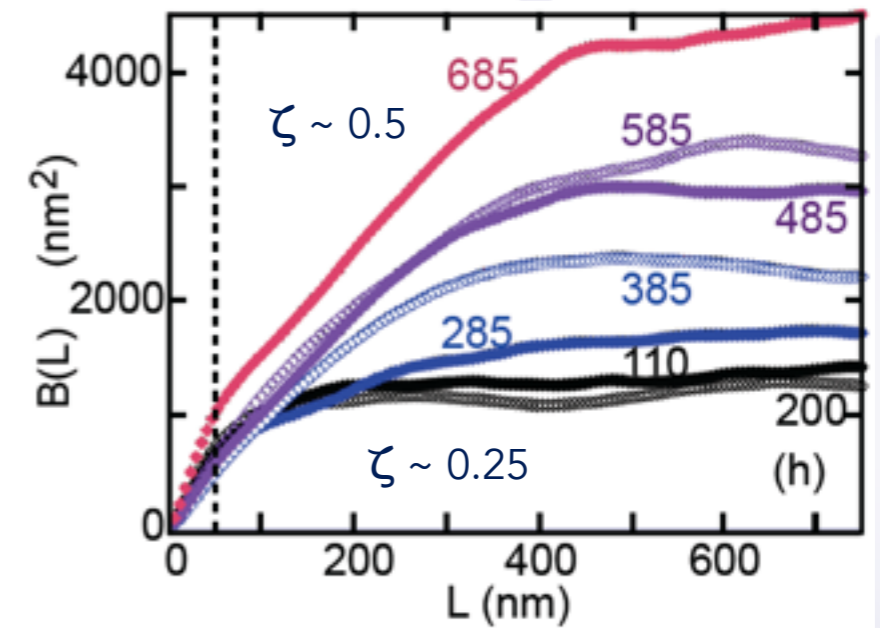
# Moving away from equilibrium



Jo, et al. PRL 102, 045701 (2009)

exploring depinning

ageing and memory effects  
after thermal quenching



Paruch, et al. PRB 85, 214115 (2012)



# Nanoscale studies of individual domain walls, switching events, and their global contribution

Want to correlate DW structure and defect interactions (specific, local) with dynamics/roughness (statistical, global) and properties (functional)

high-resolution mapping of DW evolution over long duration

Tukmantel et al. PRL. 126, 117601 (2021)  
Gaponenko, Tückmantel et al, Sci. Rep 7, 669 (2017)

correlate structural and functional measurements at multiple length scales

Croes et al., Adv. Phys. Res. 2, 2200037 (2023)  
Weymann et al. PRB 106, L241404 (2022)  
Gaponenko et al., Sci. Rep. 12, 165 (2022)  
Musy, Bulanadi et al. Ultramicroscopy 228, 113345 (2021)  
Cherifi-Hertel et al. Nat. Comm. 8, 15768 (2017)

identify physically relevant regimes/behaviours

Gaponenko et al. npj Comp. Mat. 7, 163 (2021)  
Griffin, Gaponenko et al, Adv. Mat. 32, 2002425 (2020)  
Domingo et al., Nanoscale 11, 17920 (2019)  
Griffin, Gaponenko et al, npj Comp. Mat. 5, 85 (2019)



Iaroslav Gaponenko



Philippe Tückmantel



Ralph Bulanadi



Loïc Musy



Christian Weymann



Kumara Cordero-Edwards

<https://github.com/paruch-group>

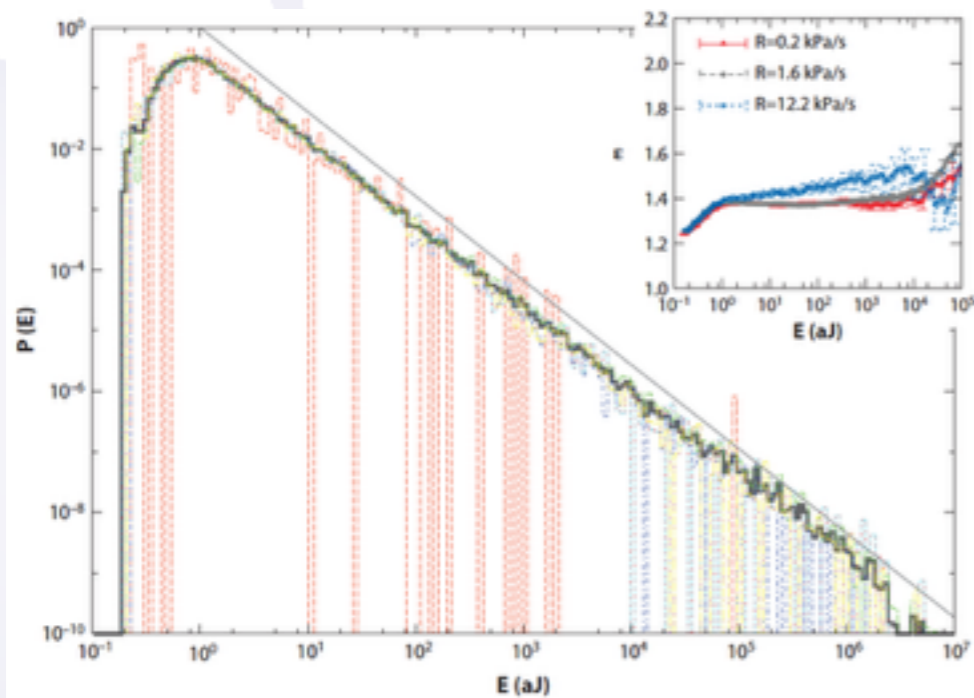
# Bridging approach - linking the local and global switching dynamics in ferroelectrics



Eckhart Salje

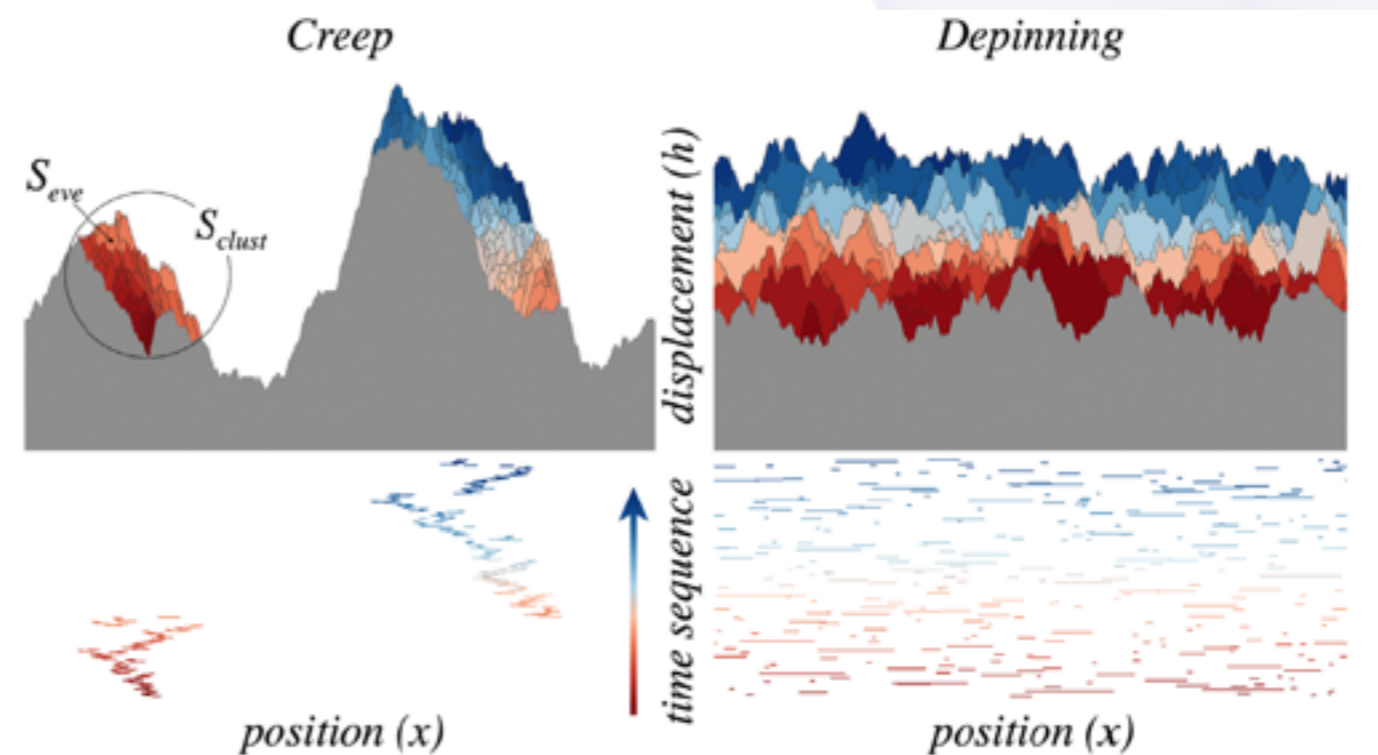


Thierry Giamarchi



Salje, Dahmen. *Ann. Rev. Cond. Mat. Phys.* 5, 233 (2014)

Size/Power distribution of slip avalanches in compressed porous media and ferroelastic crystals



Ferrero et al. *PRL* 118, 147208 (2017)

Distinguishing creep and depinning from avalanche statistics

# PZT thin films with different defect densities

Tuckmantel et al. PRL. 126, 117601 (2021)

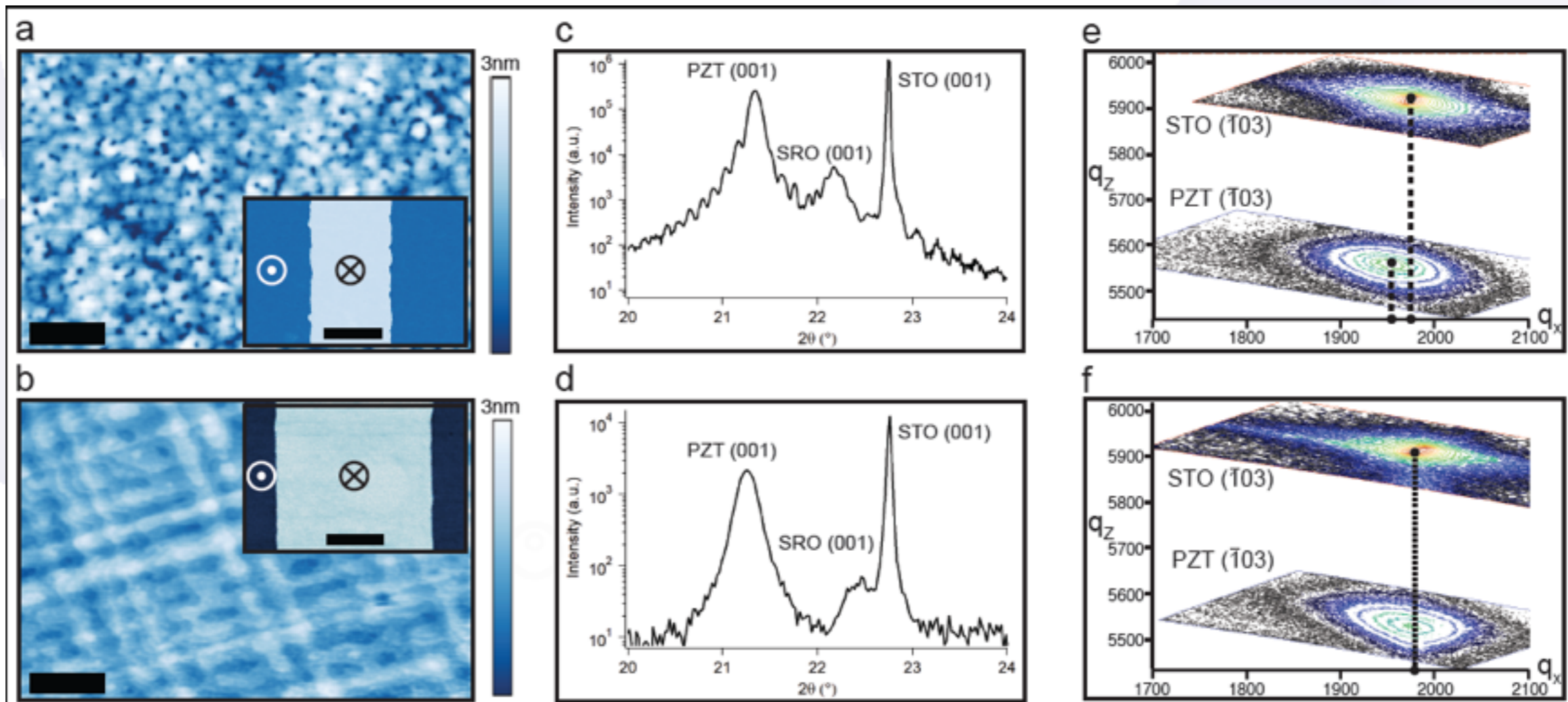


Philippe Tückmantel

Control density and type of defects during thin film growth

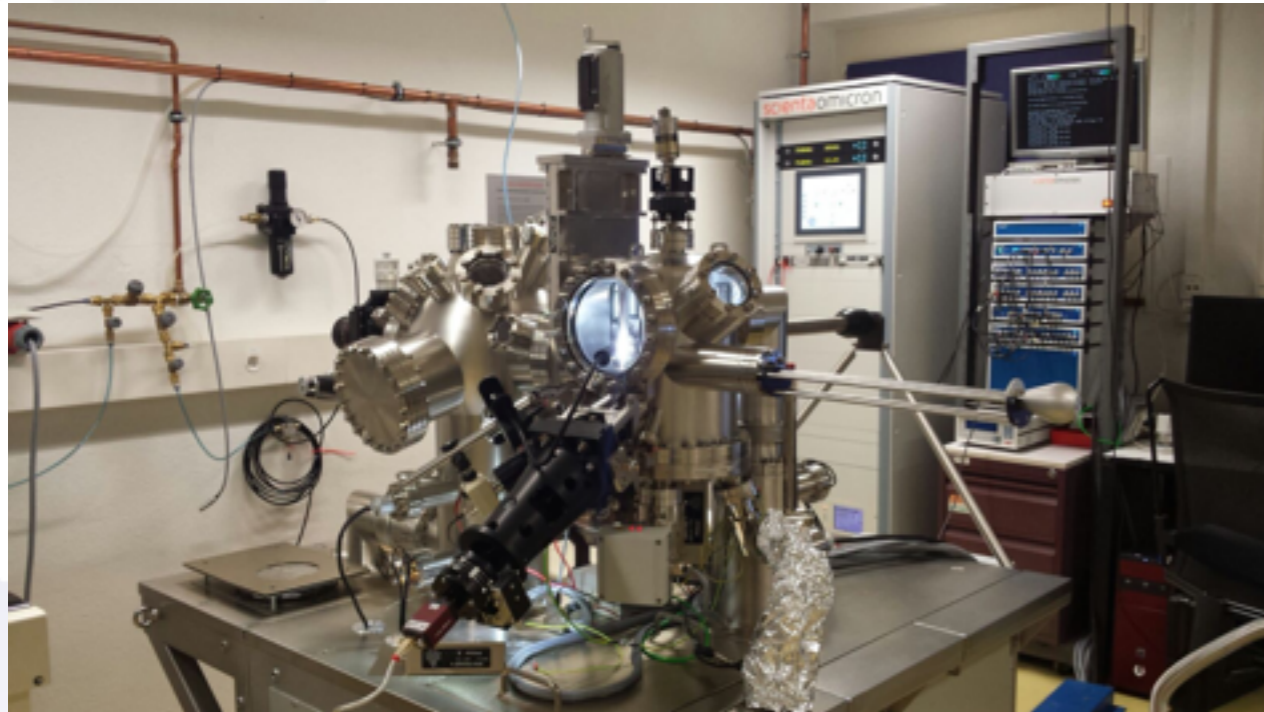
rough AFM written domain walls, in-plane strain relaxation  
-> higher density of stronger pinning sites, extended defects

PZT<sub>RFS</sub>

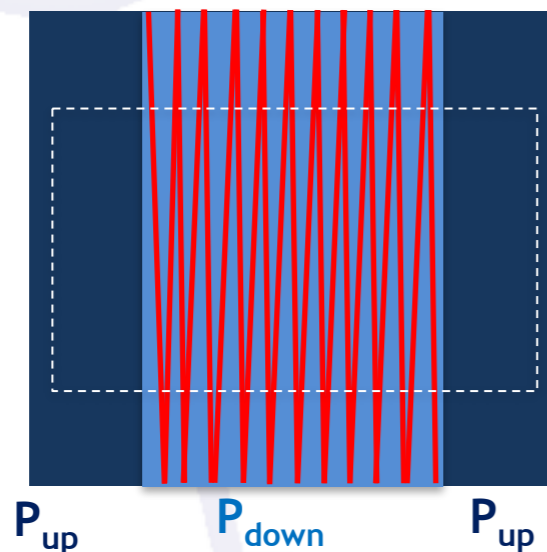


smooth AFM written domain walls, fully strained in-plane  
-> higher density of point defects

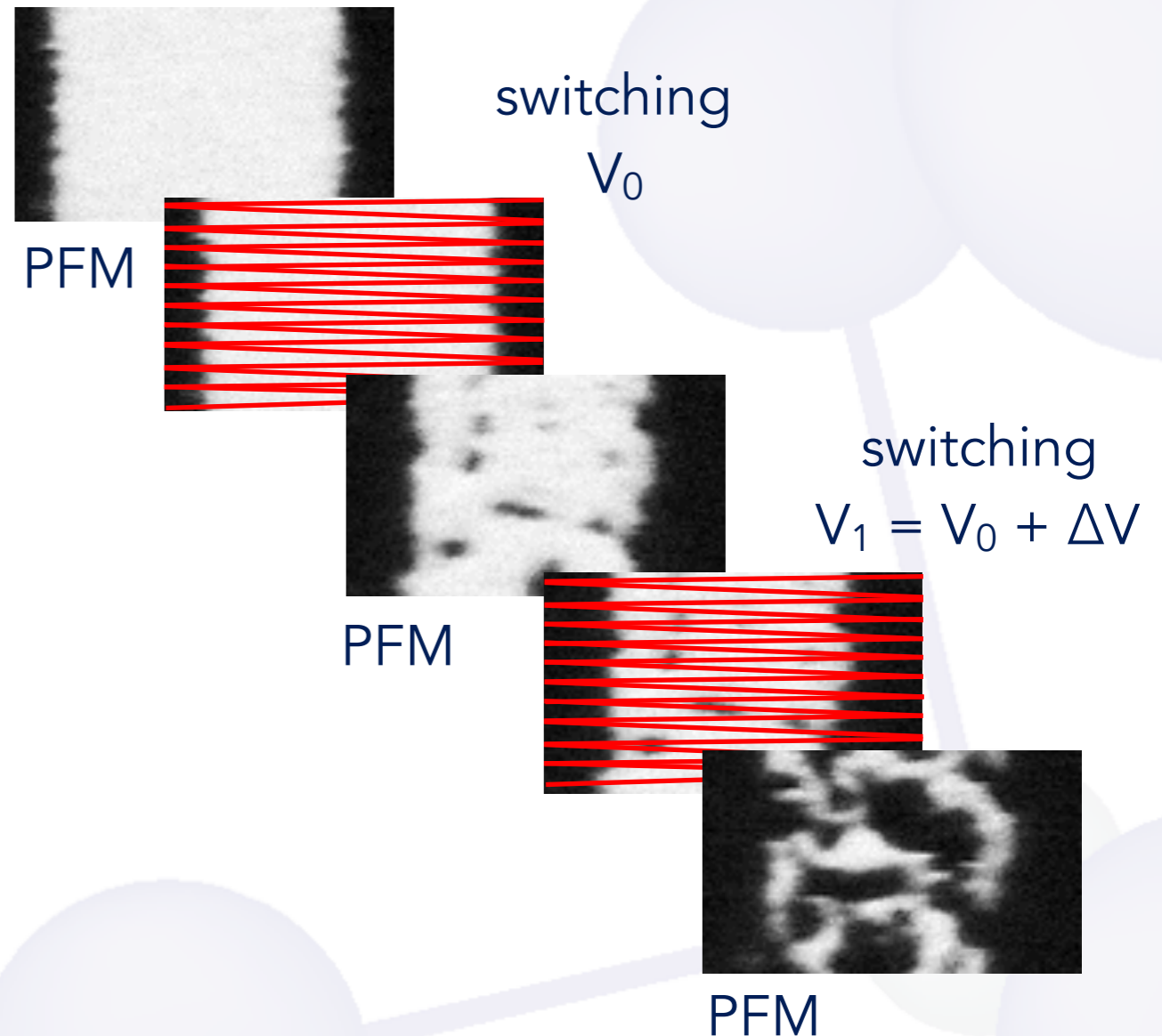
# UHV measurements of polarisation switching



Stripe domain structures written in as-grown monodomain  $P_{UP}$  films

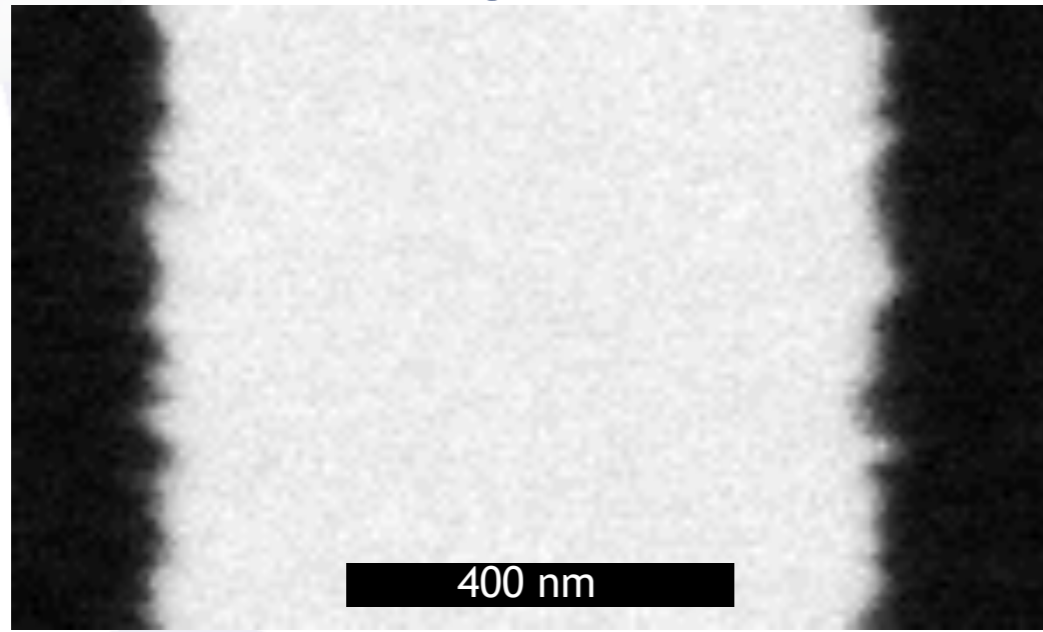


Alternate PFM scans with switching scans at incrementally increasing bias or at constant bias

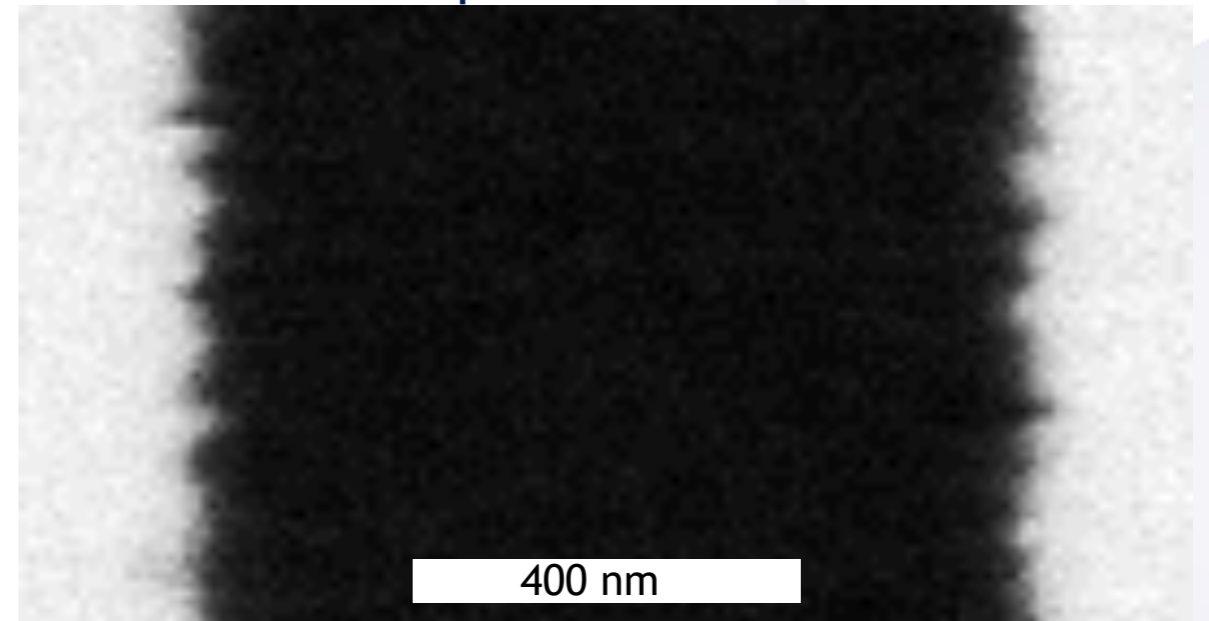


# Locally mapping polarisation switching

PZT<sub>RFS</sub> negative bias



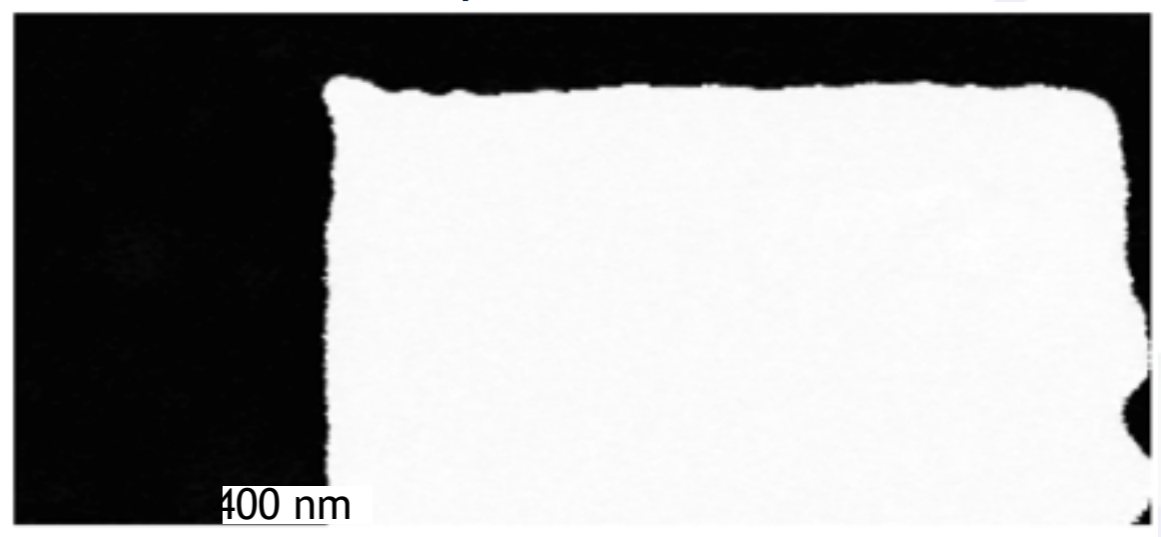
PZT<sub>RFS</sub> positive bias



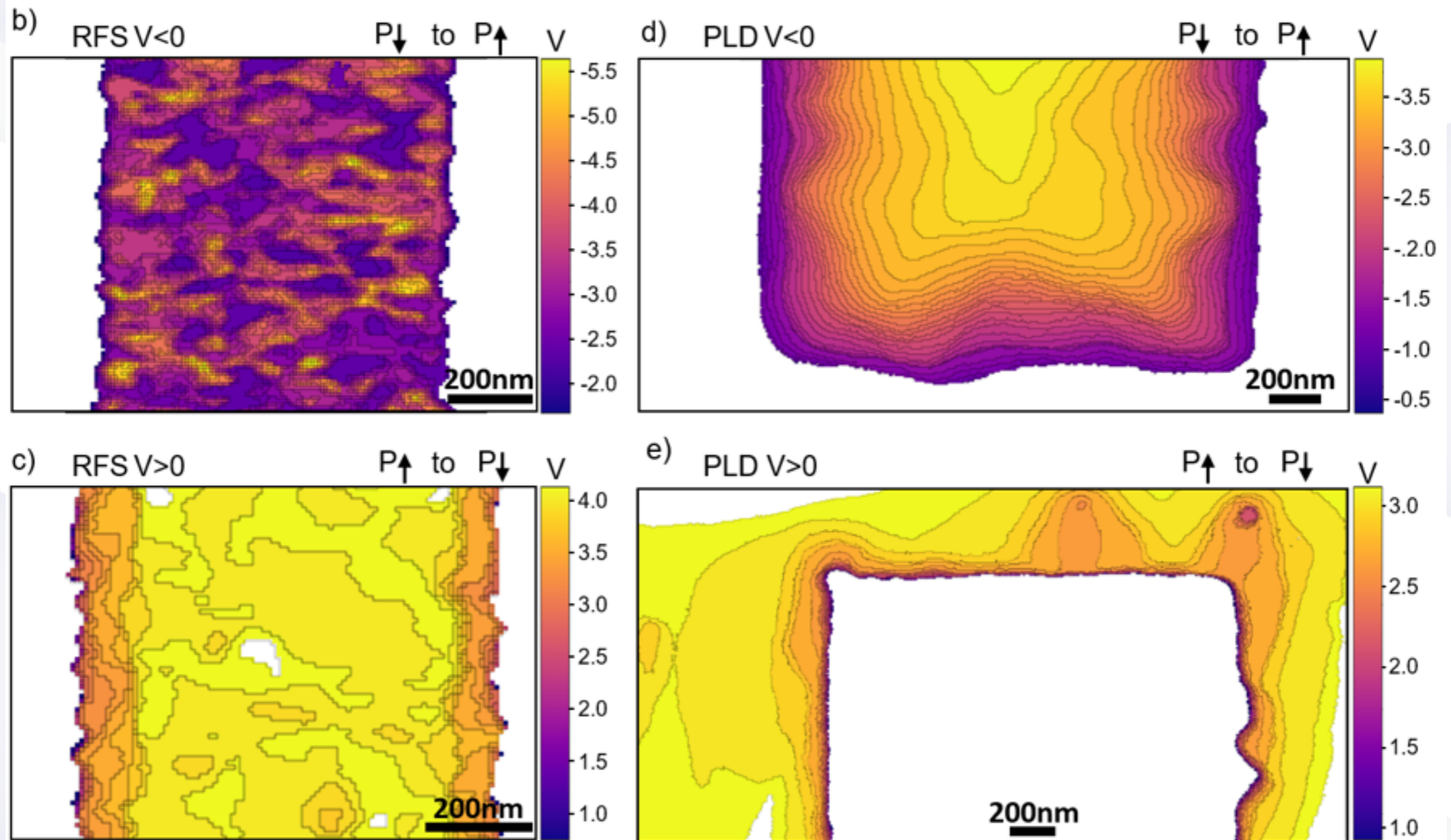
PZT<sub>PLD</sub> negative bias



PZT<sub>PLD</sub> positive bias



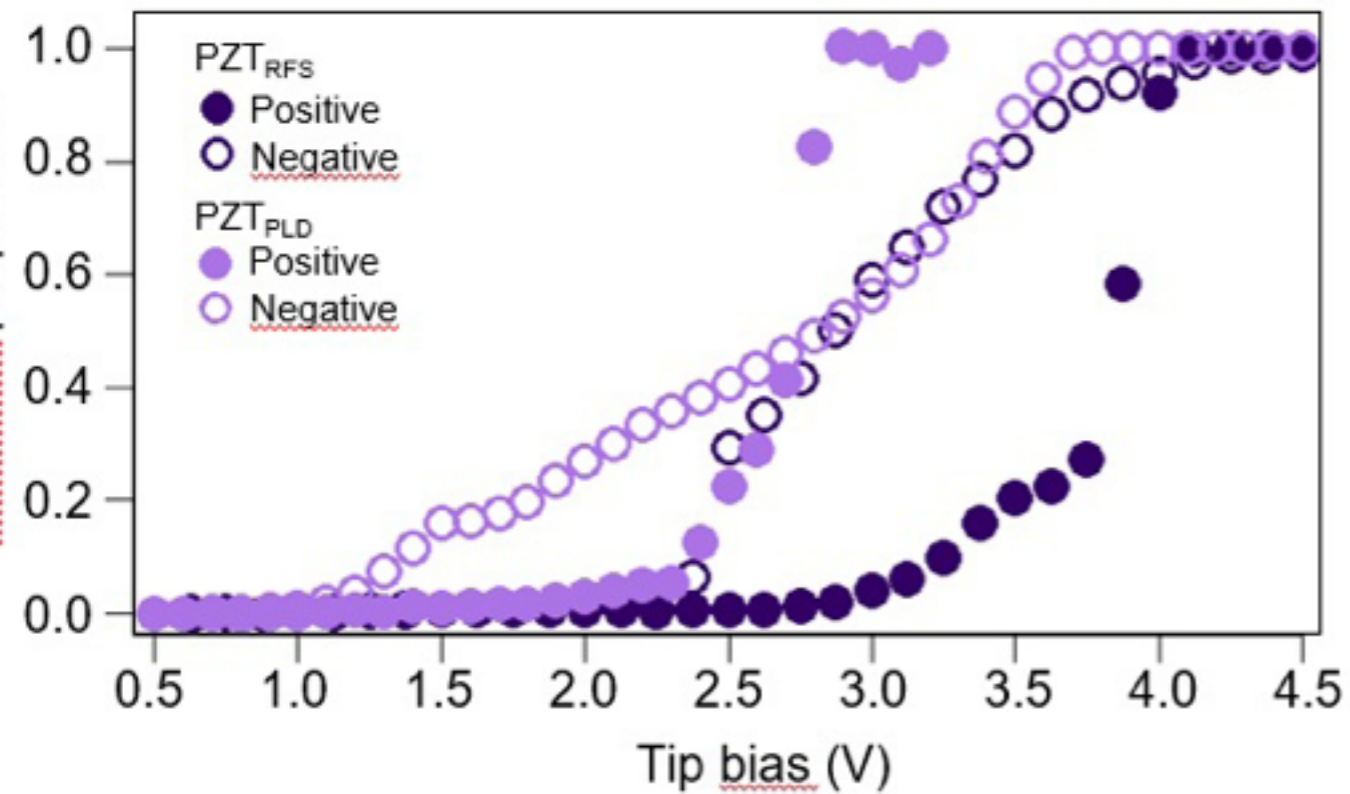
# Locally mapping polarisation switching



Lower switching threshold in  $PZT_{PLD}$

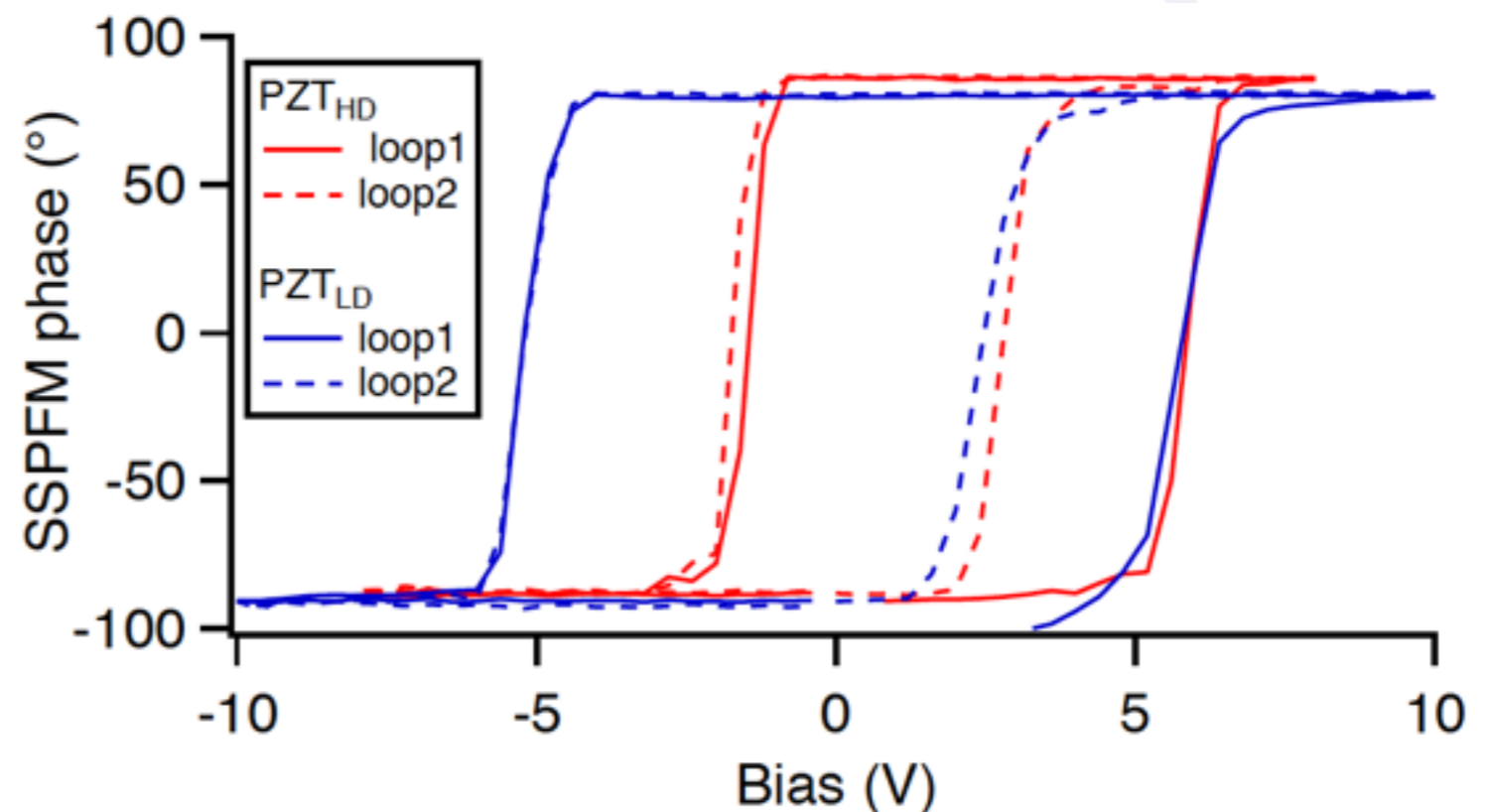
Lower threshold for negative bias switching (**written** areas) in both

# Switching dynamics - polarity AND history

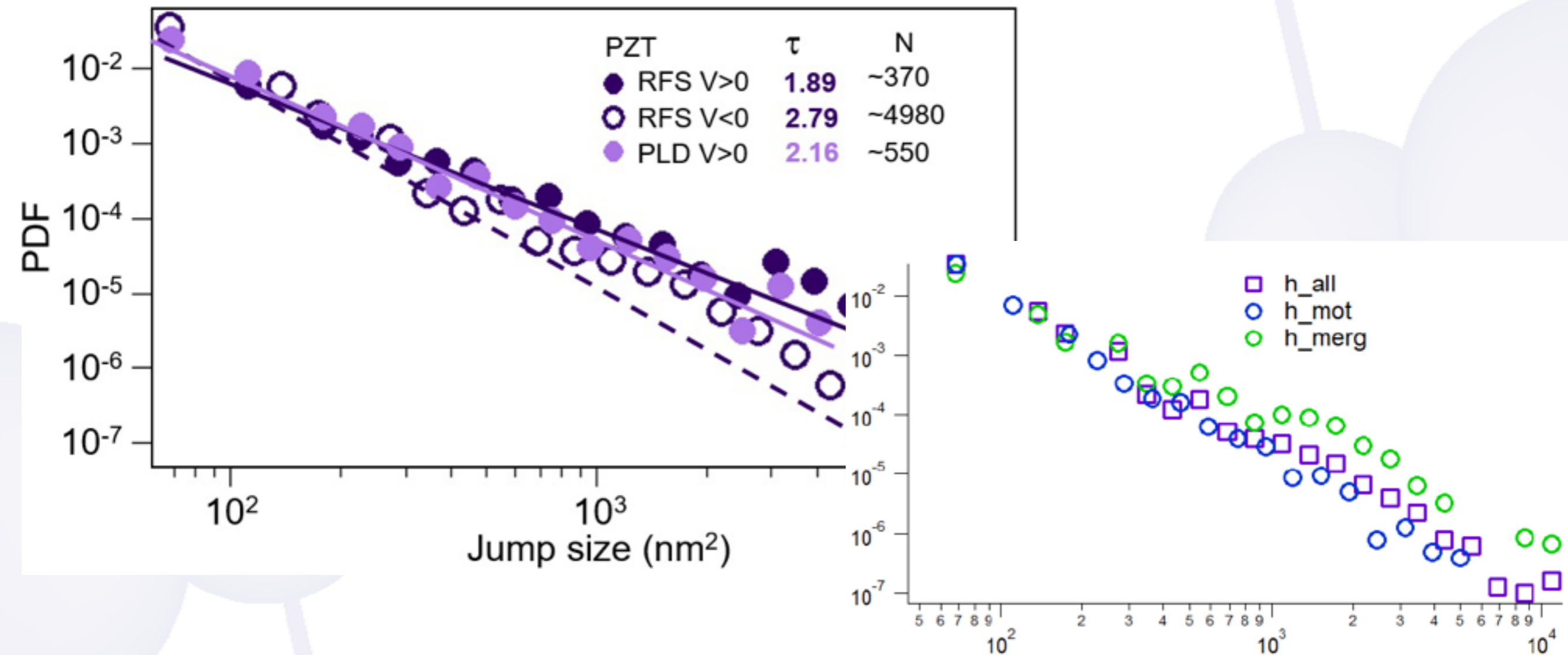


Highly asymmetric switching under positive vs. negative bias

Strong influence of a prior switching cycle which modifies the disorder/defect landscape



# Identify contributions to size spectrum from nucleation, DW motion and domain merging



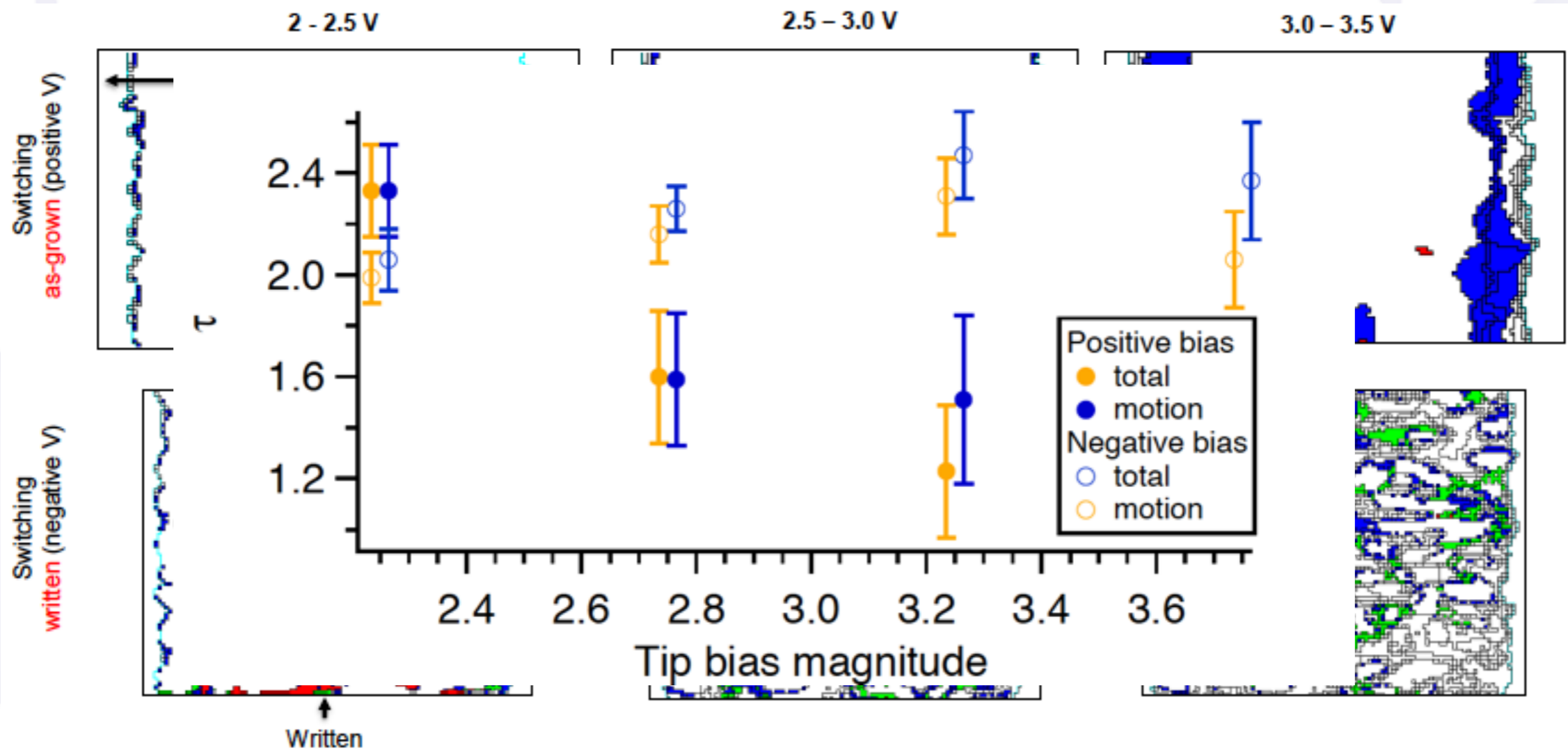
Avalanche size spectrum exponent sensitive to intrinsic defect landscape and defect injection during writing

DW motion events increase  $\tau$ , merging events decrease  $\tau$



# Effect of pinning strength on jump size exponent

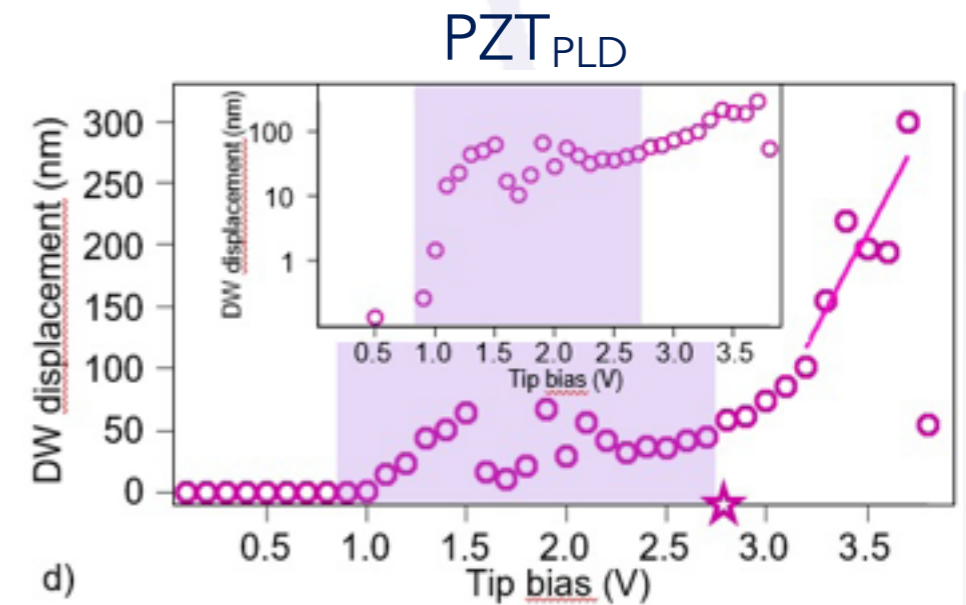
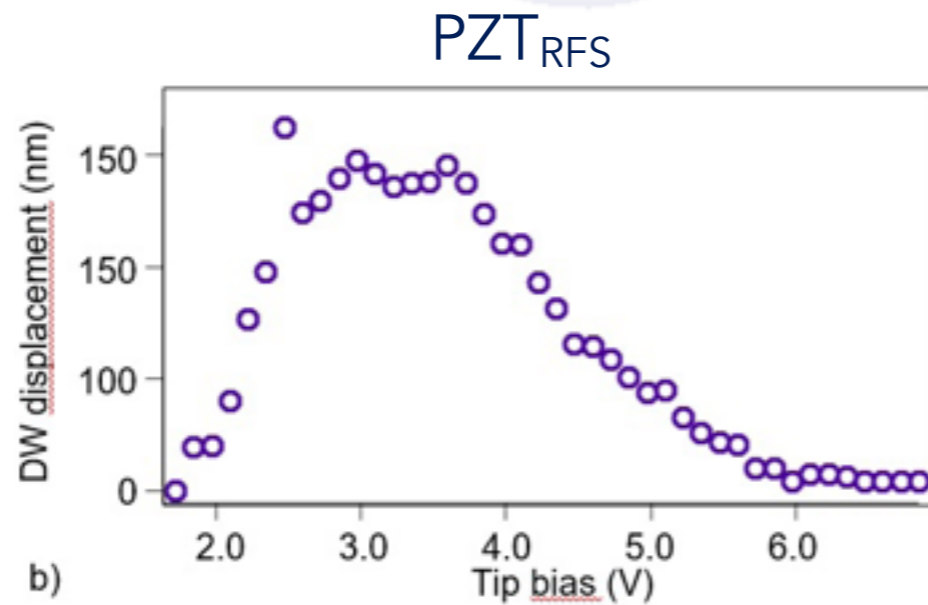
In as-grown areas, switching events occur further from initial DW position with increasing tip bias



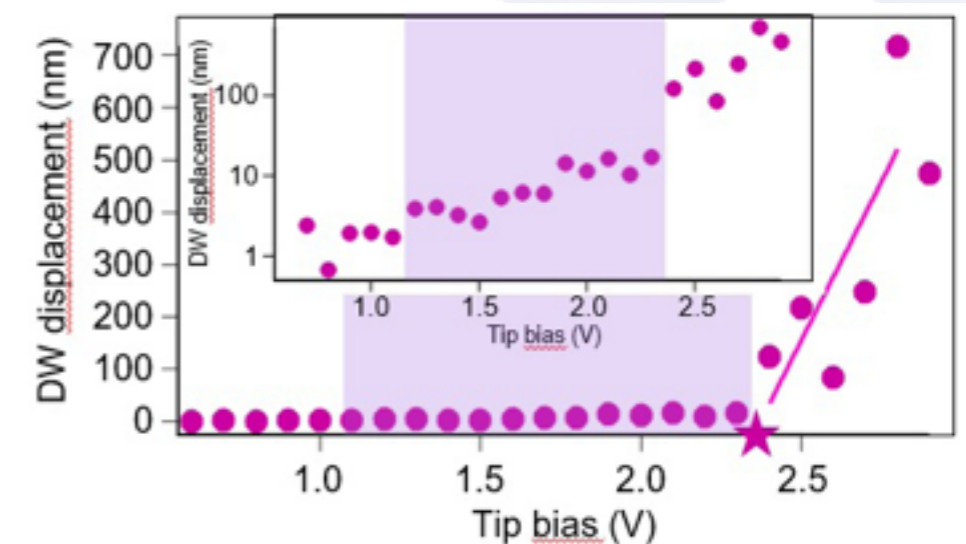
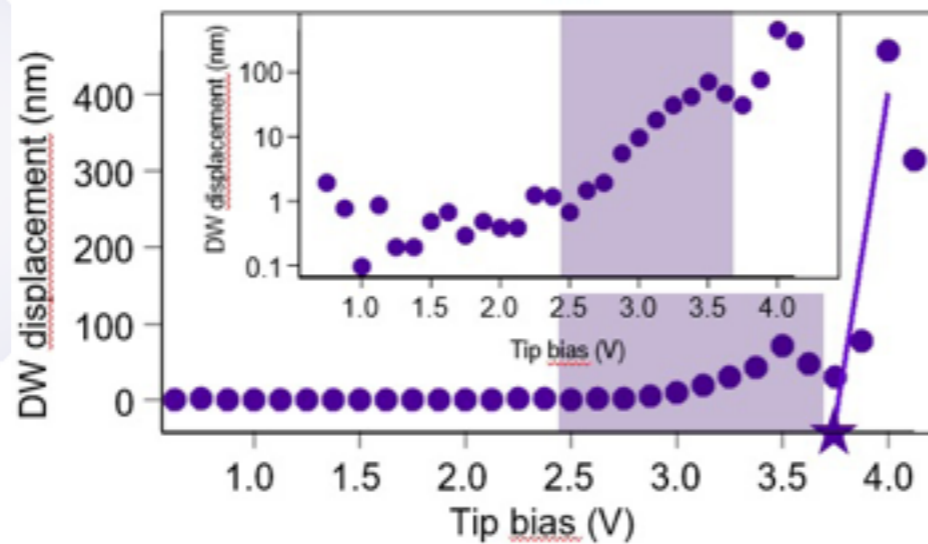
In previously switched areas, switching dominated by nucleation, possibly as a result of defect redistribution/injection during writing

# Identifying creep and depinning regimes

negative bias  
(switching written areas)

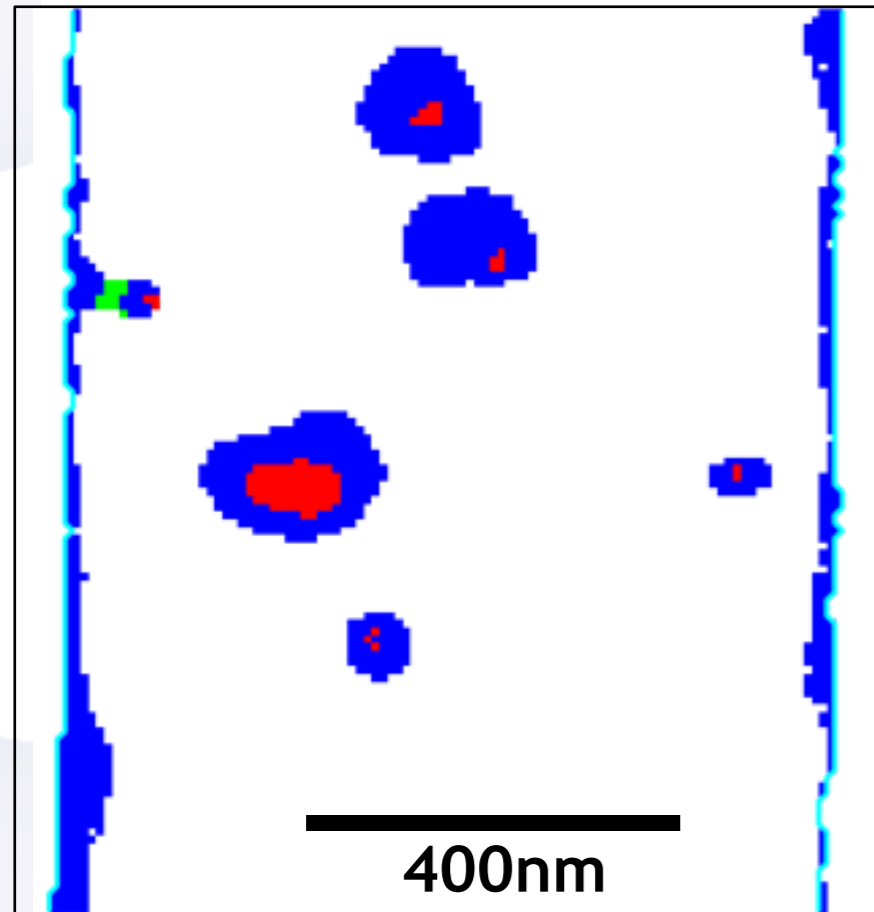


positive bias  
(switching as grown areas)



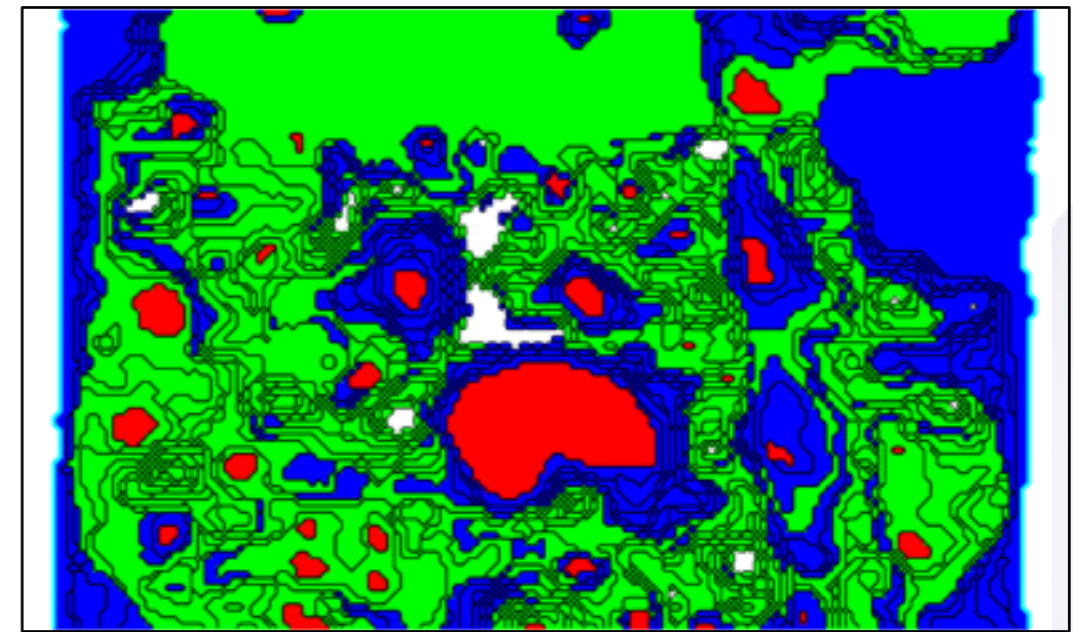
Avalanche size spectrum exponent sensitive to intrinsic defect landscape and defect injection during writing

# Polarisation switching at "constant" voltage



**-3.5V**

PZT<sub>RFS</sub>



400nm

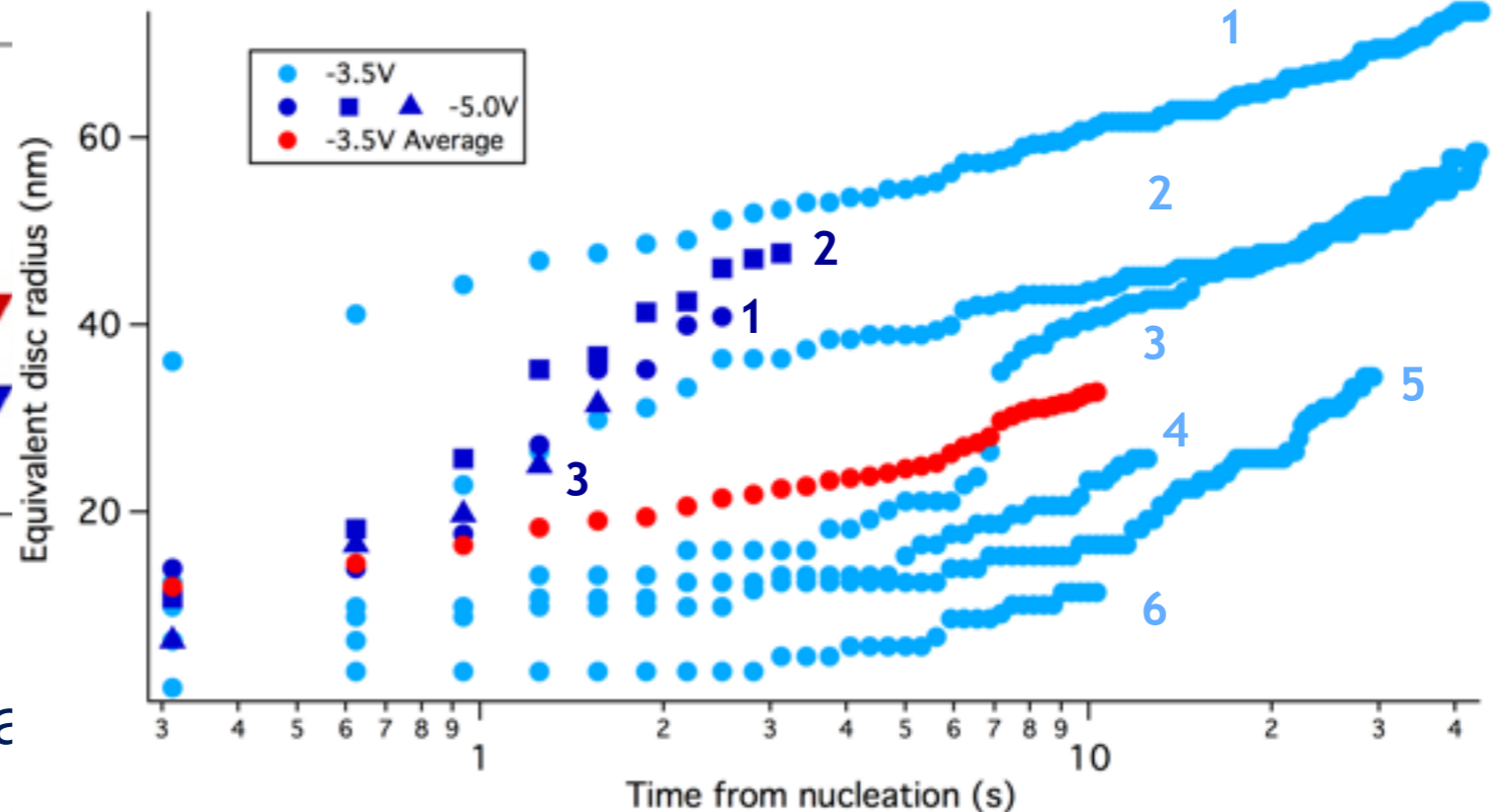
**-5.0V**



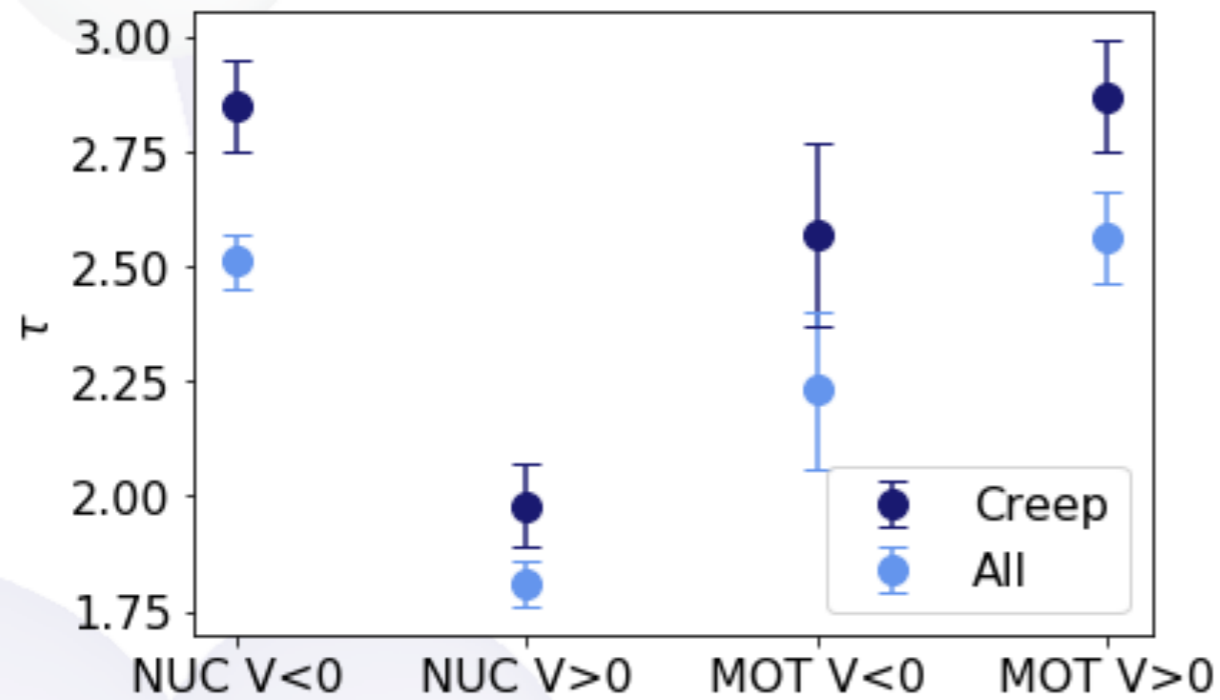
Creep-like logarithmic dependence of domain size on writing time

Tybell et al. PRL 89, 097601 (2002)

Stronger pinning  $\alpha$



# Importance of estimating the pinning force

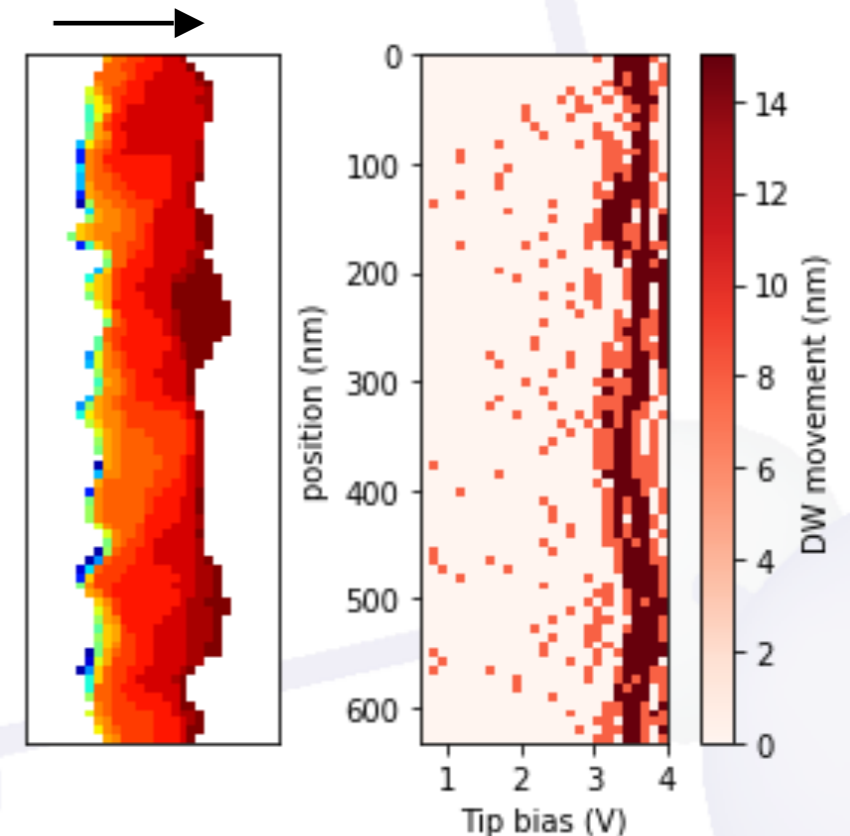


Systematic lowering of exponent values when events above the depinning threshold are included

Tukmantel et al. PRL. 126, 117601 (2021)

## Perspectives

- analysis of spatial correlations between switching events in the creep and depinning regimes
- switching dynamics studies in sample families with controlled densities of extrinsic defects
- studies of roughness and dynamics in device-relevant geometries

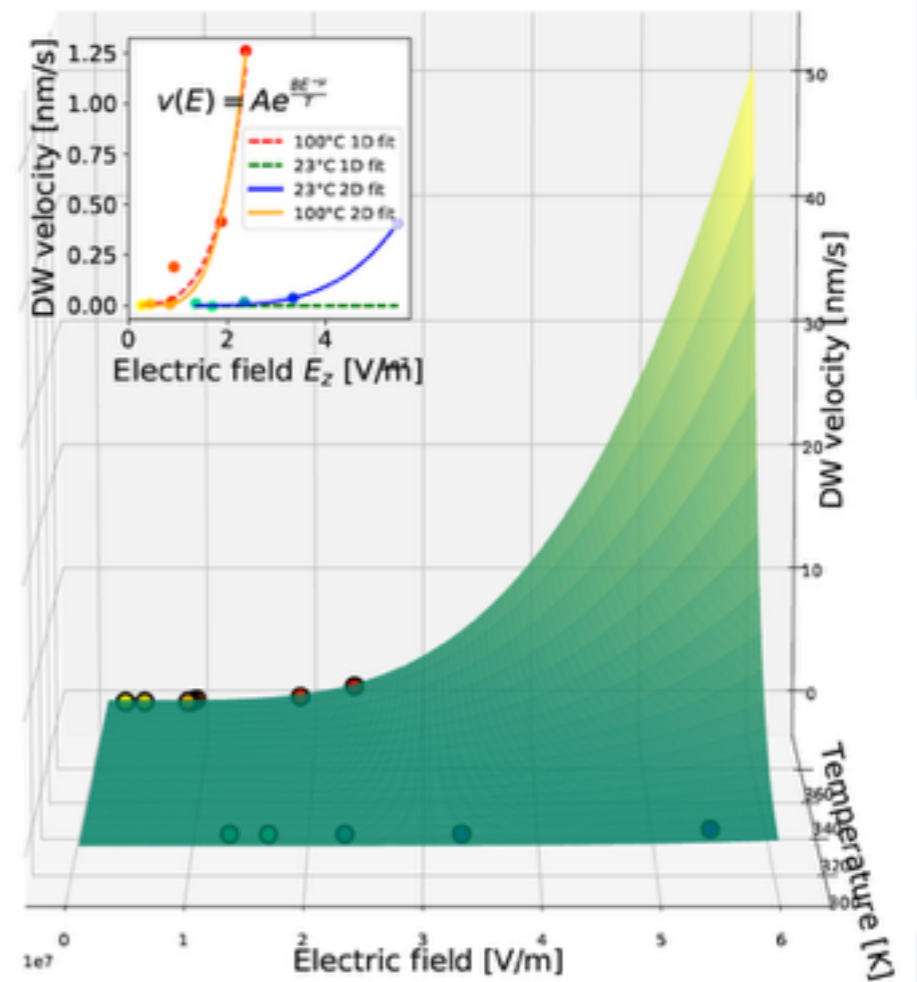
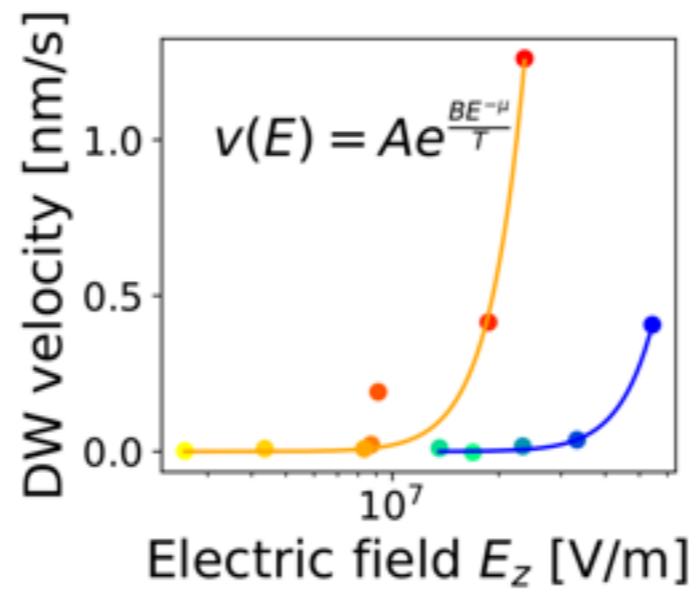
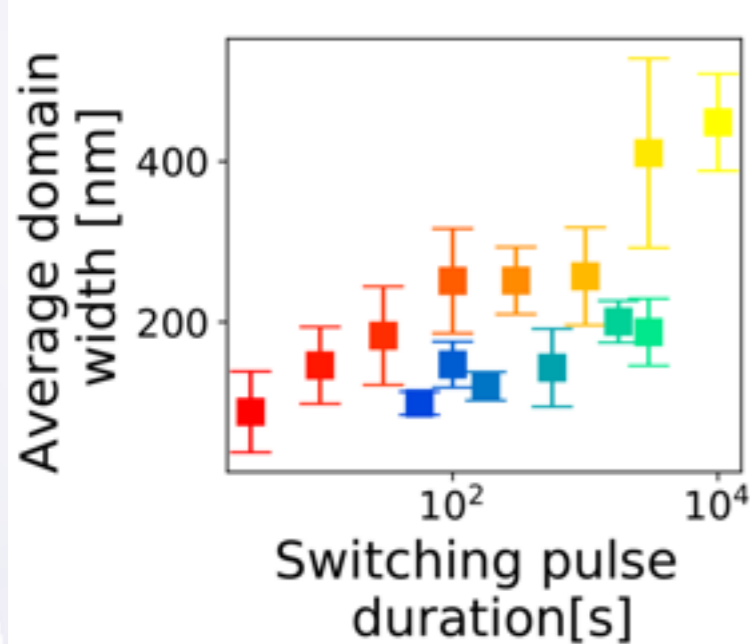
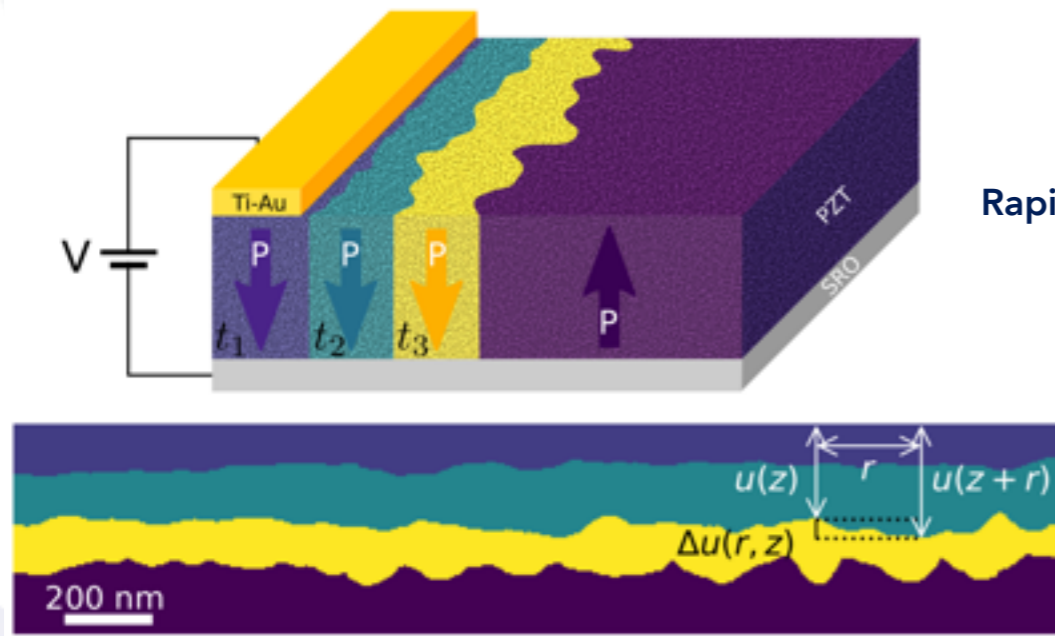


# Driving domain walls at planar electrode edges



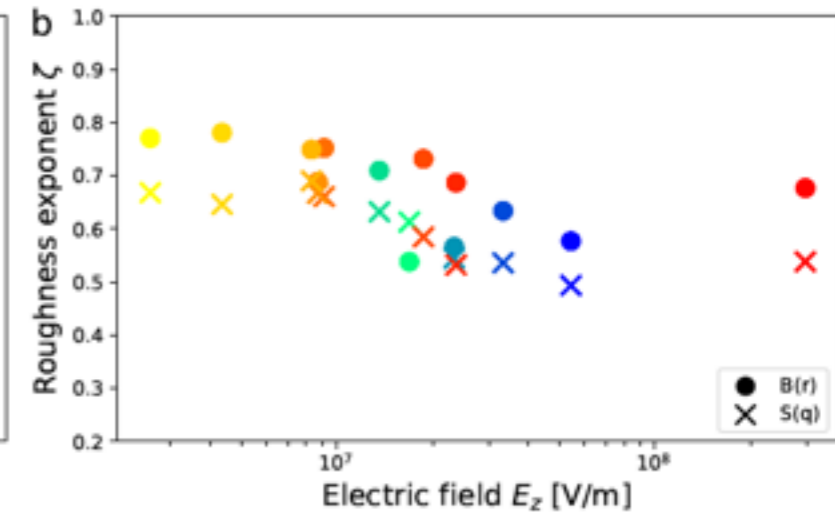
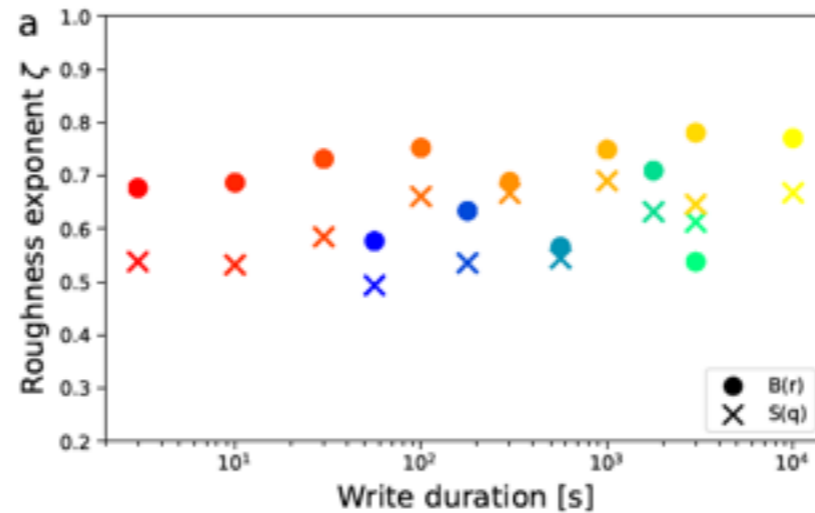
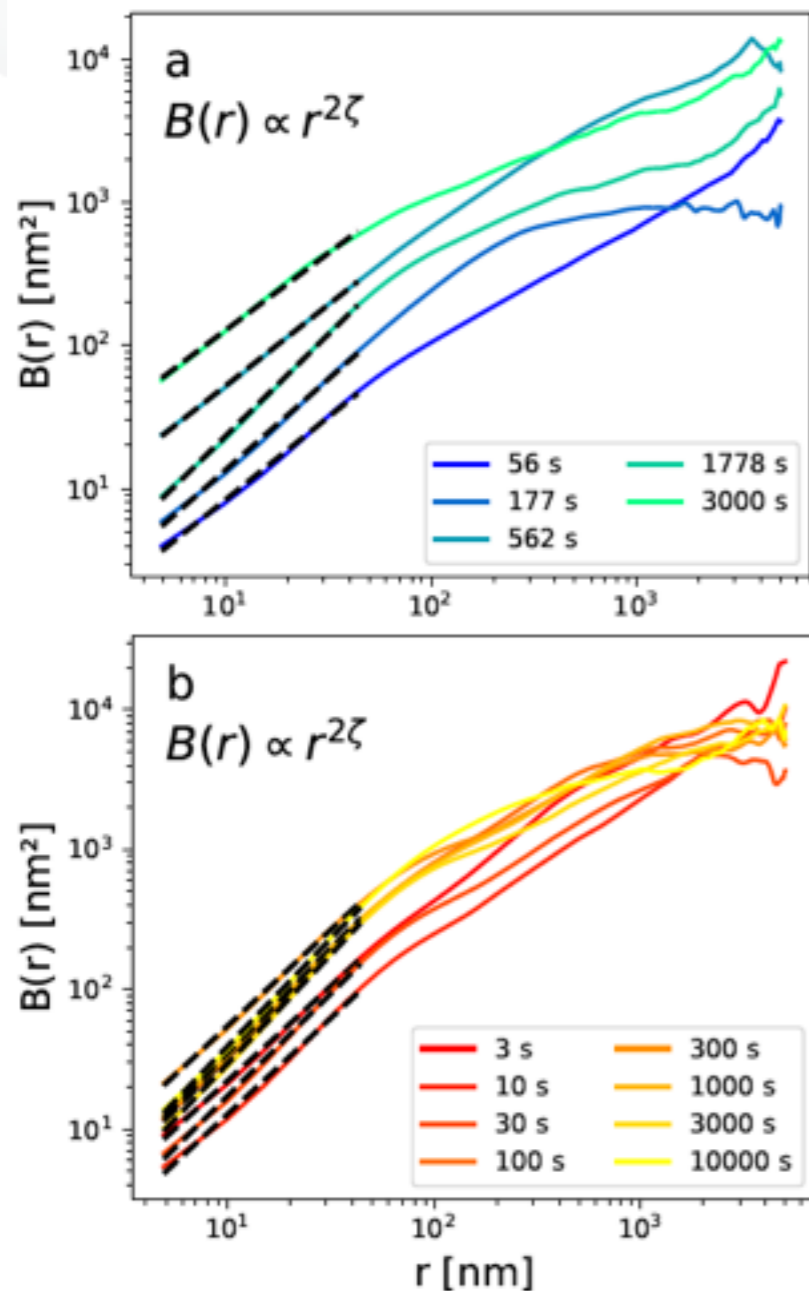
Guillaume Rapin    Sophia Ehrensperger    Nirvana Caballero

Rapin, Ehrensperger et al., APL. 119, 242903 (2021)



Domain wall dynamics as a function of driving force and temperature show strong effect of thermal activation and visible evolution of geometry

# Quantifying evolution of domain wall roughness



Significant roughening as DWs move into pristine disorder landscape  
High roughness exponent values in more "equilibrated" systems

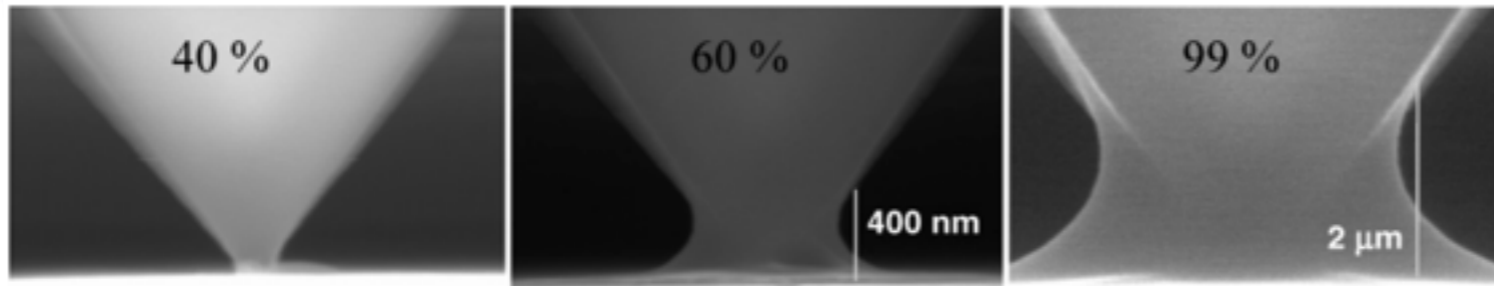
# Effects of humidity on the electric field of the SPM tip



Jill Guyonnet



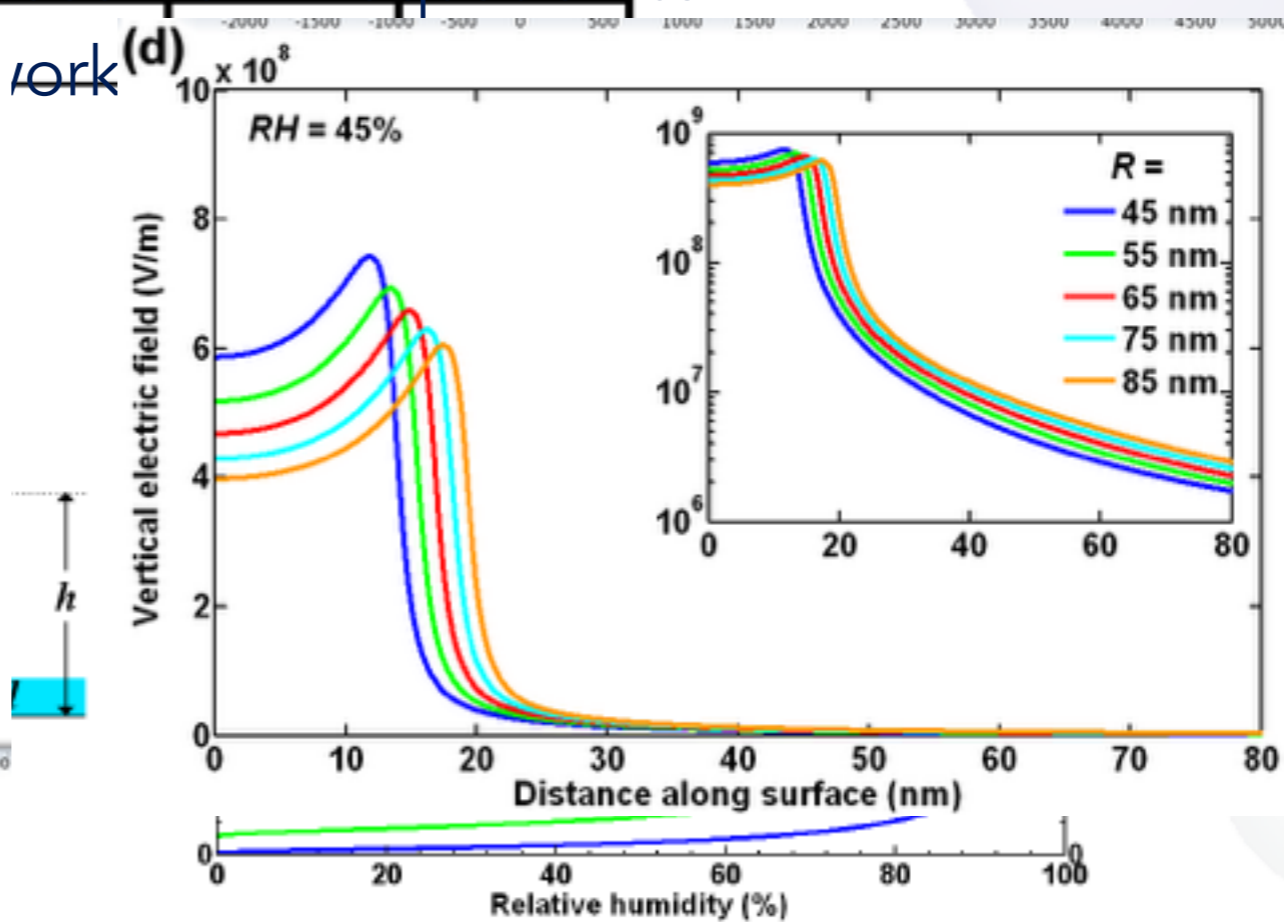
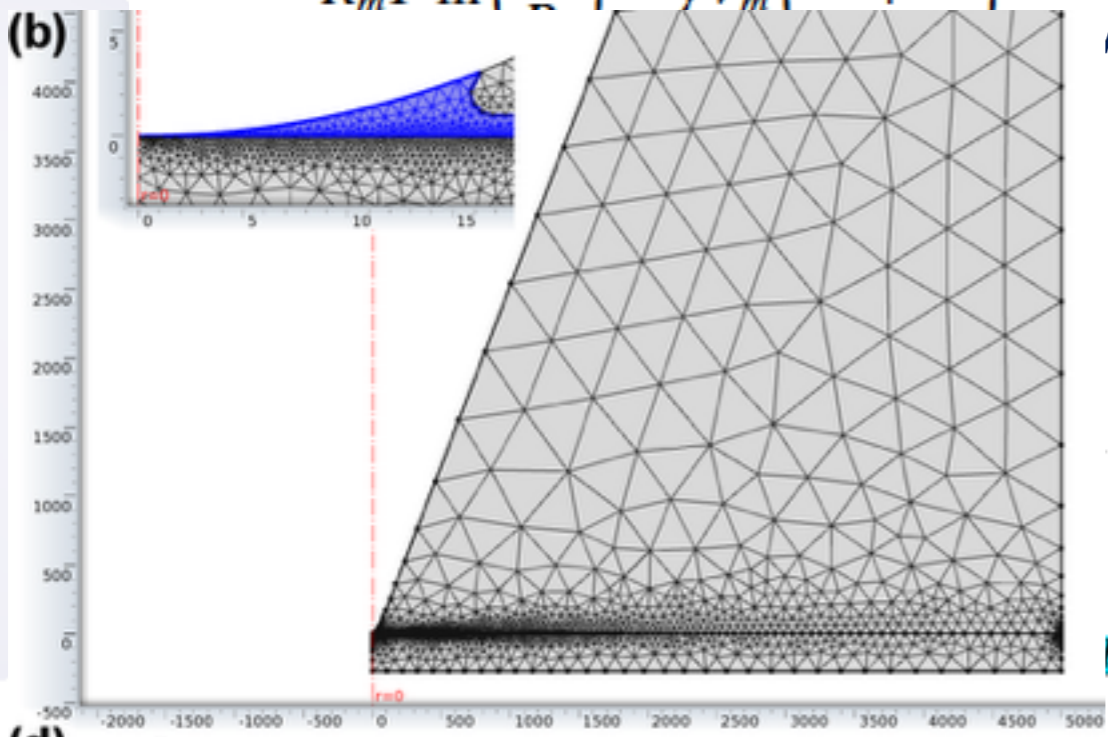
Cédric Blaser



Weeks et al., Langmuir 21, 8096 (2005)

$$10^1 R_m T \ln\left(\frac{P}{P_0}\right) = \gamma V_m \left(\frac{1}{r} + \frac{1}{R}\right)$$

use Kelvin equation to work

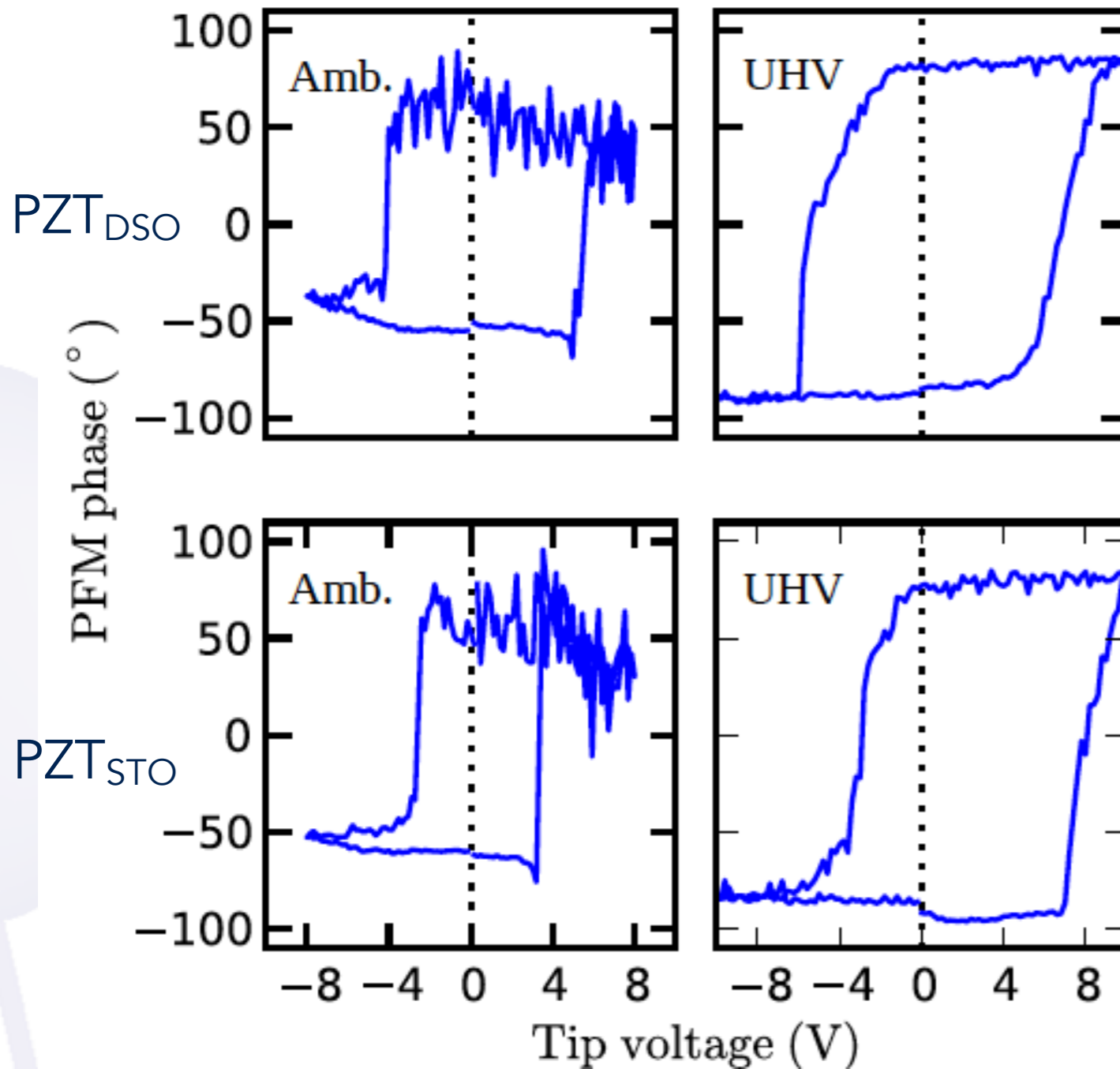


level with  
ice water

# Disorder and environmental effects in UHV and ambient conditions



Jill Guyonnet

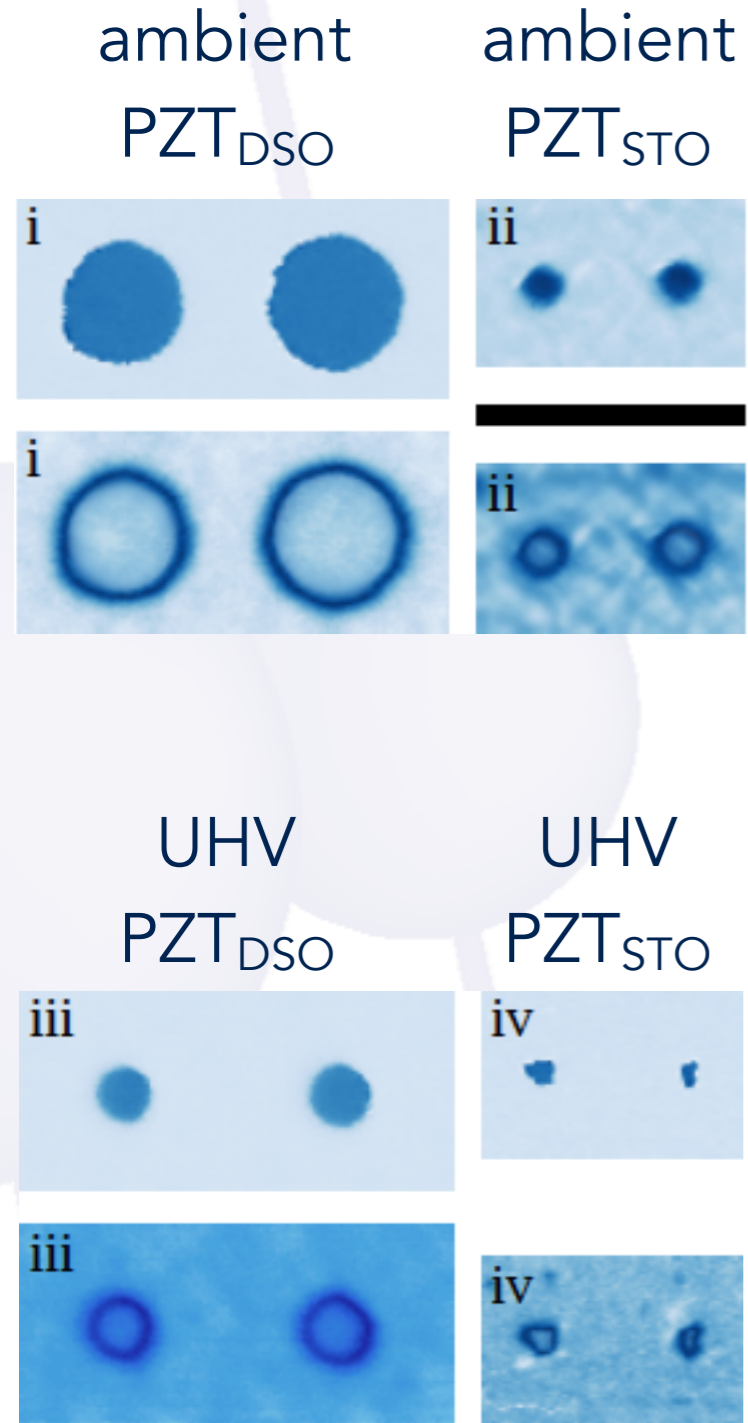


Measurements in ambient

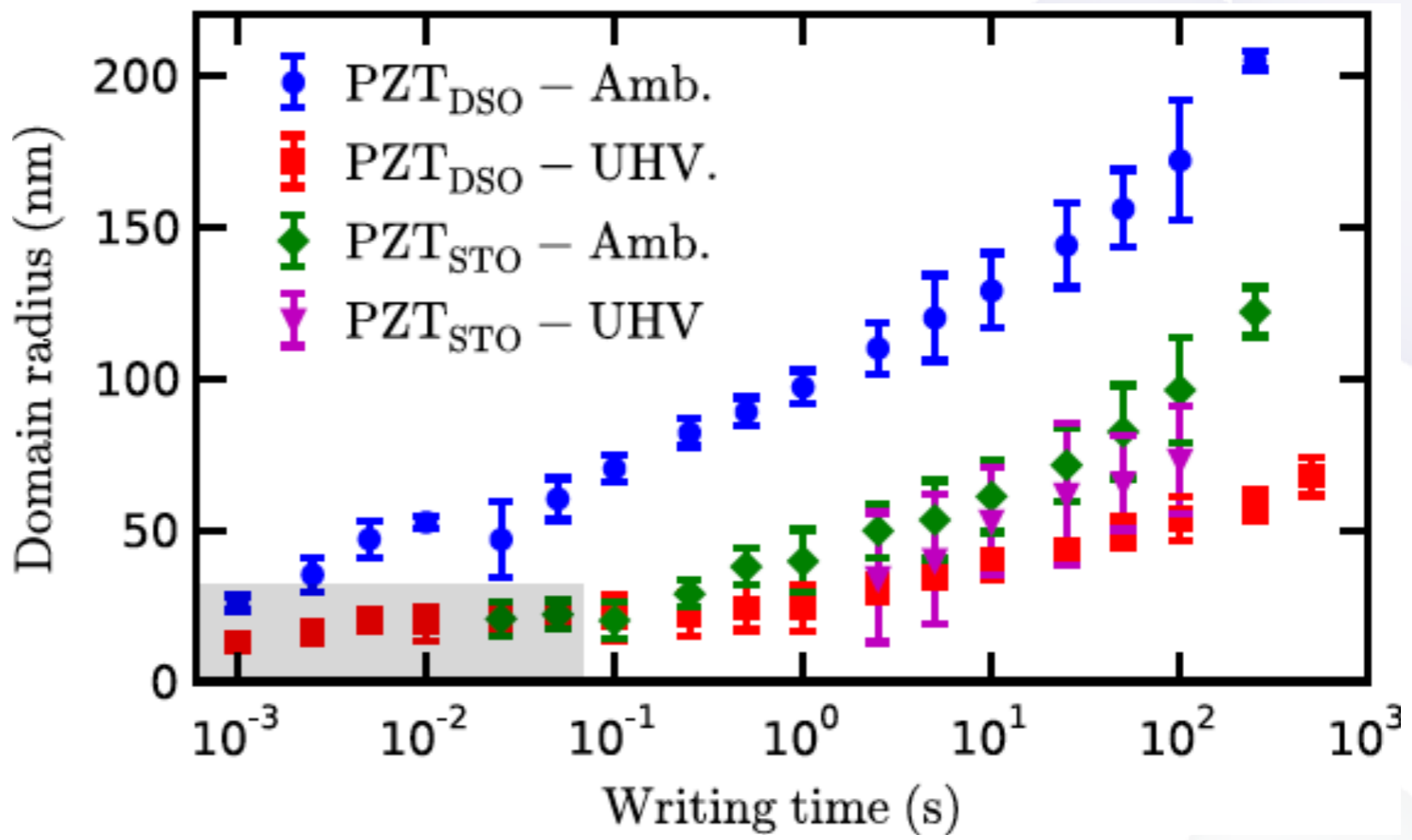
Measurements in UHV  
after short sample  
bakeout at 100°C



# Defect pinning vs screening by surface adsorbates

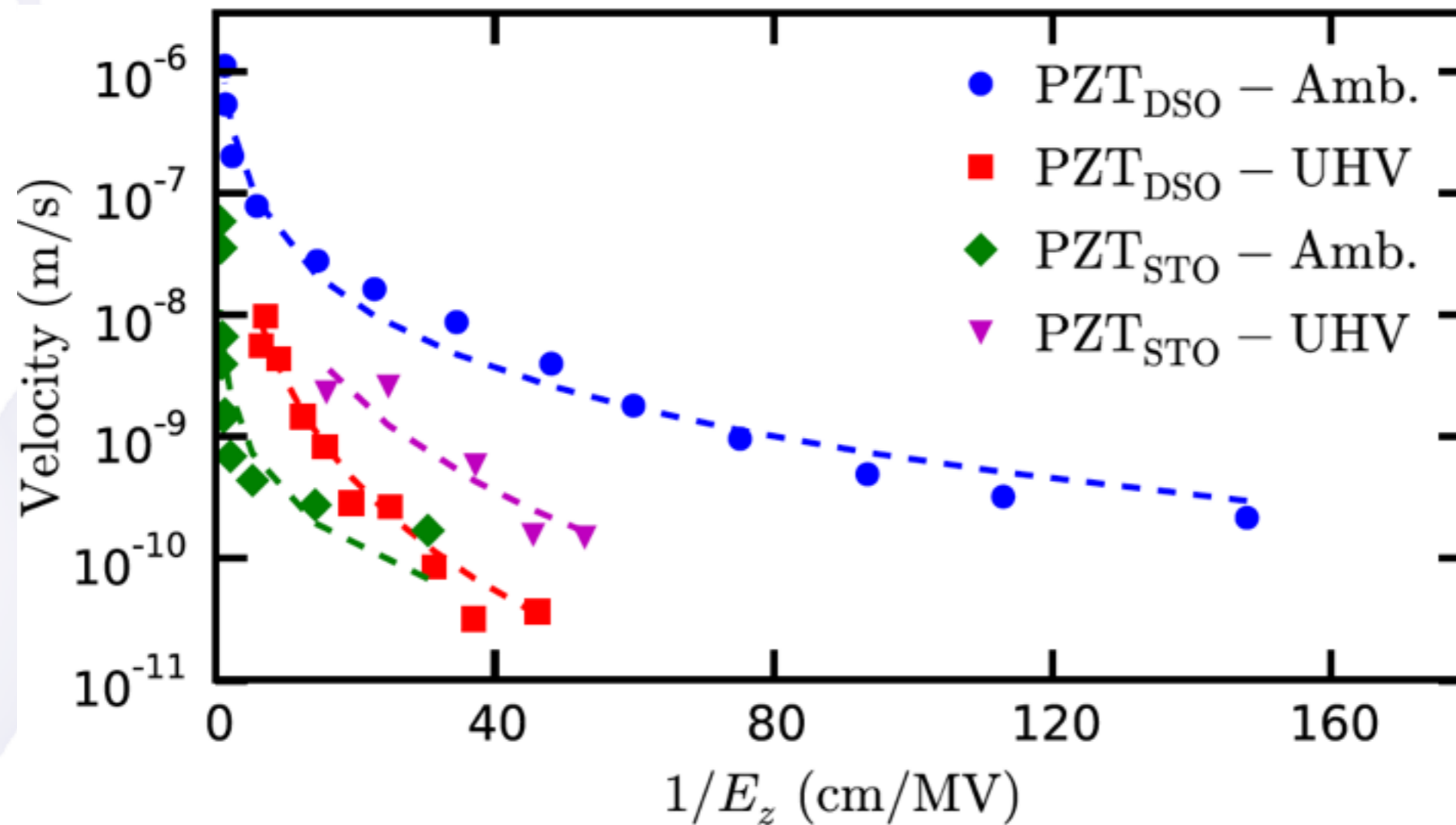


extracting dynamics 
$$v(t_{n+1}) = \frac{r(t_{n+1}) - r(t_n)}{t_{n+1} - t_n}$$



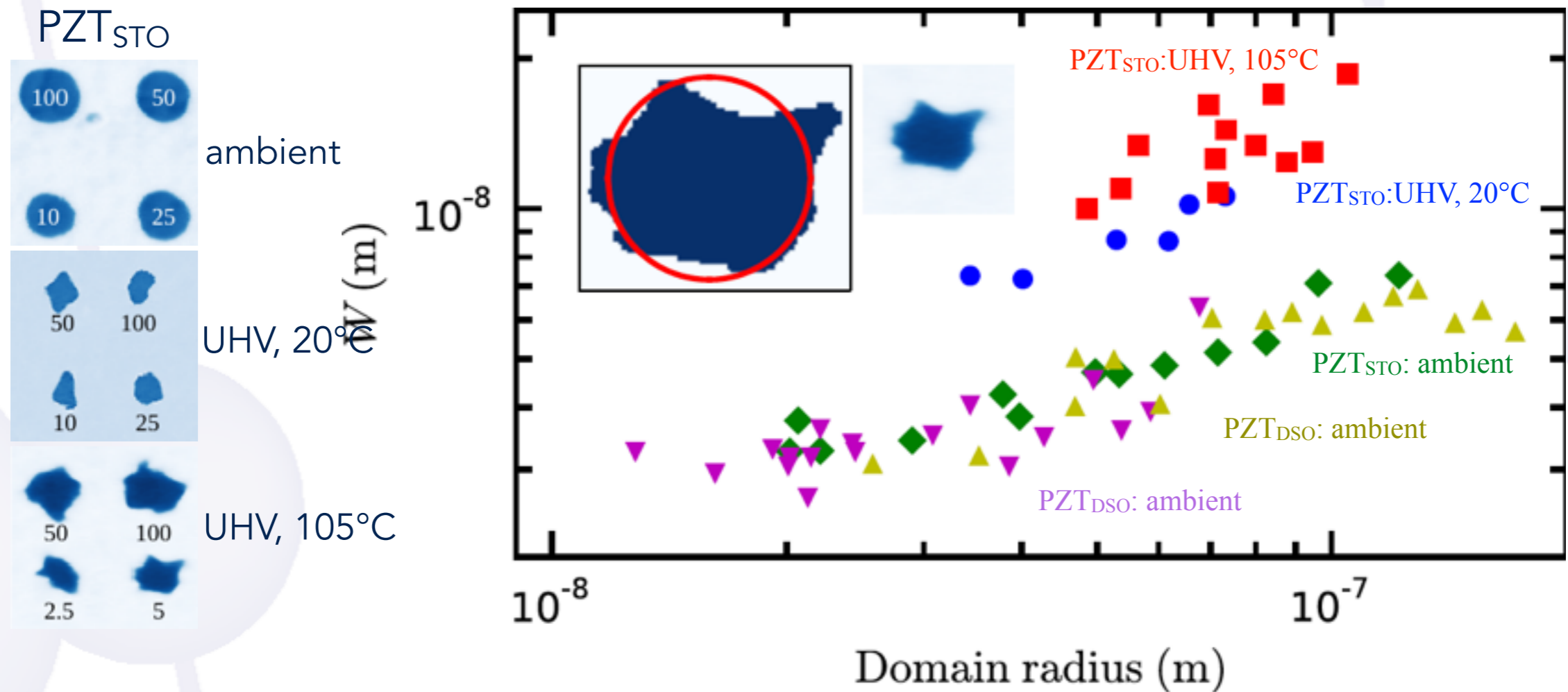
Slower domain growth in UHV  
 Smooth domain walls at ambient conditions  
 Increased roughness in more disordered films in UHV

# Domain wall creep in UHV and ambient



Surface water NOT essential for subcritical domain wall dynamics  
(suggested by Brugère et al., JAP 110, 052016 (2011))

# Domain wall roughness in UHV and ambient



$$w(r) = \sqrt{\left\langle \left[ u(z) - \langle u \rangle_r \right]^2 \right\rangle_r} : r^\xi$$

Higher domain wall roughness in UHV for films with more defects

# Numerical switching simulations in GLD framework confirm observations



Sebastian Bustingorry

$$f(\mathbf{R}) = \alpha \left( -\frac{P^2}{2} + \frac{P^4}{4} \right) + \beta \frac{|\Delta P|^2}{2} + \gamma \int \frac{PP'}{|\mathbf{R}-\mathbf{R}'|^3} d\mathbf{R}' - e(\mathbf{R}, t)P + \sqrt{T}\eta$$

double-well potential  
barrier height

$$\alpha = \alpha_0(1 + \Delta\xi)$$

random-bond  
disorder strength

domain wall  
energy

dipolar interaction

less screening = higher dipolar term

electric field

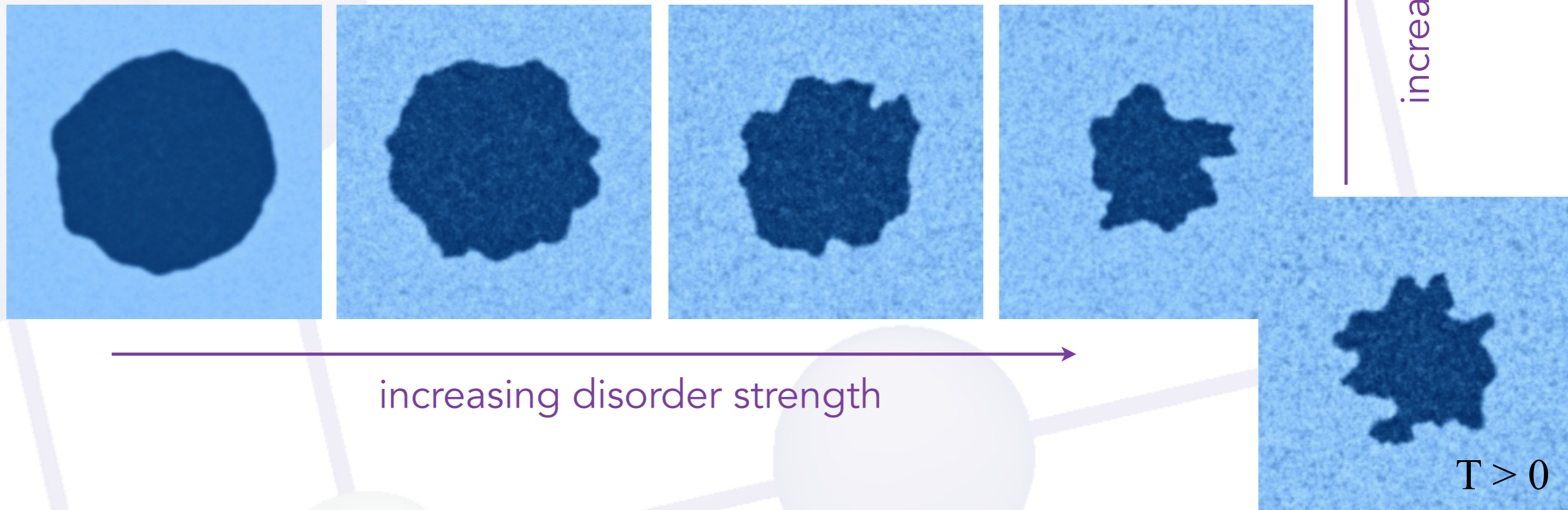
$$e(\mathbf{R}, t) = e_0/|\mathbf{R}|$$

temperature

square lattice

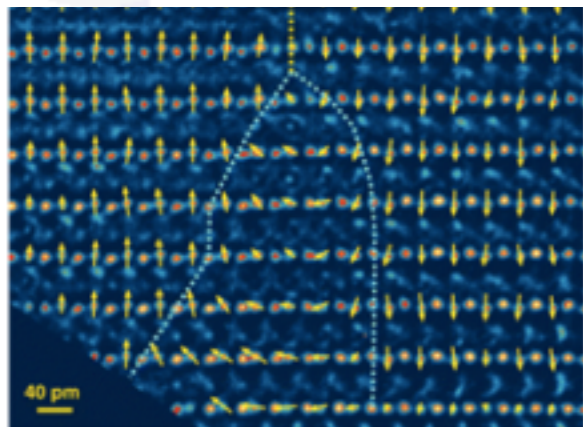
start from monodomain configuration  
apply a field at center for a given time  
let domain relax

Rougher domains and slower growth in the presence of disorder  
Surface water screening of dipolar interactions is important

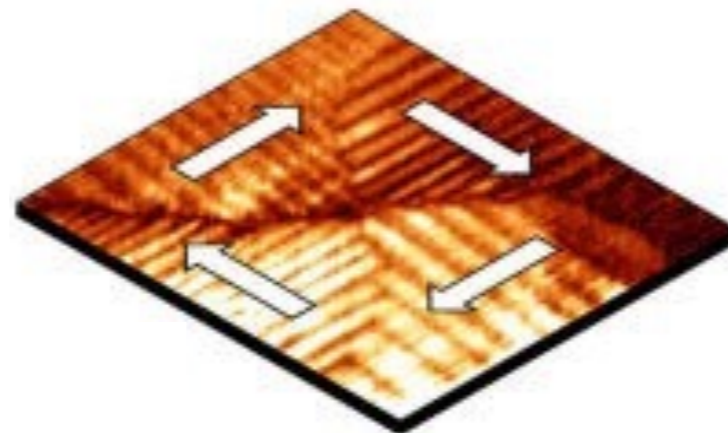


# Complex polarisation textures at the nanoscale

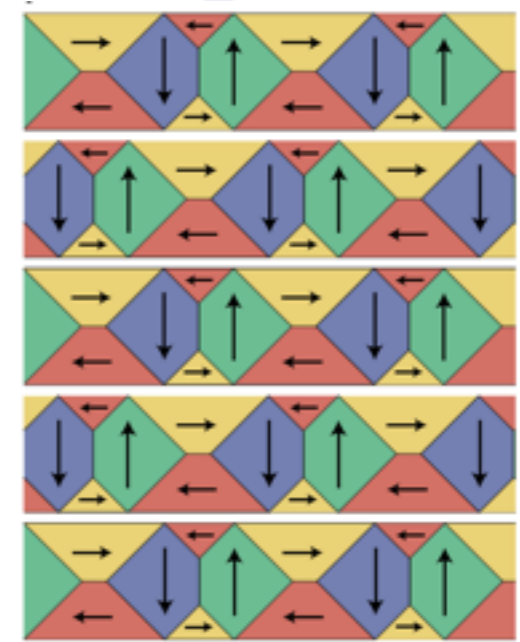
Flux-closure domains and superdomains in thin films, single crystal and superlattices



Jia et al, Science 331, 1420 (2011)

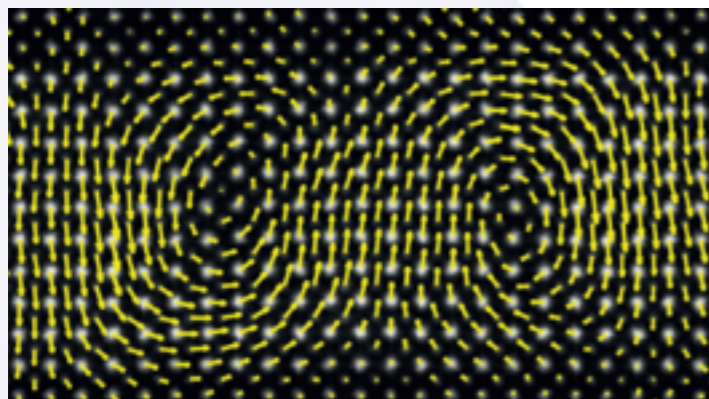


McQuaid et al, Nano Lett. 14(8) (2014)



Hadjimichael et al, Nat. Mat. (2021)  
Tang et al, Science 348, 6234 (2015)

## Polar vortices



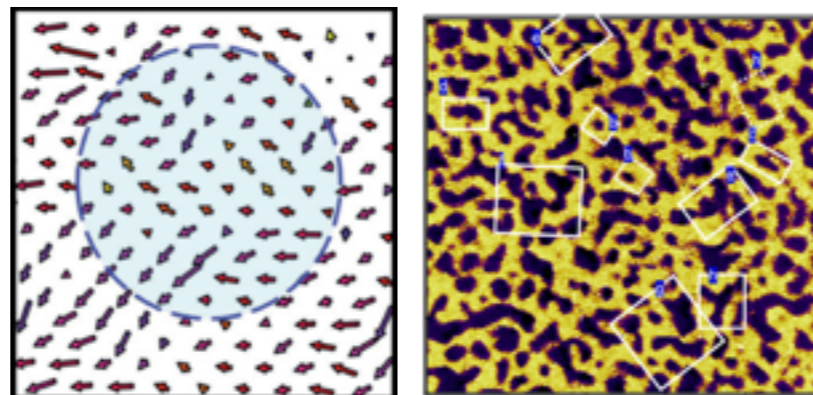
Yadav et al, Nat. 530, 198-201 (2016)

Li et al., Nat. Comm. 8, 1468 (2017)

Li et al., Nat 592, 376 (2021)

Hong et al., Nano Lett. 21, 3533 (2021)

## Bubble domain zoology

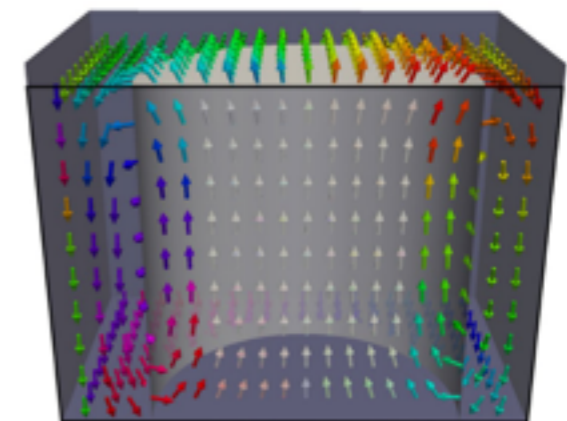


Zhang et al, Adv. Mat. 29, 46 (2017)

Nahas et al., Nat. Comm 11, 5779 (2020)

Govinden et al., PRM 5, 124205 (2021)

## Skyrmions



Das et al, Nature 568 (2019)

Gonçalves et al, Sci. Adv. 5, eaau7023 (2019)

Complex polarisation patterns arise as an interplay between strain and electrostatic boundary conditions

# Pinned elastic interfaces in biology

“can you use this physics description to look at our wound healing profiles?”

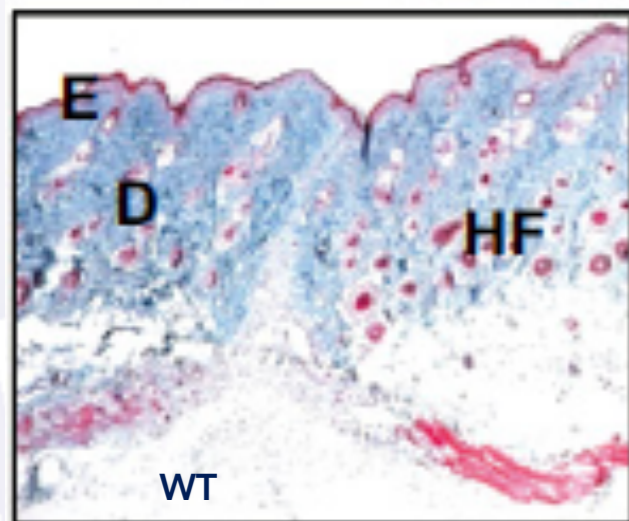
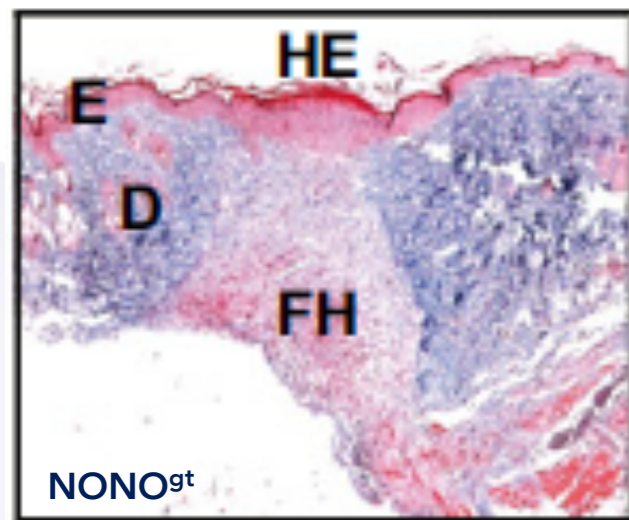


Steven Brown

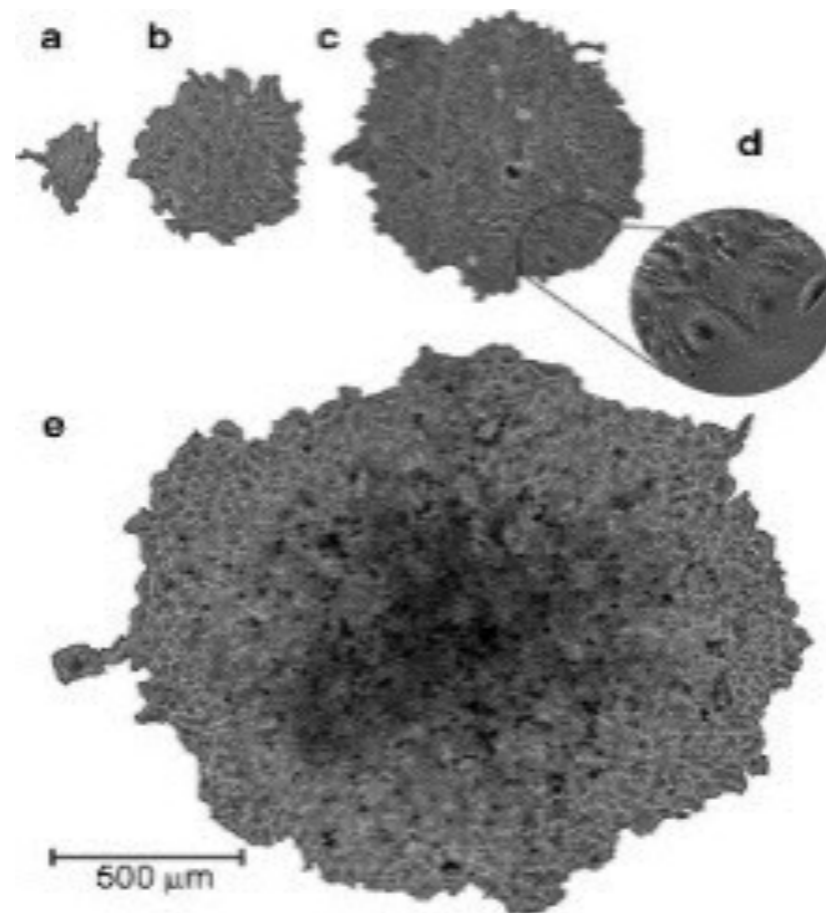


Elisabeth Agoritsas

wound healing



Kowalska et al, PNAS 110, 1592 (2013)



Muzzio et al., J. Biol. Phys. 40, 285 (2014)

Bacterial colony edges and epithelial cell fronts present universal scaling laws in morphology and dynamics characteristic of glassy systems

Vicsek et al., Phys. A 167, 315 (1990)

Fleury and Watanabe, C. R. Biologies 325, 571 (2002)

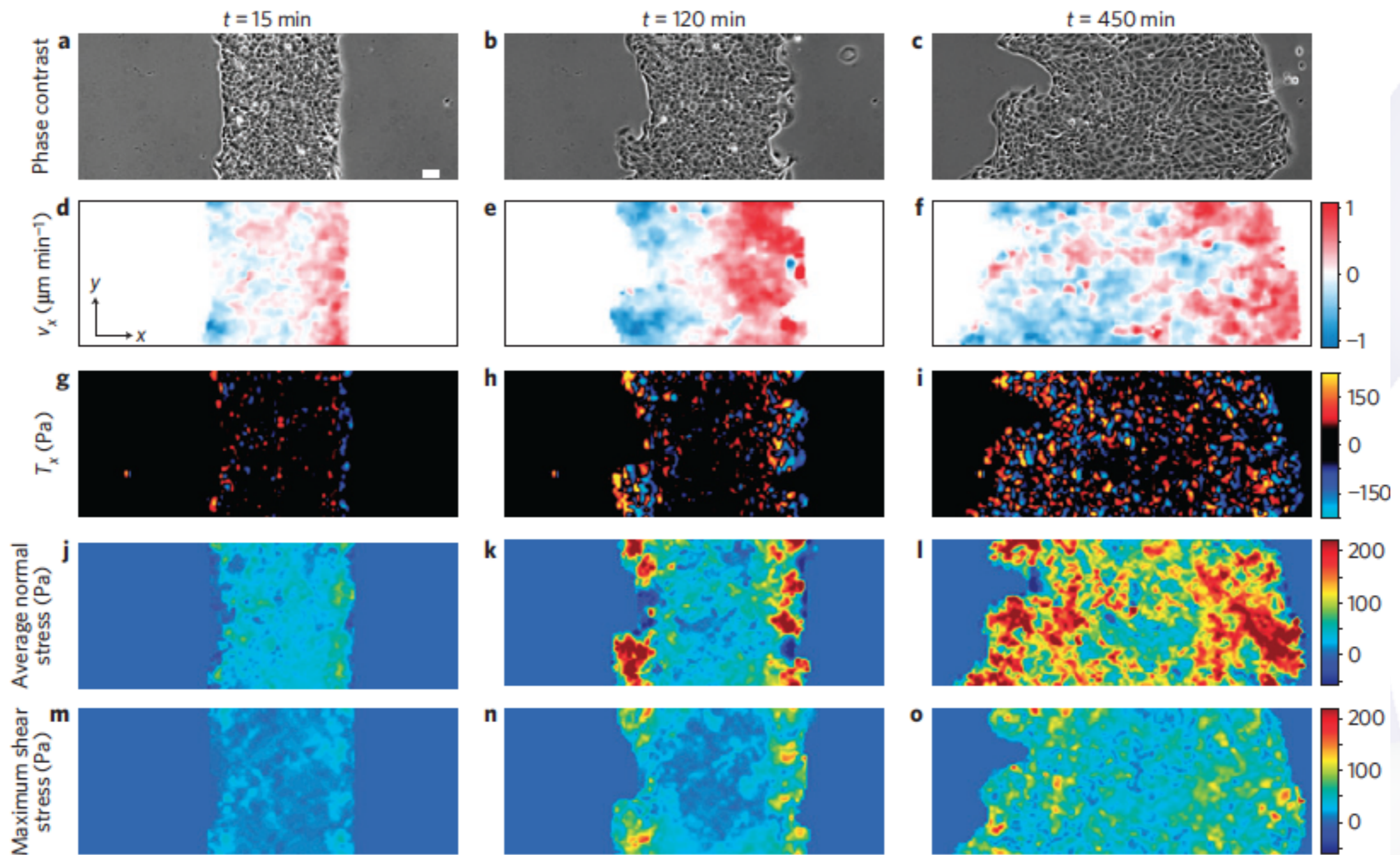
Callaghan et al., J. Stat. Phys. 122, 909 (2006)

Trepast et al., Soft Matter 4, 1750 (2008)

Bonachela et al., J. Stat. Phys. 144, 303 (2011)

Chiou et al., PLOS Comp. Biol. 8, e1002512 (2012)

# Mapping forces in moving epithelial cell fronts



Trepat et al, Nat. Phys. 8, 628 (2012)

Dickinson et al., J. Math. Biol. 31, 563 (1993)  
 Callaghan et al., J. Stat. Phys. 122, 909 (2006)  
 Khain et al., J. Stat. Phys. 128, 209 (2007)

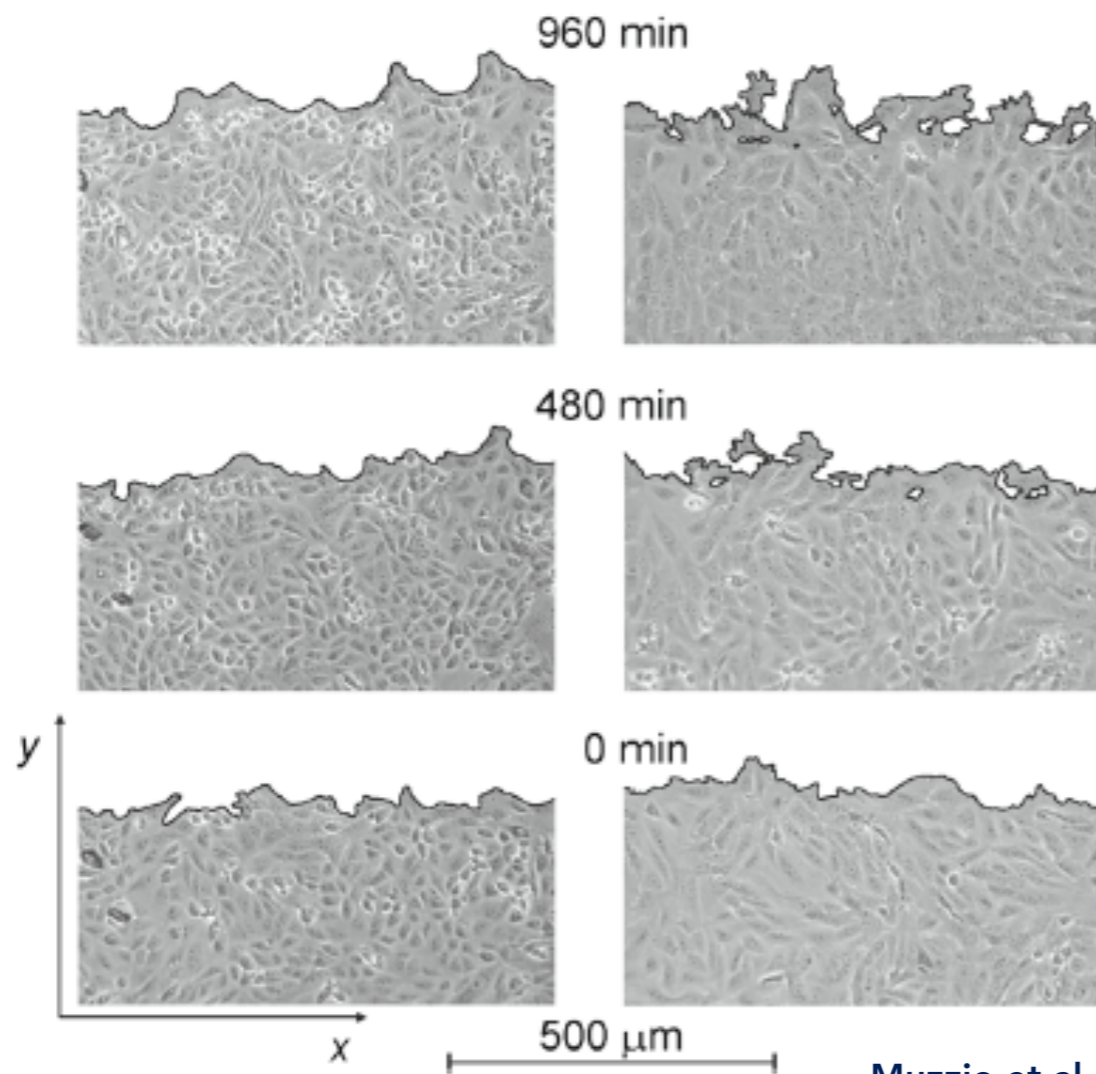
Trepat et al, Nat. Phys. 5, 426 (2009)  
 Vedula et al., Nat. Comm. 6, 6111 (2015)

Tembe et al., Nat. Mat. 10, 469 (2011)  
 Kim et al., Nat. Mat. 12, 856 (2013)



# Controlling cell colony geometry and dynamics

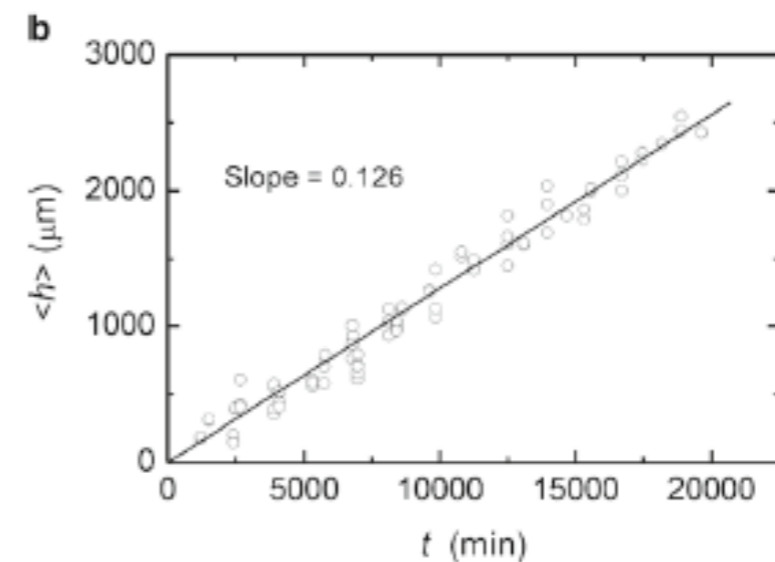
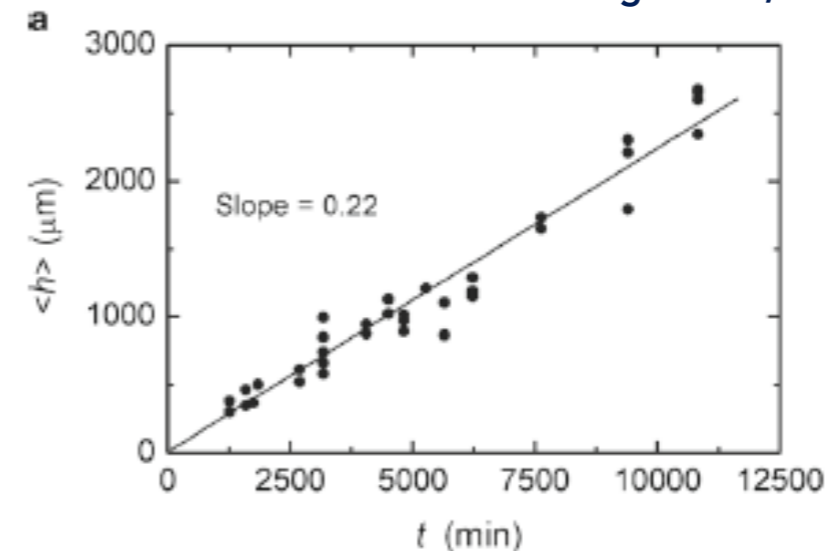
## Effects of sol vs gel medium



Vicsek et al., Phys. A 167, 315 (1990)

Huergo et al., PRE 82, 031903 (2010)

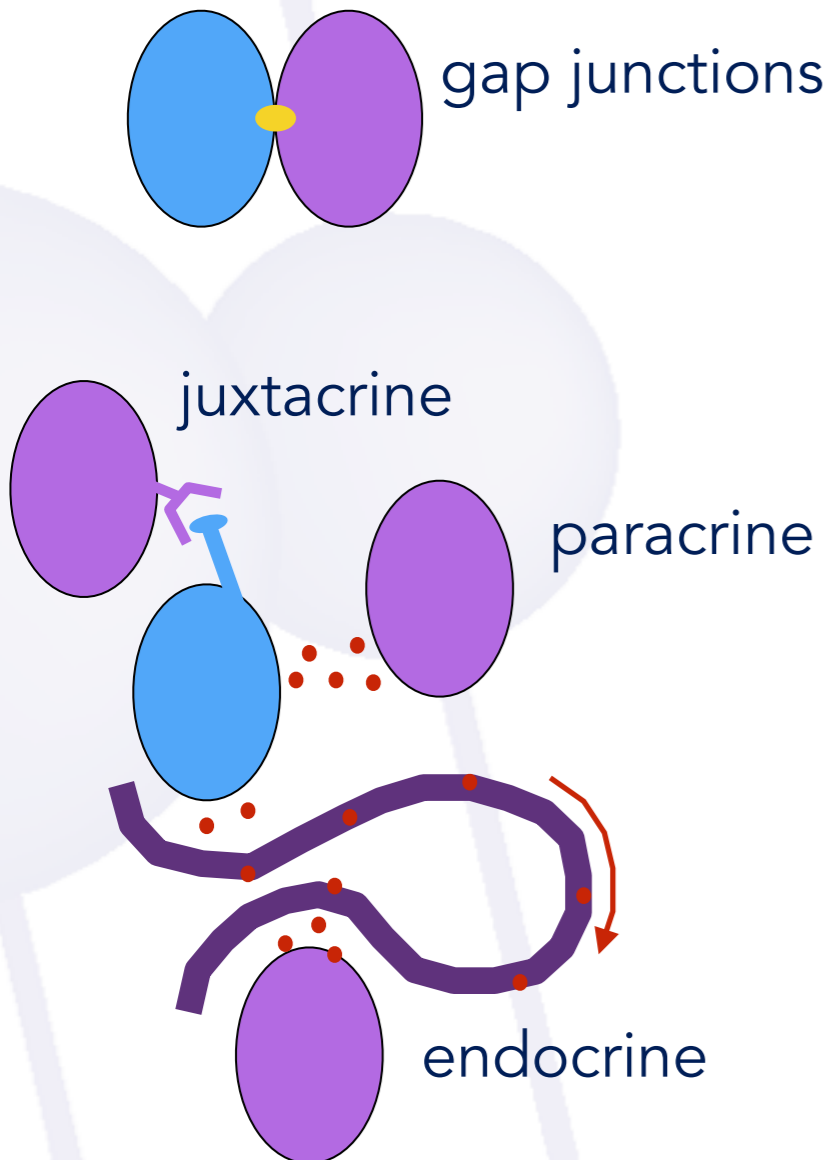
Huergo et al., PRE 84, 021917 (2011)



Can the “physics” (roughness scaling, dynamics) tell us useful information about the biological processes during front growth?

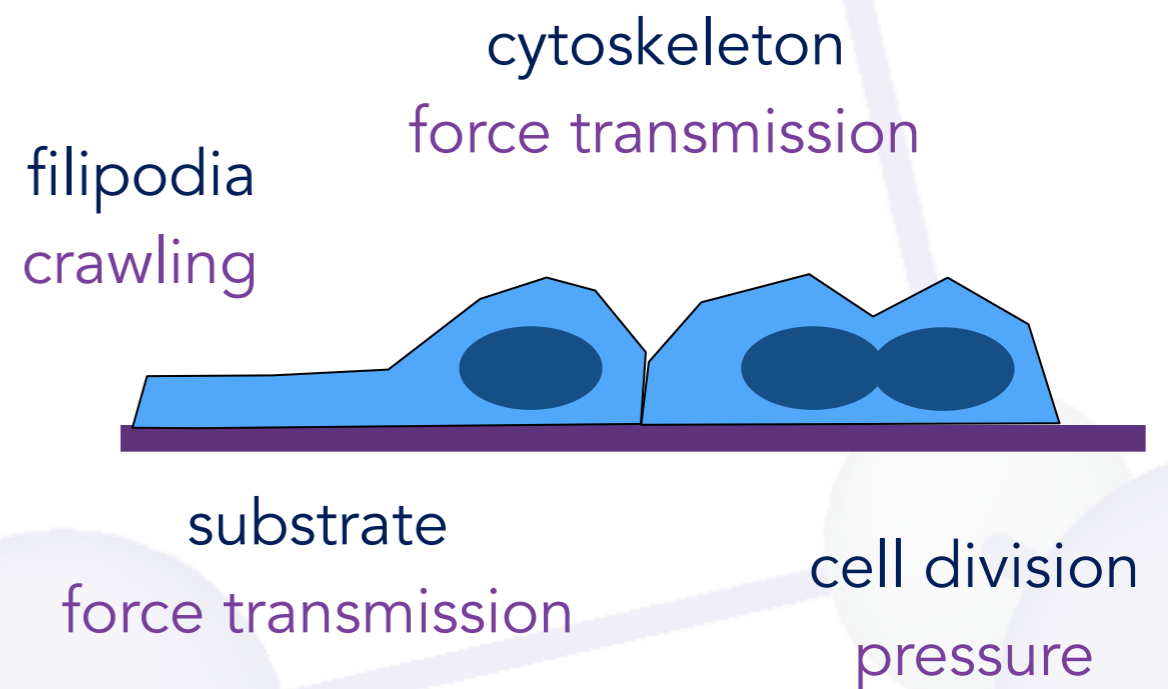
Can we correlate the roughness scaling and dynamic behaviour with specific interactions governing front behaviour from sub-cellular to multicellular level?

## chemical



cell communication  
in proliferating front

## mechanical



Can we correlate the roughness scaling and dynamic behaviour with specific interactions governing front behaviour from sub-cellular to multicellular level?

### **geometry**

- what is the roughness / scaling
- evolution
- lengthscale/regime crossovers

### **dynamics**

- what is the front displacement / speed
- global vs. local effects
- circadian/clock effects

### **inhibitor effects**

- cytochalasin B - cytoskeleton/lamellipodia/cytokinetics
- colchicine - microtubules/spindle/mitosis
- meclofenamic acid (MFA) - gap junctions
- forskolin - cAMP levels

# Experimental setup (physicists doing biology)

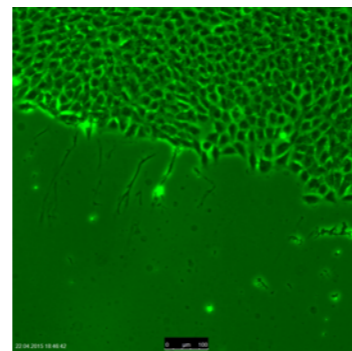
scratch assay: silicon insert liftoff from plate of confluent epithelial RAT1 cells, ideal 1D front model system



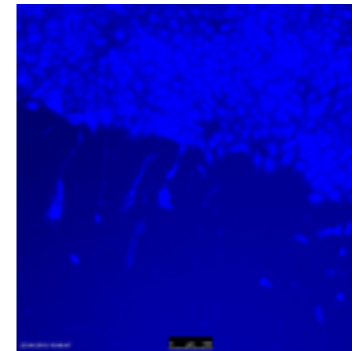
Benedikt  
Ziegler



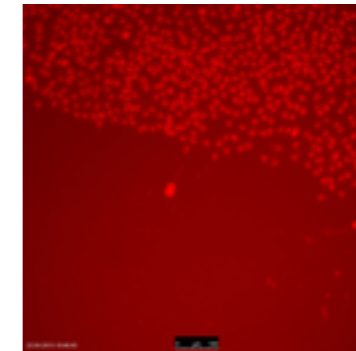
Guillaume  
Rapin



Optical



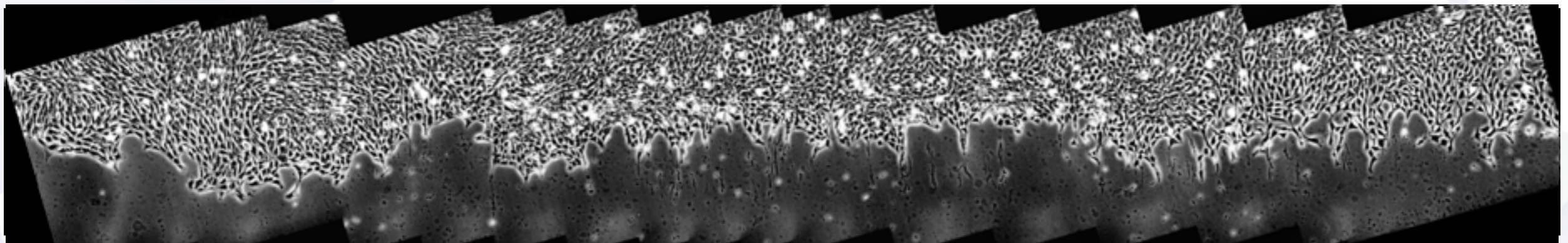
Cytoplasm



Nuclei

cytoplasm and nuclei staining, GFP labelling

fluorescence microscopy of front at 4 hour intervals

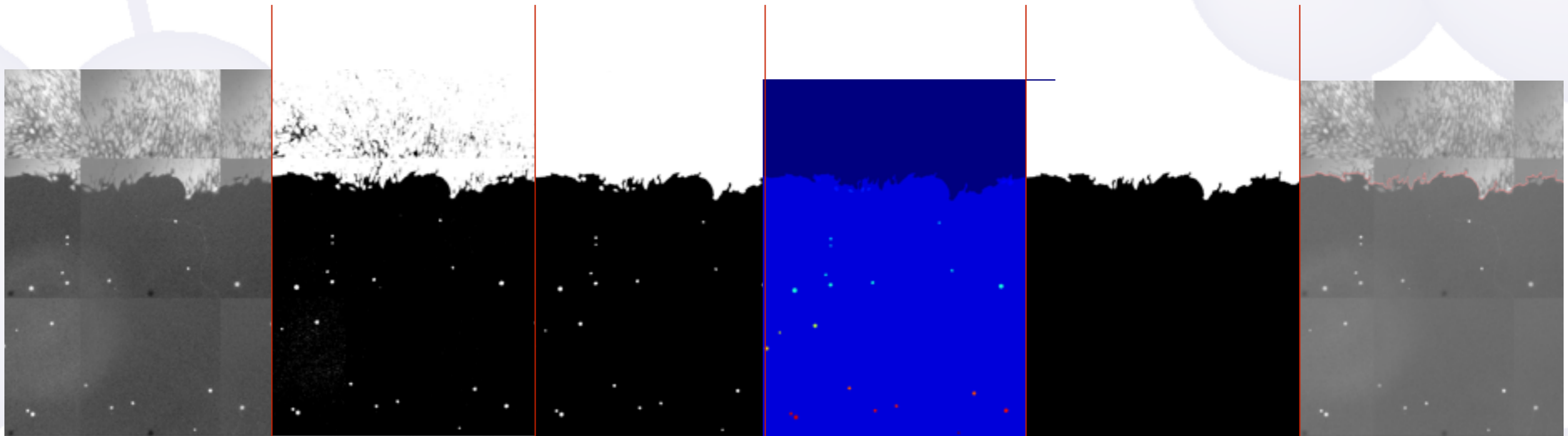


# Measuring cell front roughness and dynamics



panorama of stitched front images 6.0 cm

identifying continuous front as  
largest subdomain



binarisation and noise cleaning

extracting  
front position  
for analysis

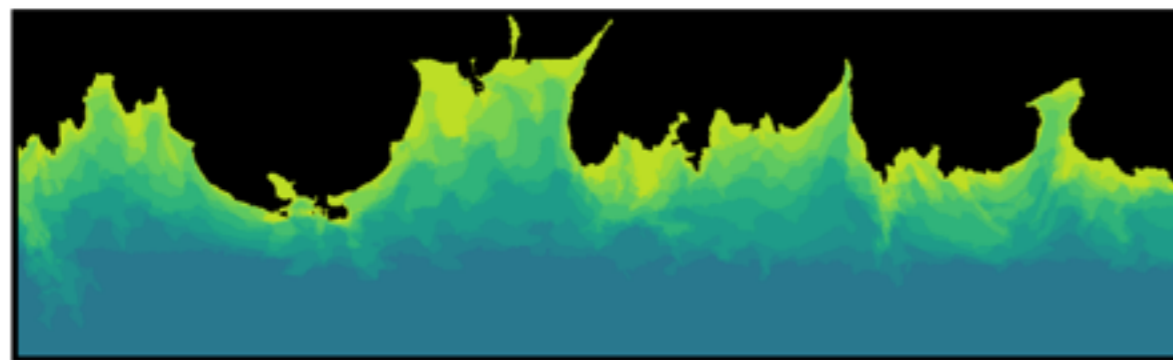
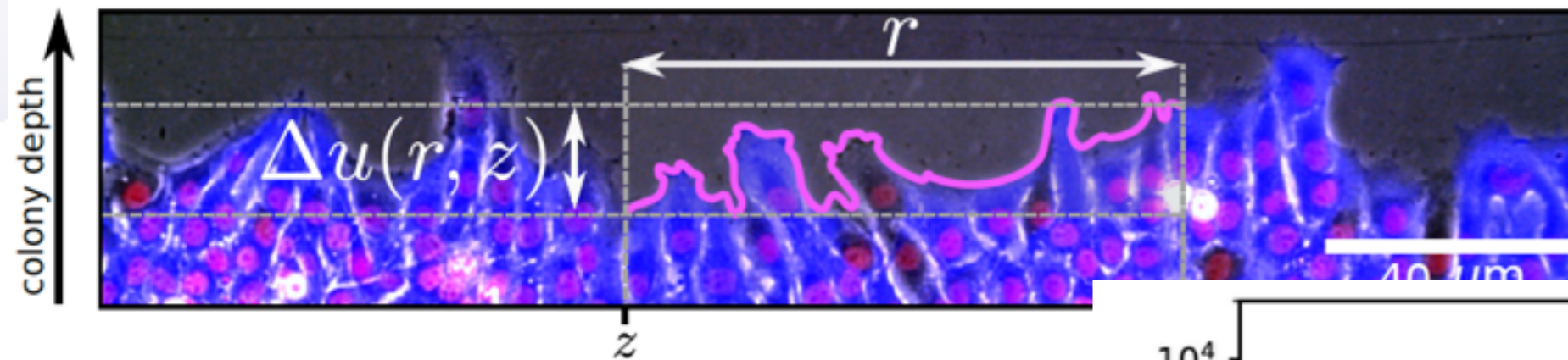
# Front proliferation under control conditions



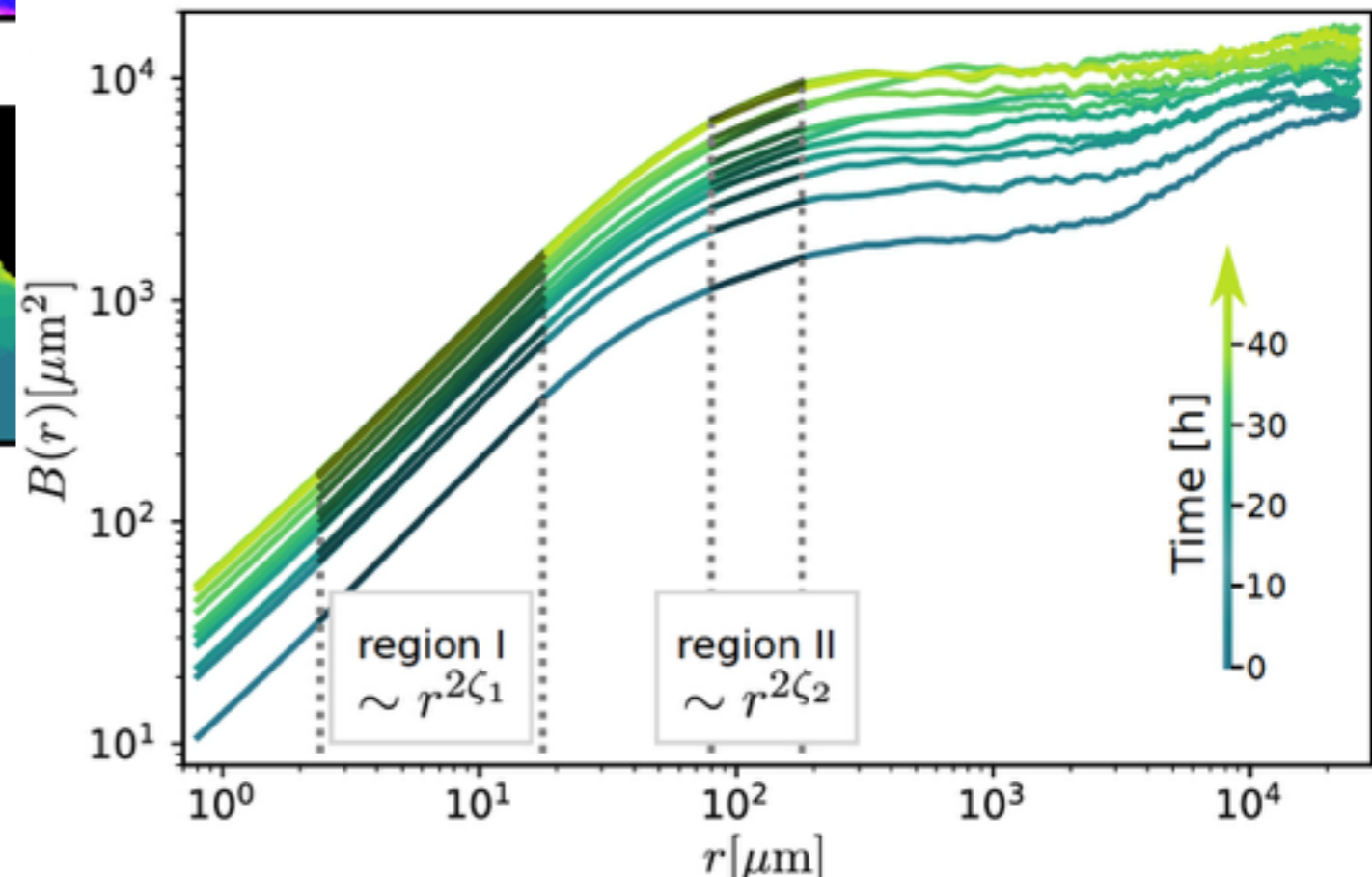
Nirvana Caballero



Guillaume Rapin



Rapin, Caballero et al. npj Sci. Rep. 11, 8869 (2021)

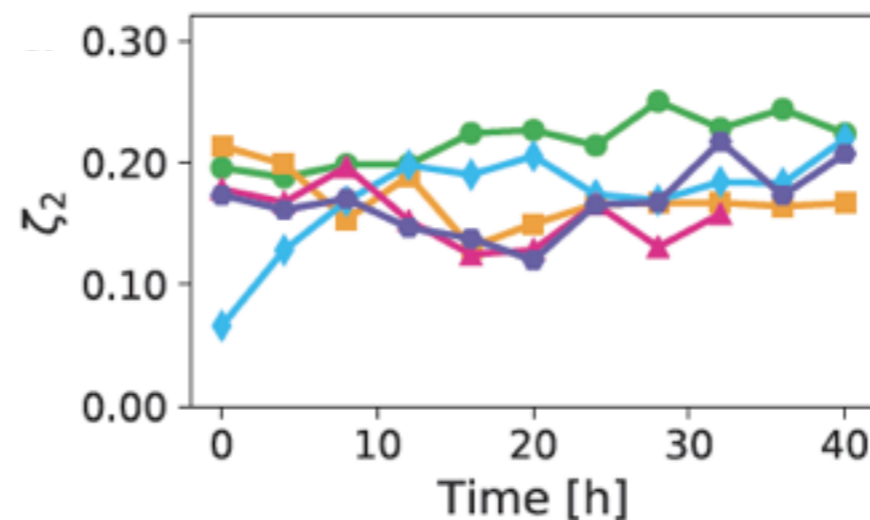
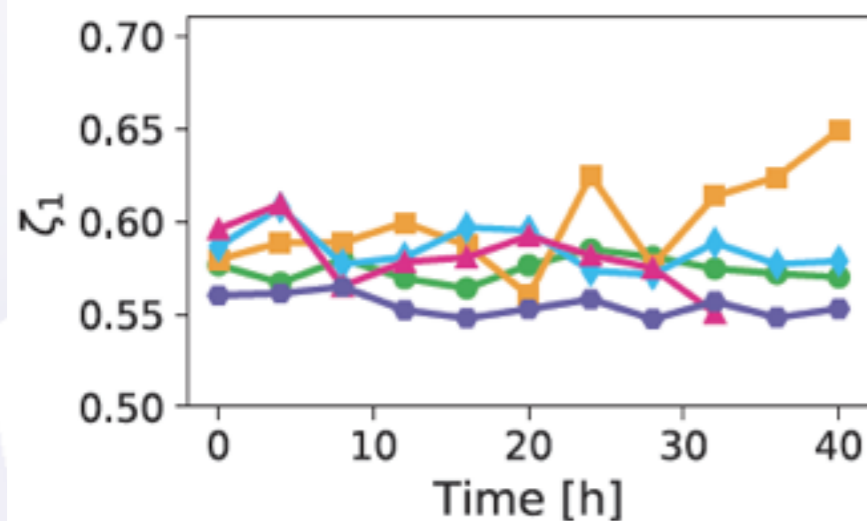
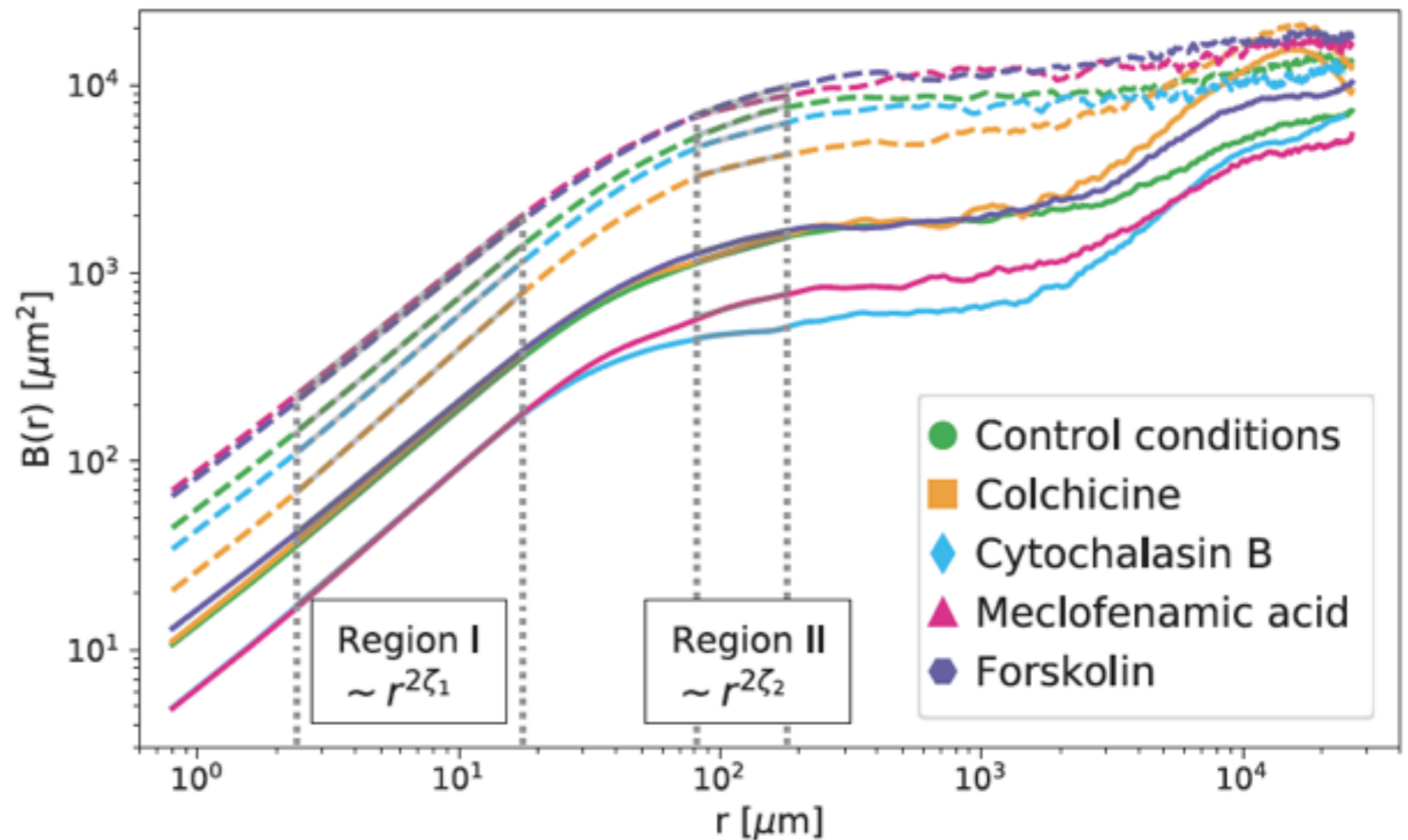
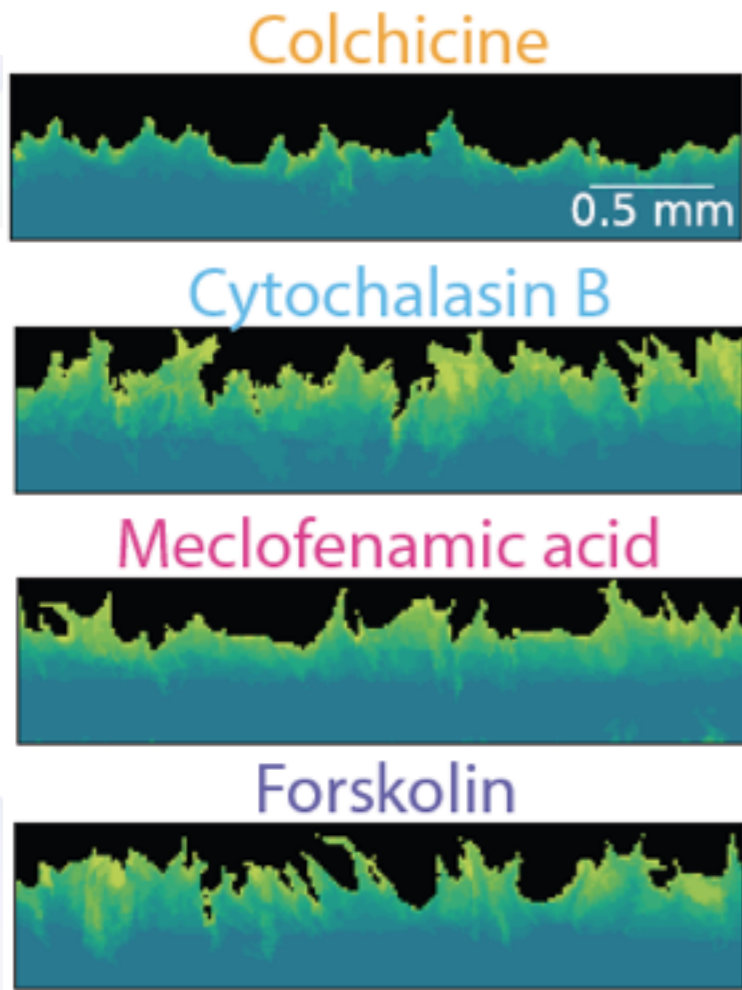


Saturation of front roughness at high length scales

Roughness scaling with  $\zeta \sim 0.2$  at few-cell lengthscales

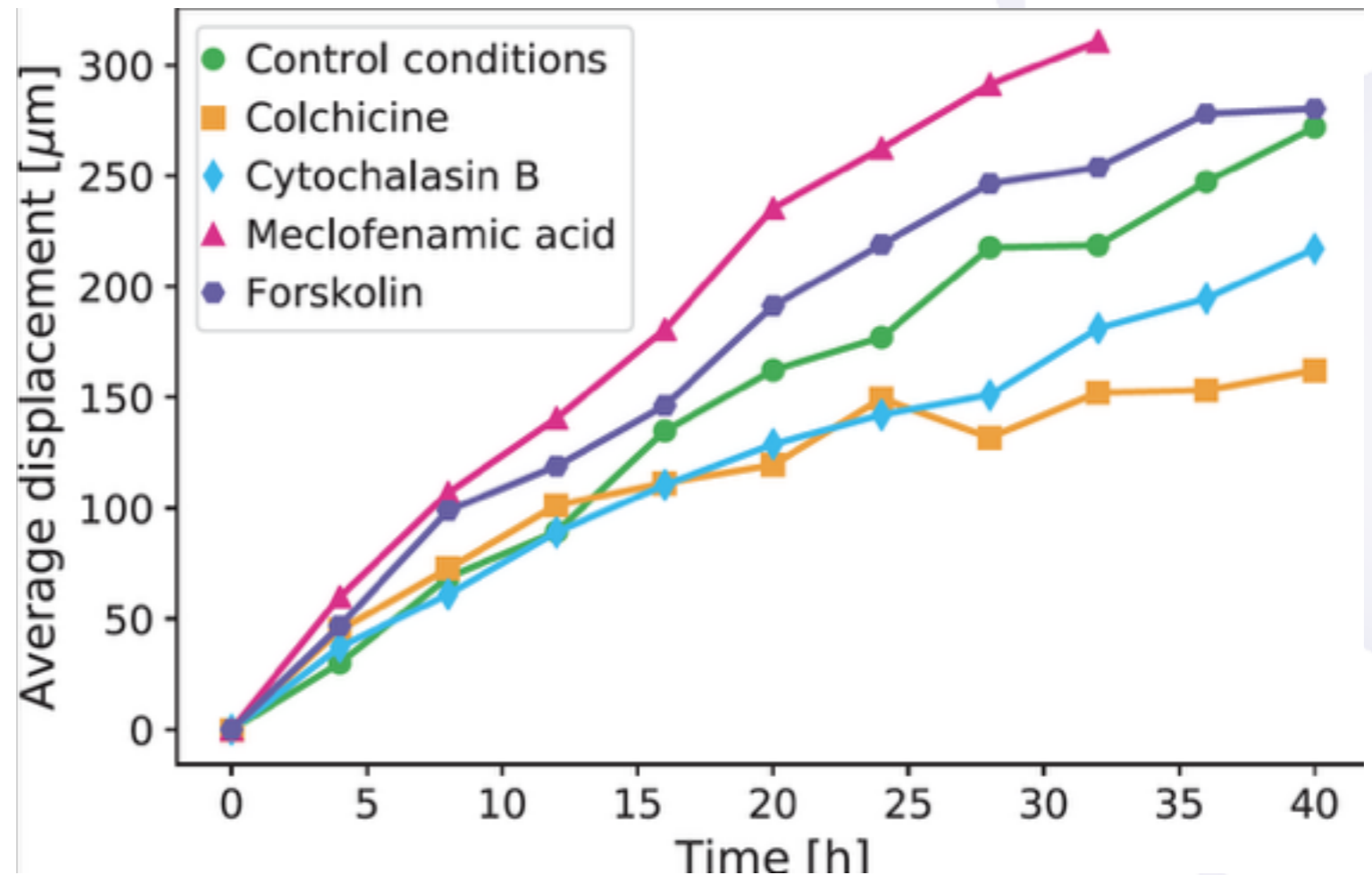
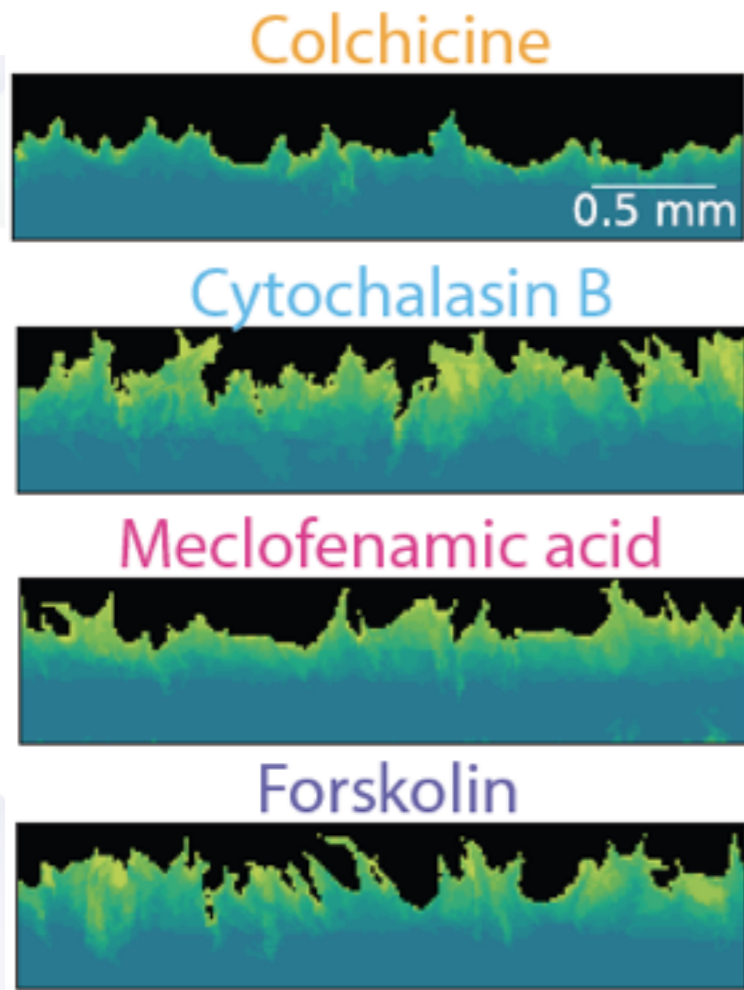
Roughness scaling with  $\zeta \sim 0.6$  at sub-cell lengthscales

# Targeting different interactions using inhibitors



Inhibitors do not appear to have significant effects on the roughness exponent values but modulate the roughness itself

# Targeting different interactions using inhibitors



Inhibiting cell division by colchicine and disrupting cell motility/cytoskeleton via cytochalasin-B significantly slows front motion and decreases roughening, while MFA inhibition of gap junctions and forskolin activation of c-AMP accelerate front motion and increase roughening



# Comparison with numerical simulations



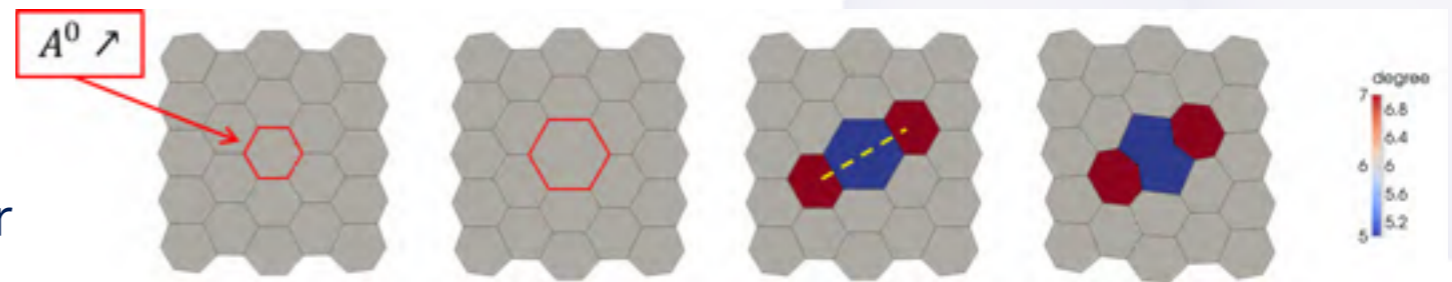
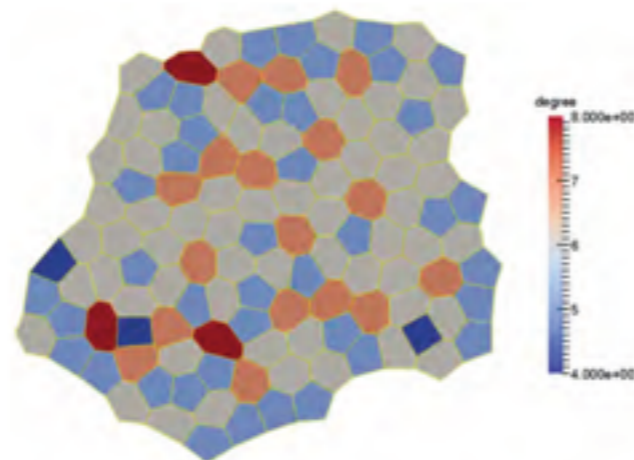
Aziza Merzouki Bastien Chopard

[epicells.unige.ch](http://epicells.unige.ch)

$$H = \sum_{\text{all cells } \alpha} \frac{1}{2} K_{\alpha} (A_{\alpha} - A_{\alpha}^0)^2 + \sum_{\text{all cells } \alpha} \frac{1}{2} \Gamma_{\alpha} L_{\alpha}^2 + \sum_{\text{all edges } e_{ij}} \Lambda_{i,j} L_{i,j}$$

Merzouki et al, Soft Matter 12, 4745 (2016)

2D vertex model of confluent cell layer incorporates cell area elasticity, cell perimeter contractility and intercell line tension, developed to model mechanical properties of epithelial sheet

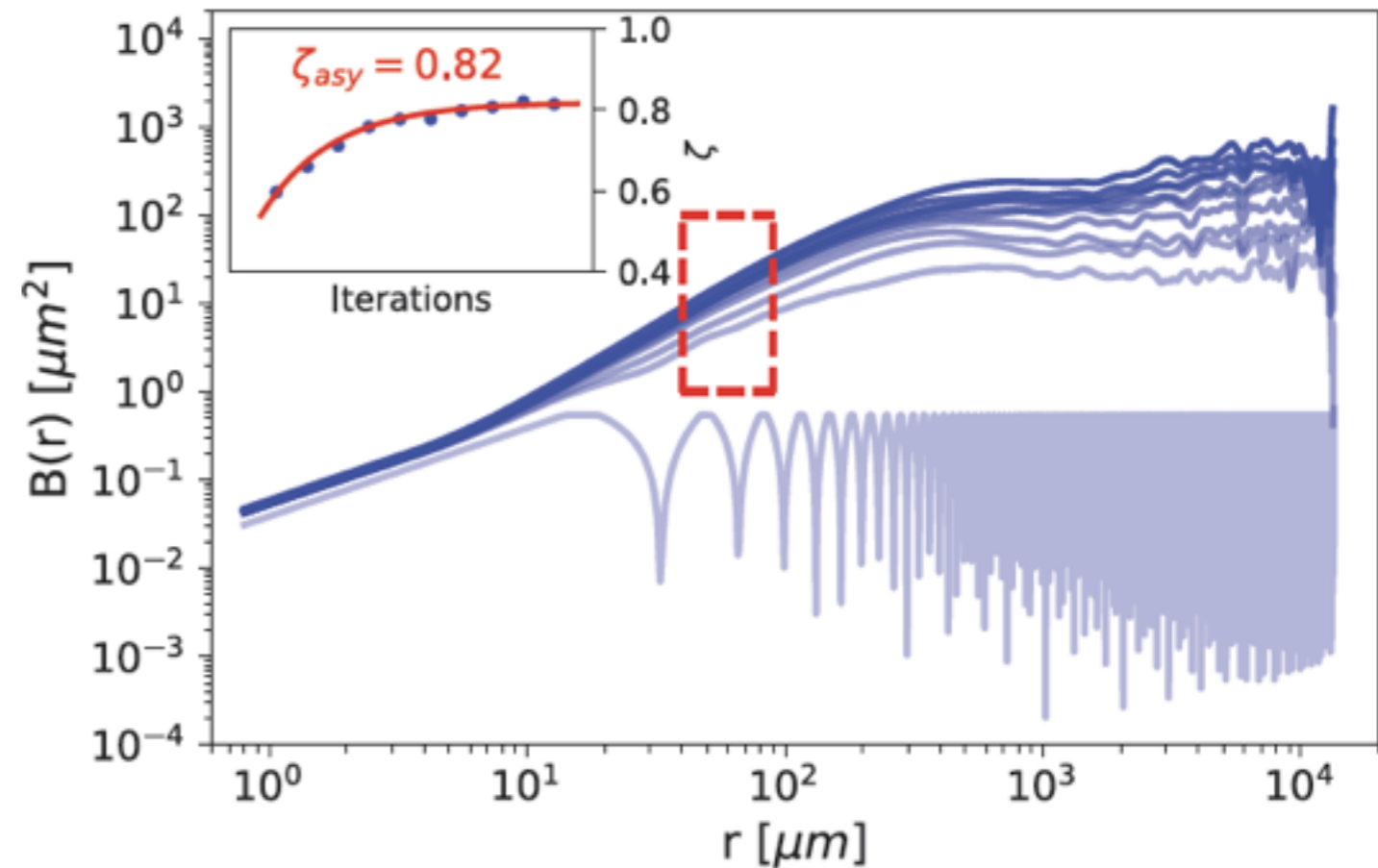
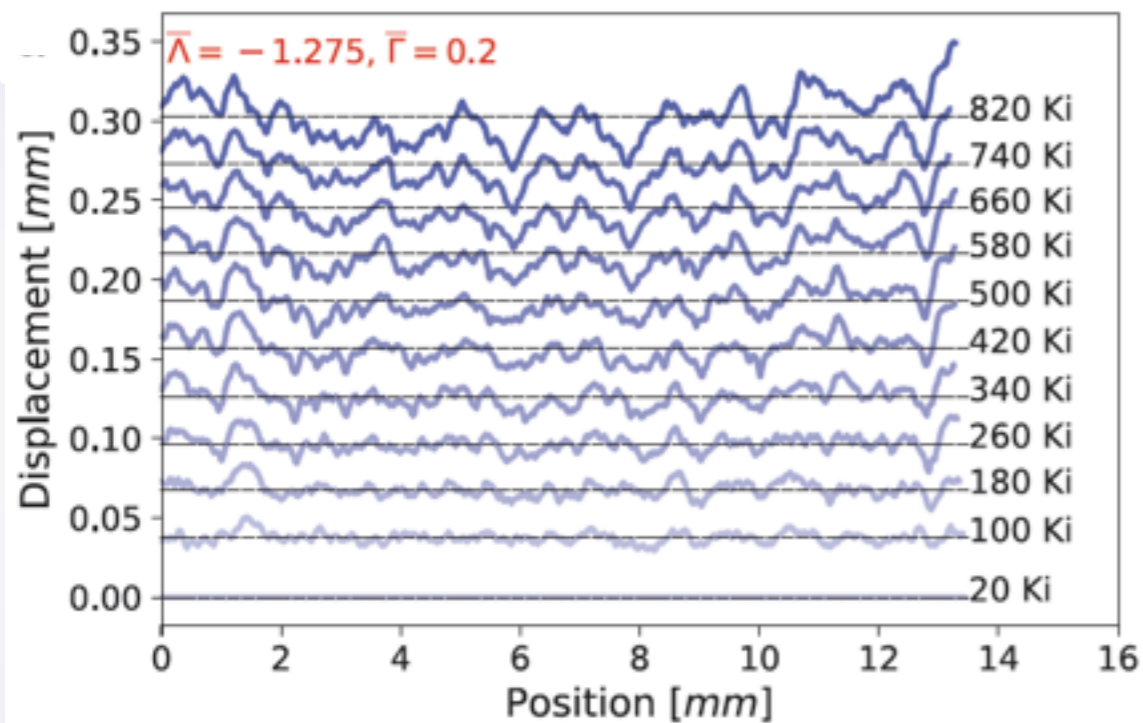
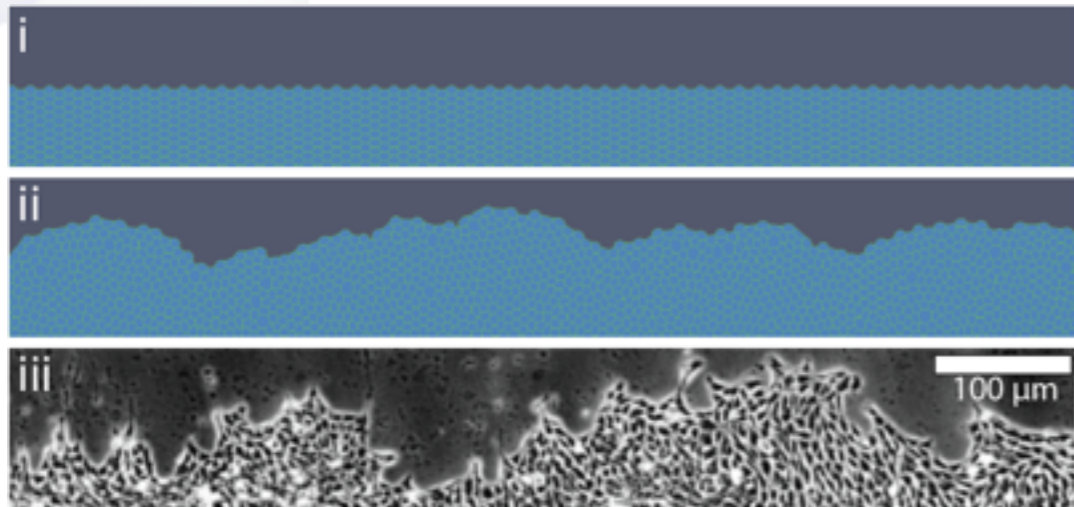


- set original vertex positions, minimise  $H$
- probability of cell growth at adjustable rate up to fixed threshold
- probability of cell division based on random / oldest first/biggest first choice, always along shortest edge-edge axis
- adjustable elastic constraints set boundary conditions (wall vs. medium)
- minimise  $H$ , iterate

# Comparison with numerical simulations

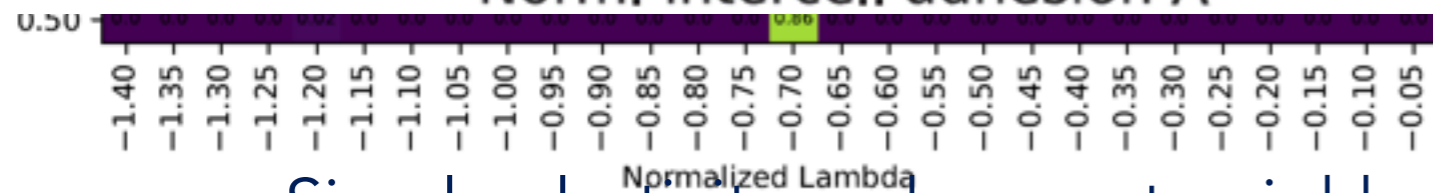
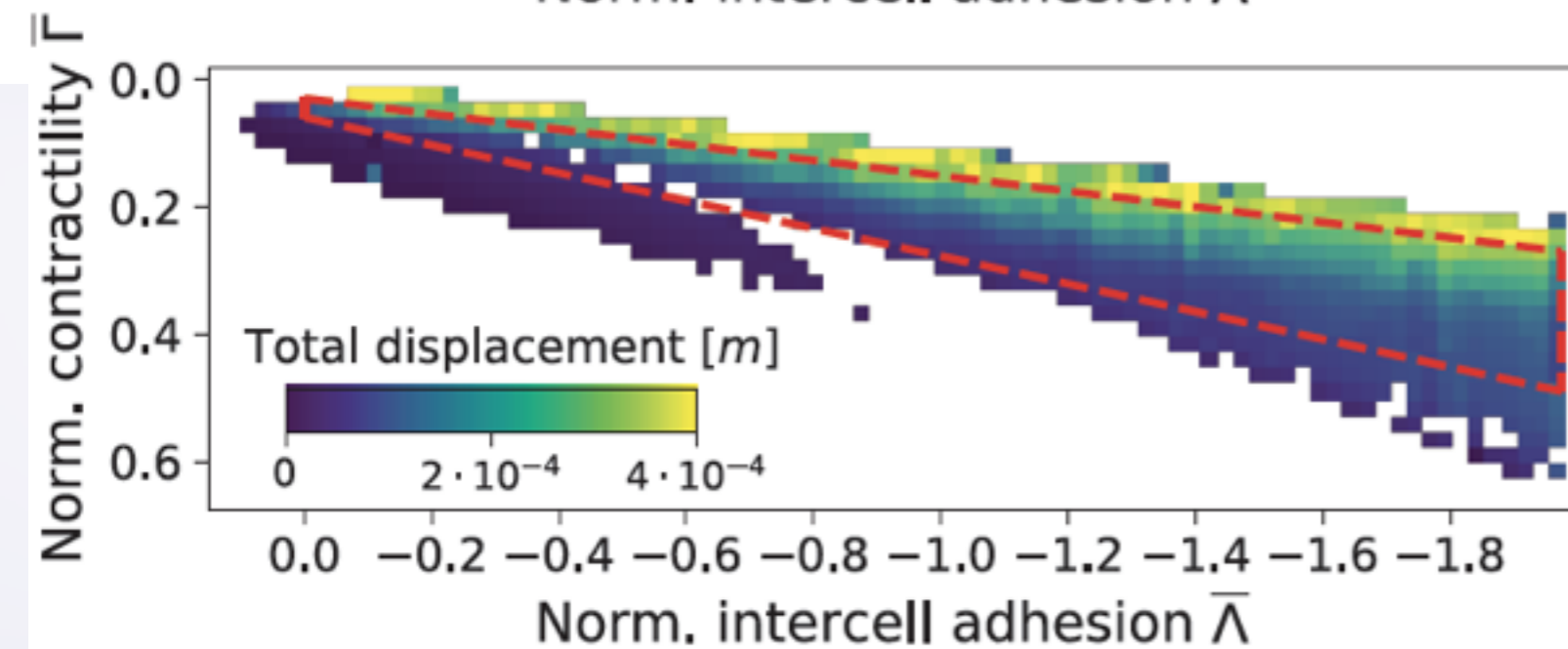
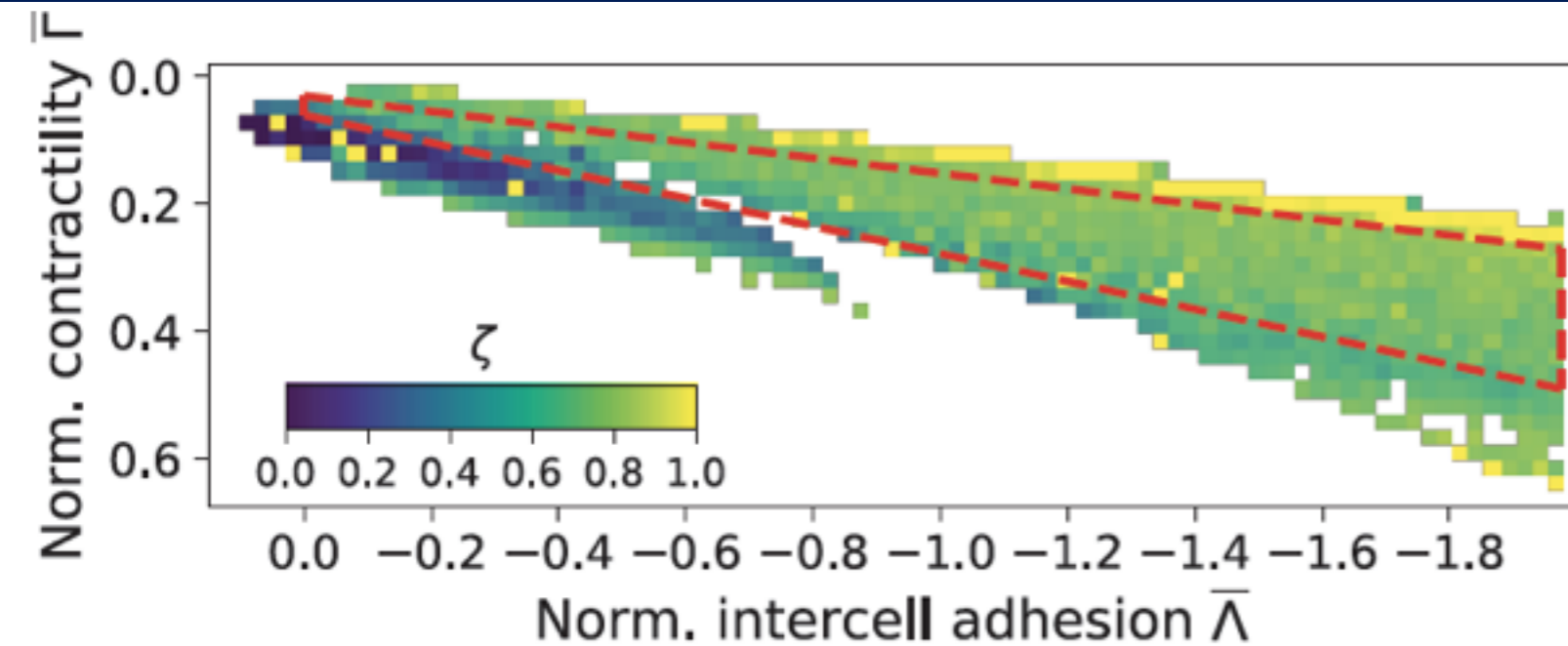


Iaroslav  
Gaponenko

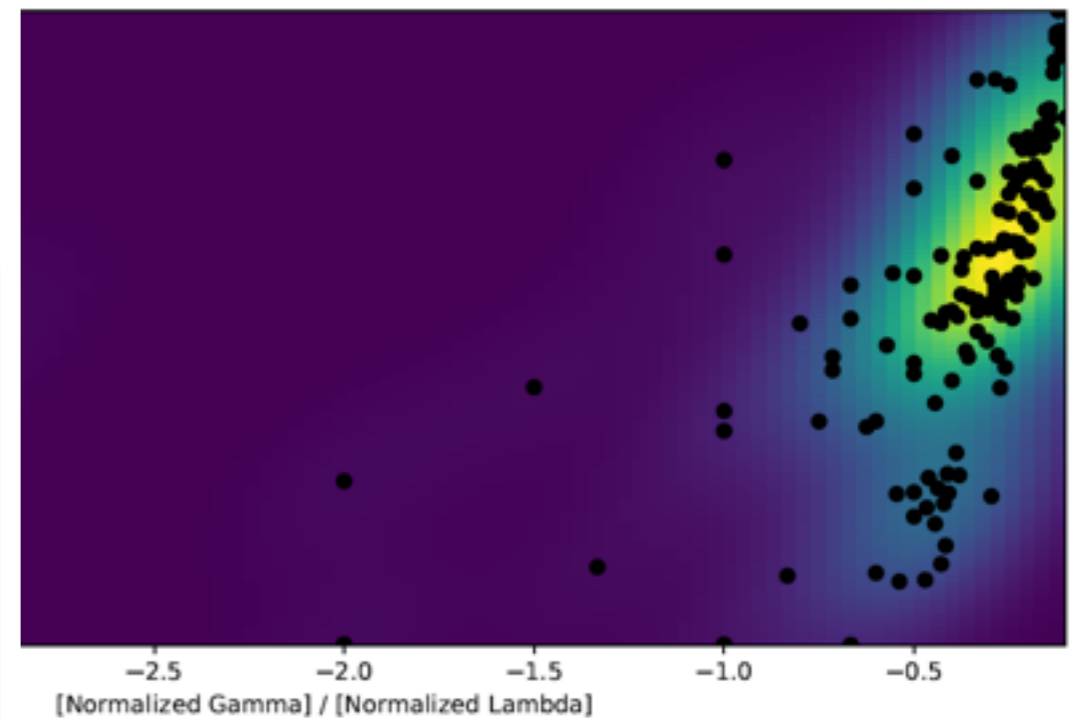


Tissue relevant information as well as cell front position and roughness can be extracted from each simulation run

# Mapping out a roughness “phase diagram”



key parameter for simulation viability is ratio between normalised cell perimeter contractility and intercell line tension



$\zeta$  values ranging from 0.4 - 1.0, with optimum of around 0.65

Rapin, Caballero et al. npj Sci. Rep. 11, 8869 (2021)

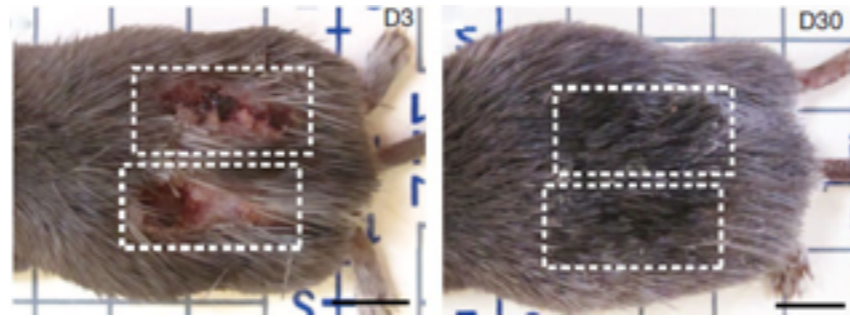
Simple elasticity and nearest neighbour interactions do not reproduce the lower zeta values /second power law scaling regime

# Perspectives

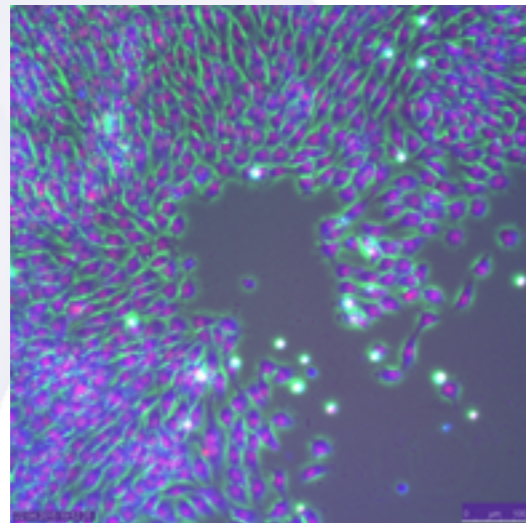
- compare epithelial cell fronts from known pathological and prolific wound healing phenotypes



Spiny mice: *Acomys*



Seifert et al, Nat. 489, 561 (2012)



- explore effects of varying front curvature, cell size, clock gene mutations, substrate mechanics

- use measurements of cell front roughness to suggest potential interaction at play in wound healing mutations of unknown origin



# Thank you !

Iaroslav Gaponenko  
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Benedikt Ziegler  
Sophia Ehrensperger

Jambunathan Karthik, Lane W. Martin

Steven Brown

Aziza Merzouki, Bastien Chopard

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Alejandro Kolton, Sebastian Bustingorry

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UniGE



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