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Phase-field and Monte Carlo simulations of ferroelectric domain structures: Two simple cases

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Group page http://pld.nju.edu.cn/

Acknowledgement

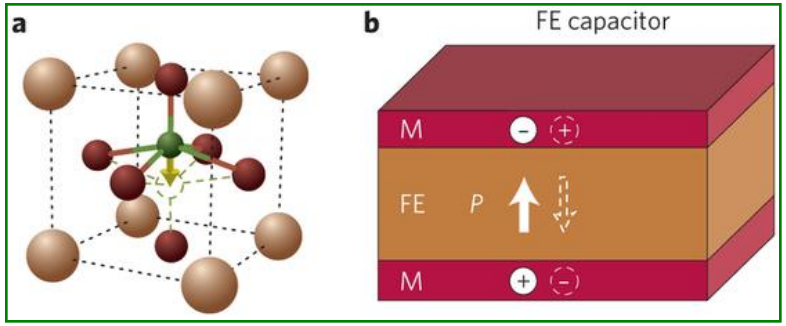
- **P. Chu,** **Y. Zhang,** **Y. L. Xie**



- **Funding Agencies: NSFC & 973 Programme**

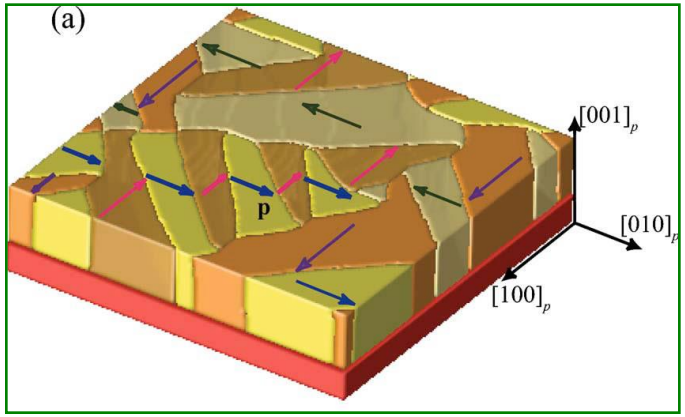
Background: domain

- **Ferroelectricity**



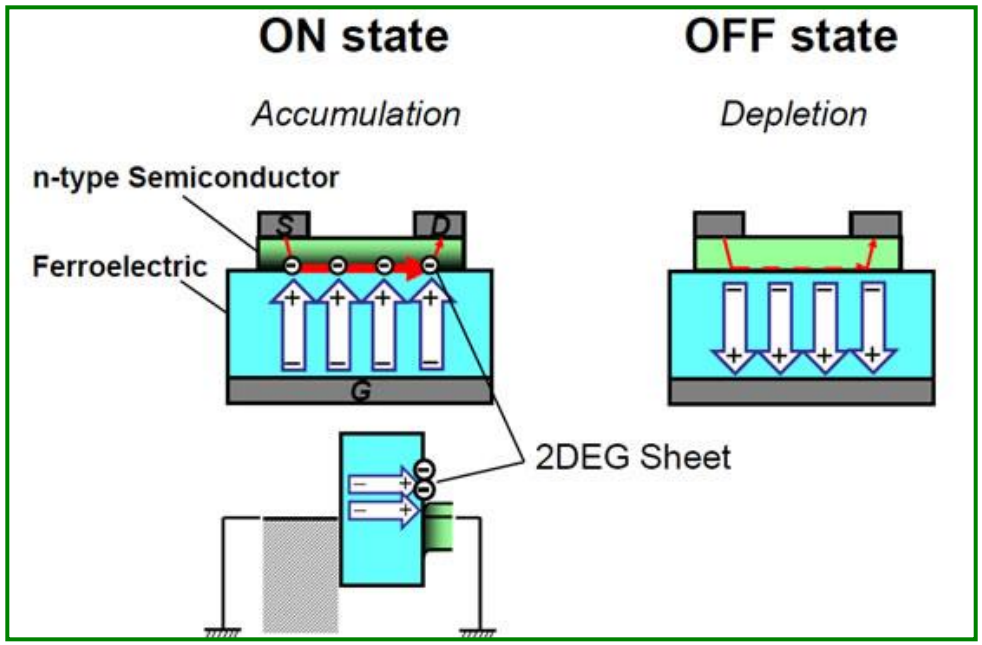
Polarization

E.Y.Tsymbal & A.Gruverman, NM 12, 602 (2013)

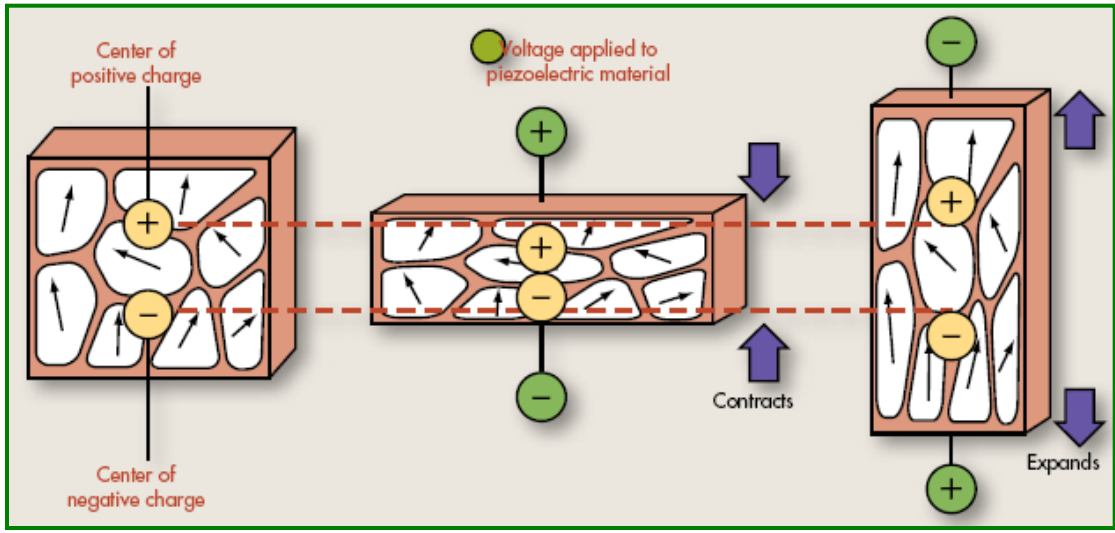


Domain

Gopalan Group



Memory devices



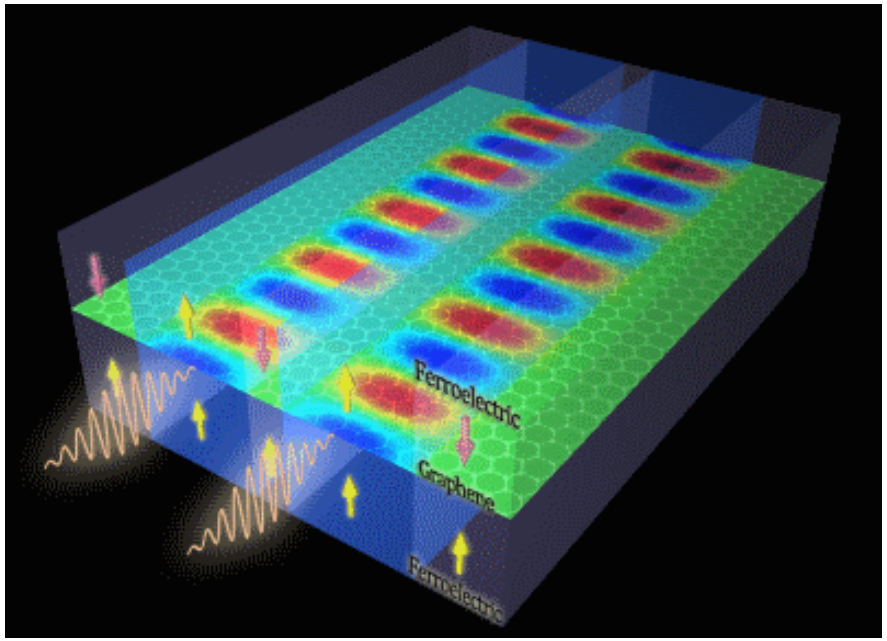
Sensor & actuator devices

Work 1: microwave dielectric response

- 90^{o} domain structure contribution
- External normal strain effect

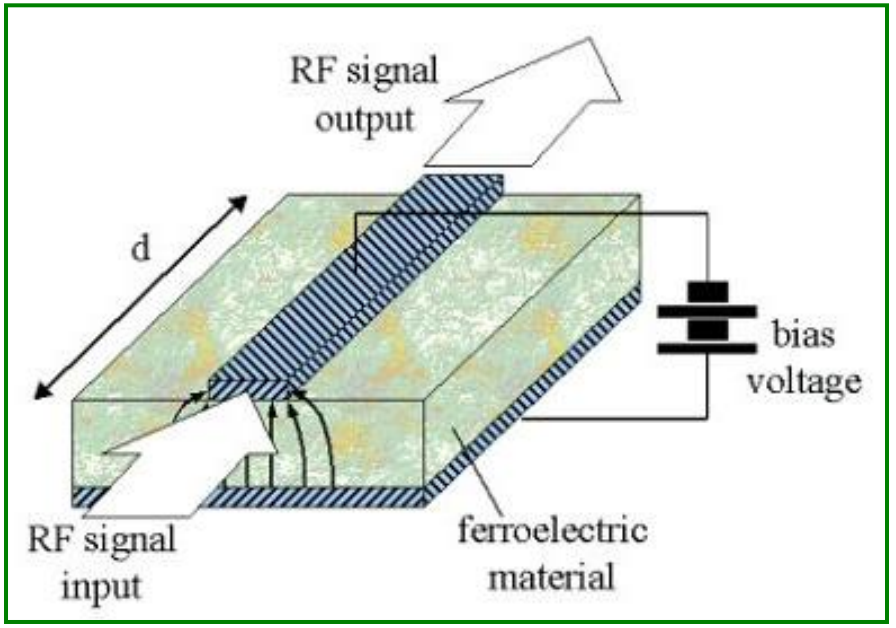
Background: domain

- **Dielectric microwave**

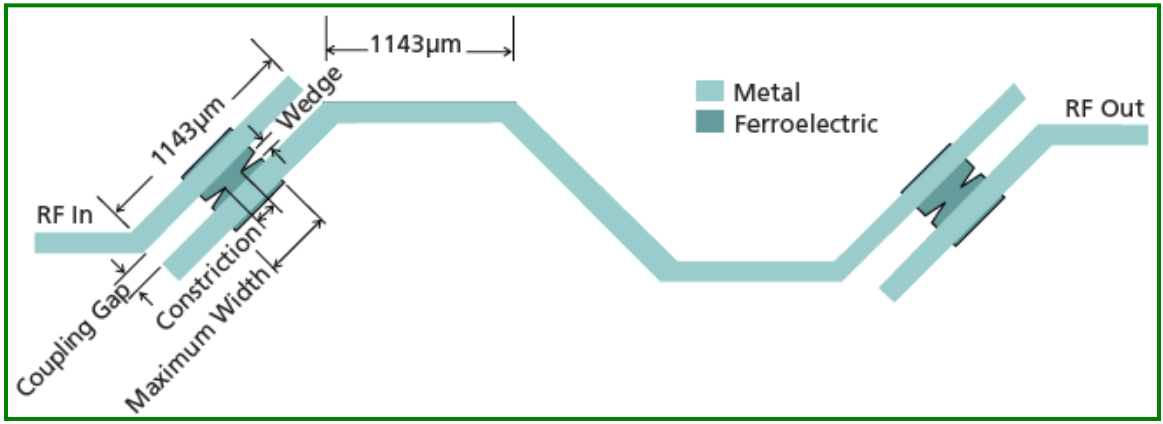


MIT

Terahertz optical memories boost density 10-times by sandwiching high-mobility graphene between two layers of ferroelectric materials



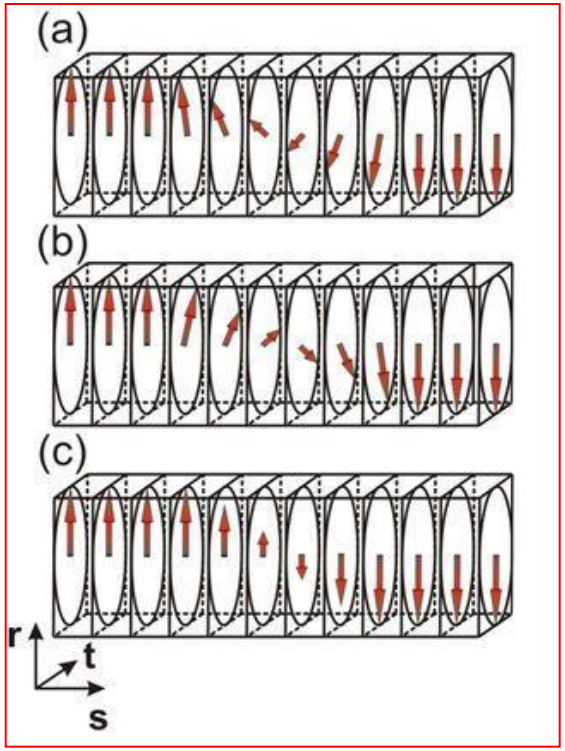
Ferroelectric phase shifter

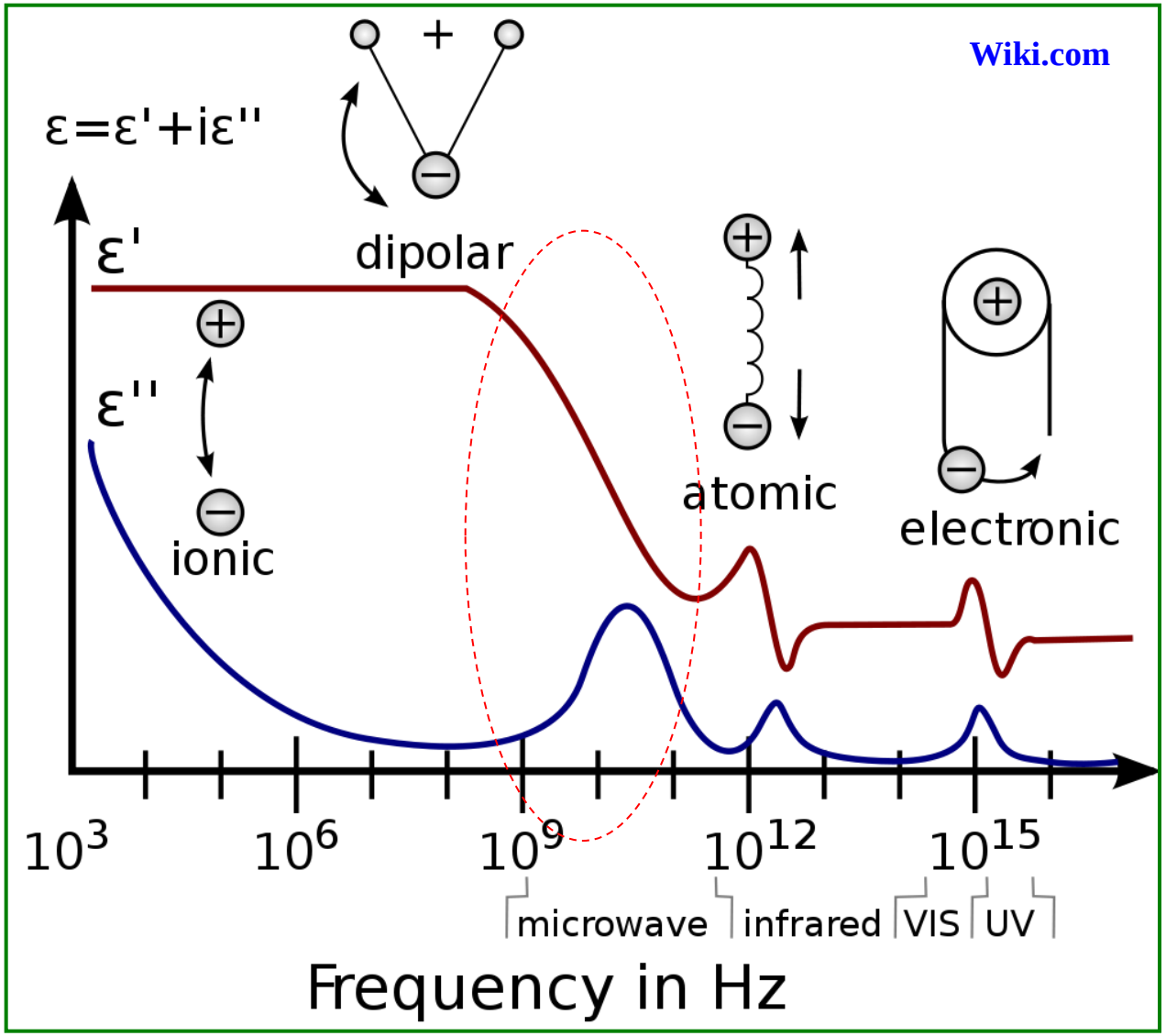


One-pole microstrip filter with etched ferroelectric layer

Motivations: domain structure

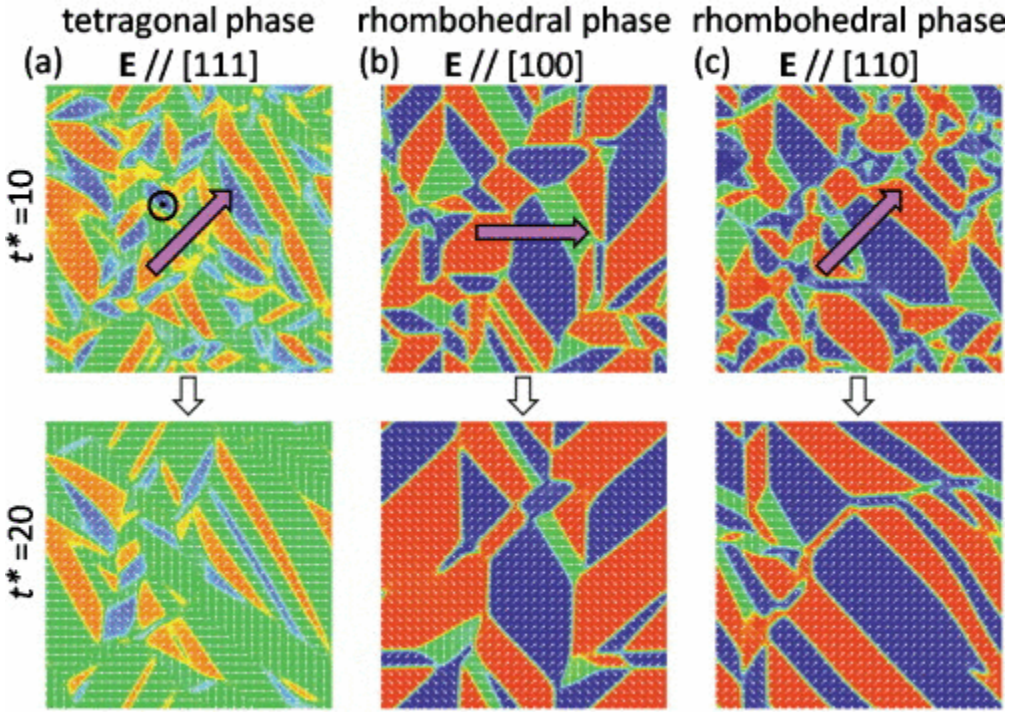
- **Domain structures and high-*f* dielectric response**

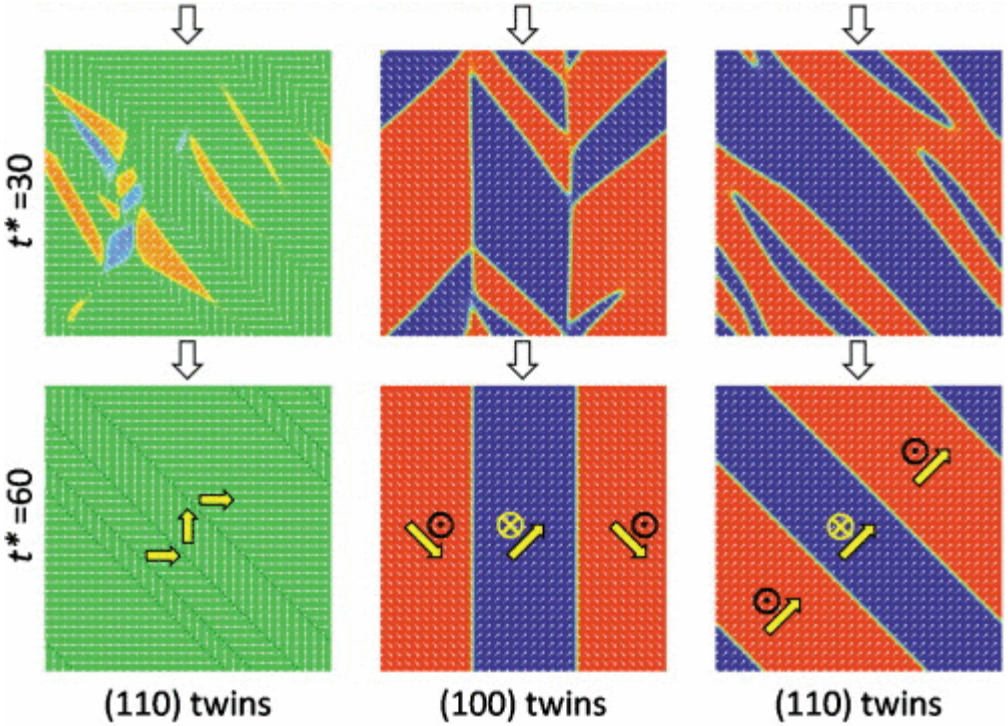




Work 1: microwave dielectric response

- **Phase-field method**





$BaTiO_3$ From W.F.Rao et al, APL 97, 162901 (2010)

Work 1: microwave dielectric response

- **Thermodynamics**

$$F = F_{ld} + F_g + F_{dd} + F_{el} + F_{es} + F_{se}$$

$$\frac{\partial P(r,t)}{\partial t} = -D\frac{\delta F}{\delta P(r,t)}$$

$$P(t) = \int_{-\infty}^{t} \varepsilon(t-t')E_{ext}(t')dt'$$

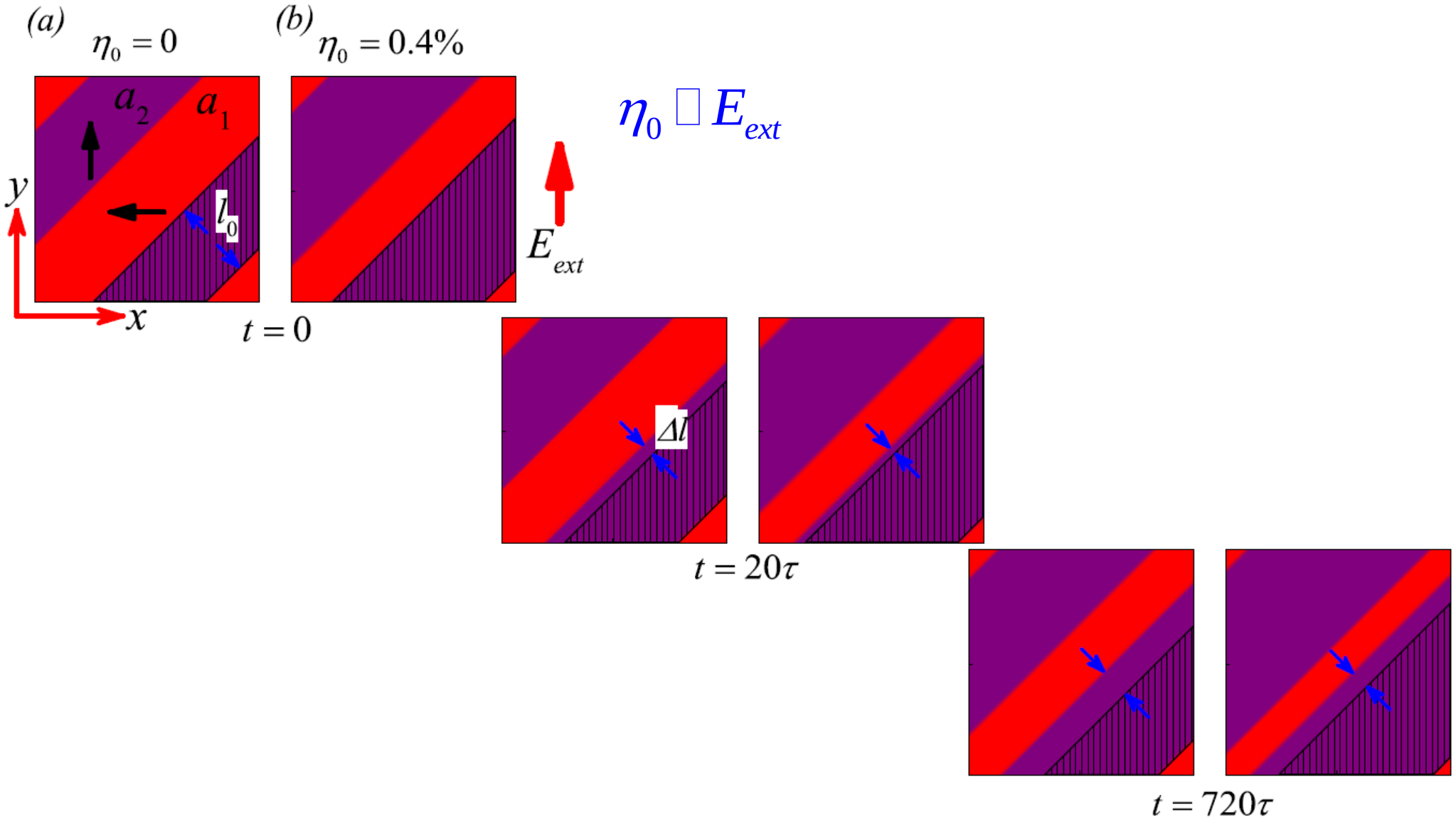
$$P(\omega) = \varepsilon(\omega)E_{ext}(\omega)$$

Physical parameters chosen for the simulation ($\tau^{-1} = |A_1|D$). All these parameters appear in the dimensionless form.

Parameter (unit)	Value	Parameter (unit)	Value	Parameter (unit)	Value
L	64~256	A_1^* ($\|A_1\|$)	-1.00	A_{11}^* ($A_{11}P_0^2/\|A_1\|$)	-0.24
A_{12}^* ($A_{12}P_0^2/\|A_1\|$)	2.50	A_{111}^* ($A_{111}P_0^4/\|A_1\|$)	0.49	A_{112}^* ($A_{112}P_0^4/\|A_1\|$)	1.20
G_{11}^* ($G_{11}/A_1^2\|A_1\|$)	1.60	G_{12}^* ($G_{12}/A_1^2\|A_1\|$)	0.00	G_{44}^* ($G_{44}/A_1^2\|A_1\|$)	0.80
G'^*_{44} ($G'_{44}/A_1^2\|A_1\|$)	0.80	C_{11}^* ($C_{11}/\|A_1\|P_0^2$)	2.75	C_{12}^* ($C_{12}/\|A_1\|P_0^2$)	1.79
C_{44}^* ($C_{44}/\|A_1\|P_0^2$)	0.543	q_{11}^* ($q_{11}/\|A_1\|$)	0.143	q_{12}^* ($q_{12}/\|A_1\|$)	-0.0074
q_{44}^* ($q_{44}/\|A_1\|$)	0.0157	τ^* (τ)	0.0004		

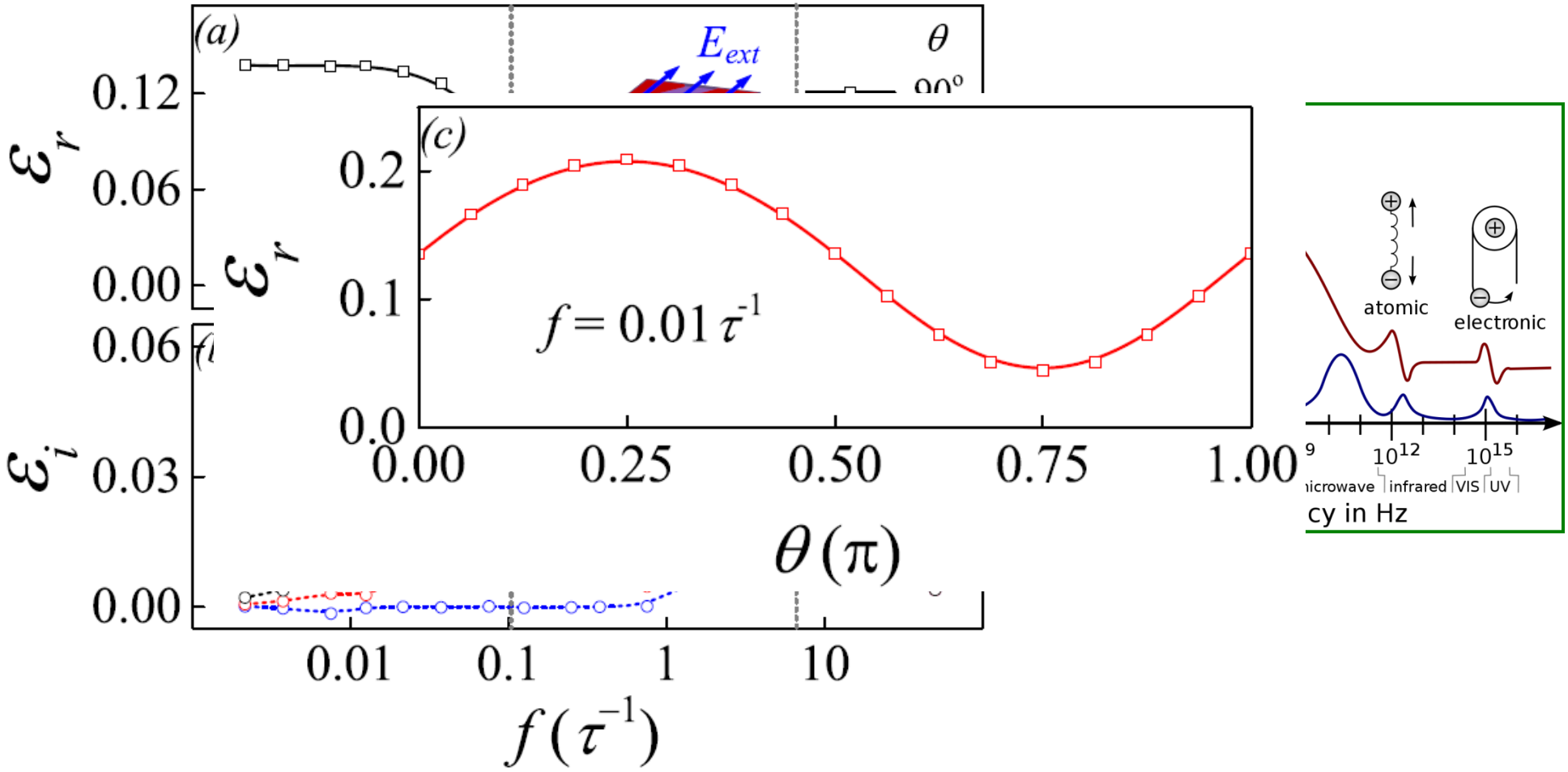
Work 1: microwave dielectric response

- **Domain wall motion with electric bias**



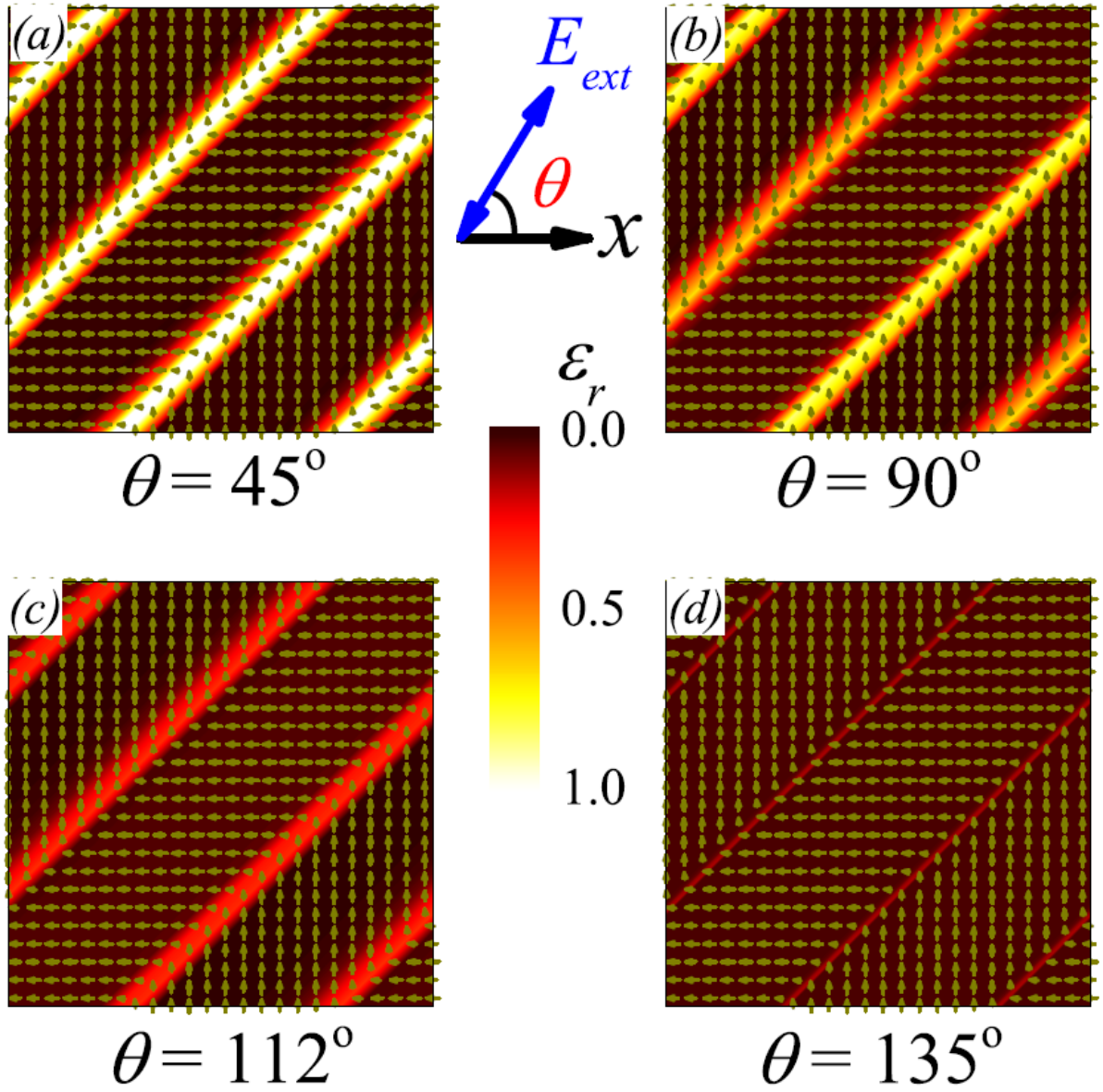
Work 1: microwave dielectric response

- **High-*f* dielectric response**



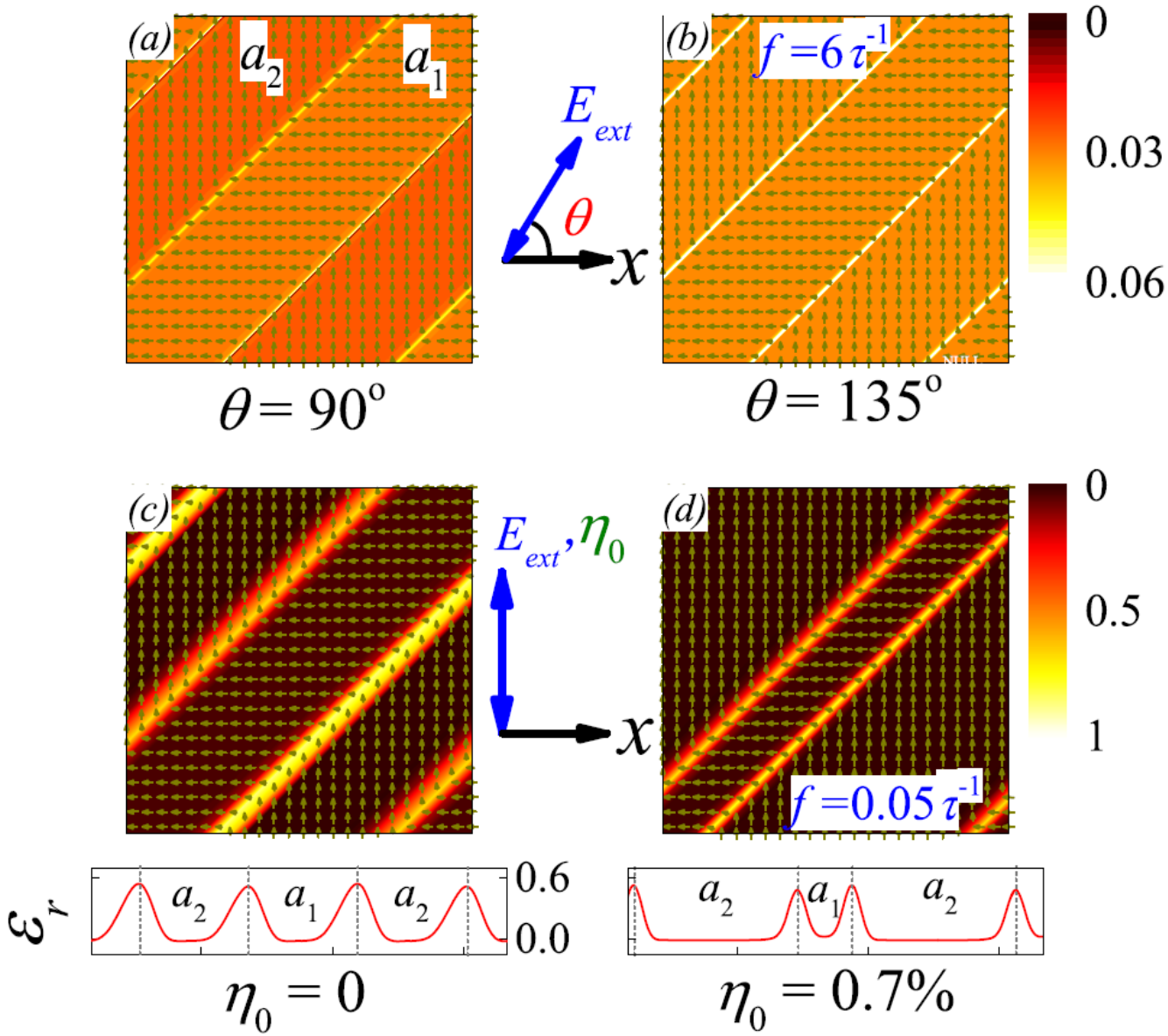
Work 1: microwave dielectric response

- **Domain response: η_0=0**



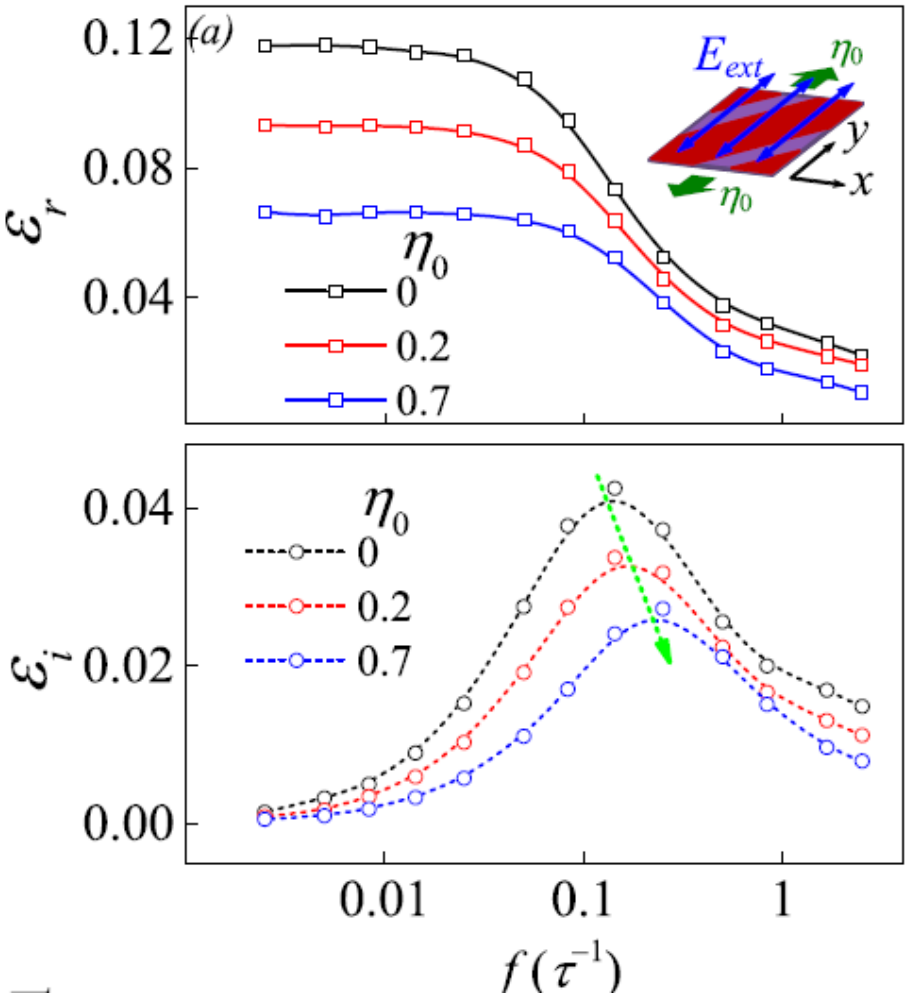
Work 1: microwave dielectric response

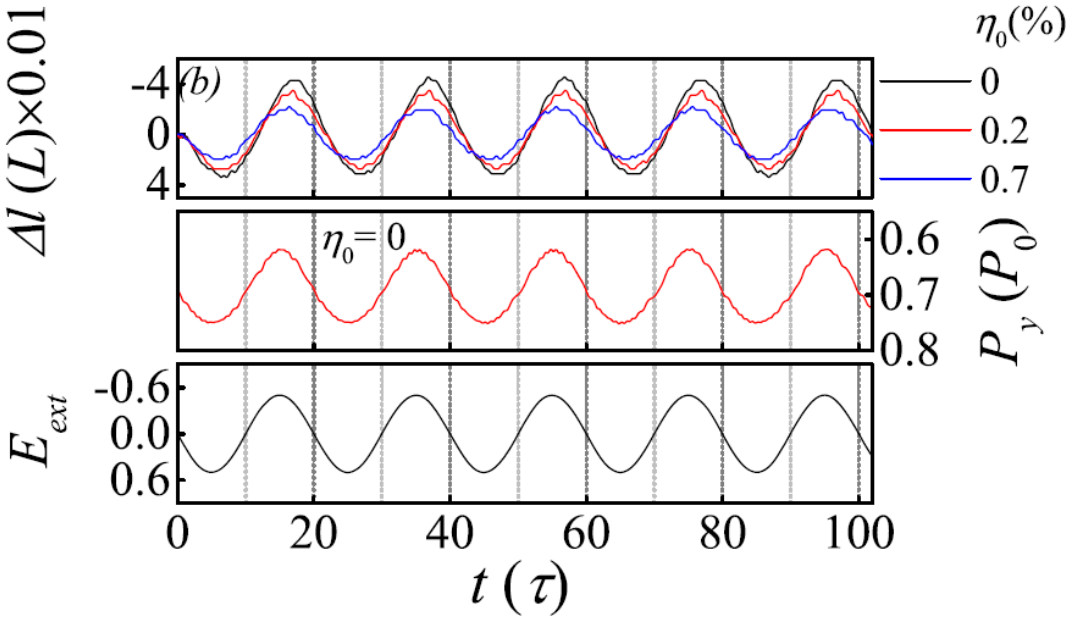
- **Domain response: $\eta_0 \neq 0$**



Work 1: microwave dielectric response

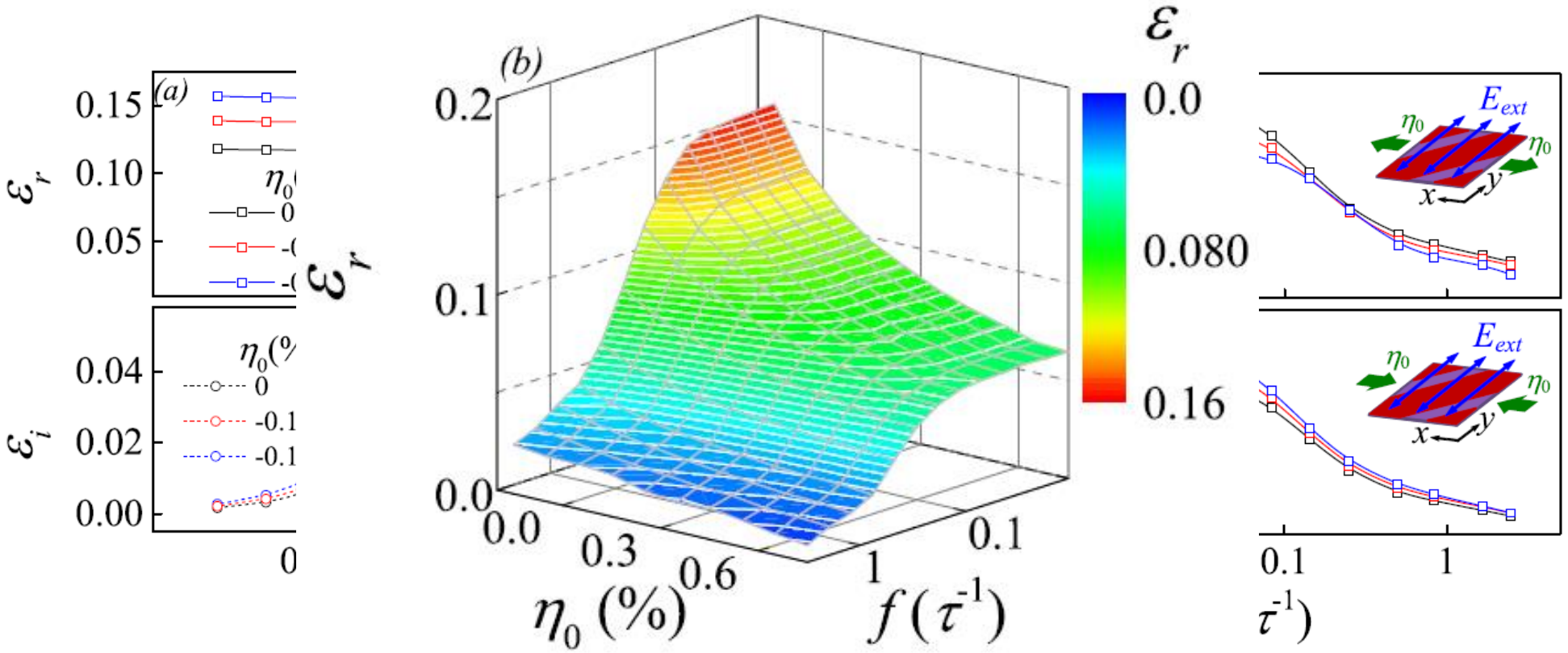
- **Domain response: $\eta_0 \neq 0$**





Work 1: microwave dielectric response

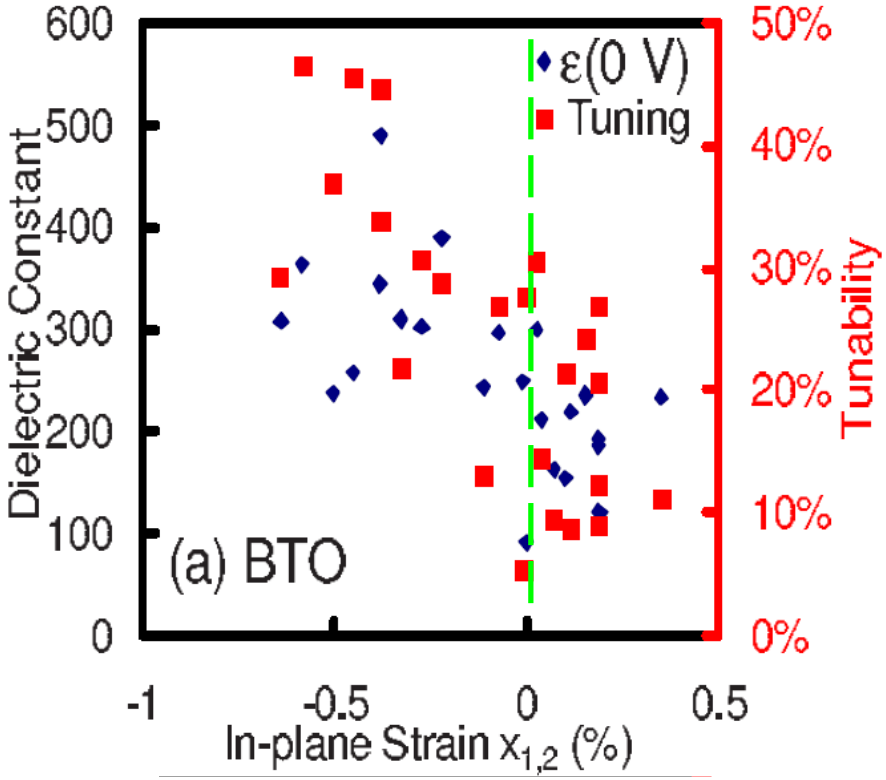
- **Domain response: $\eta_0 \neq 0$**



Work 1: microwave dielectric response

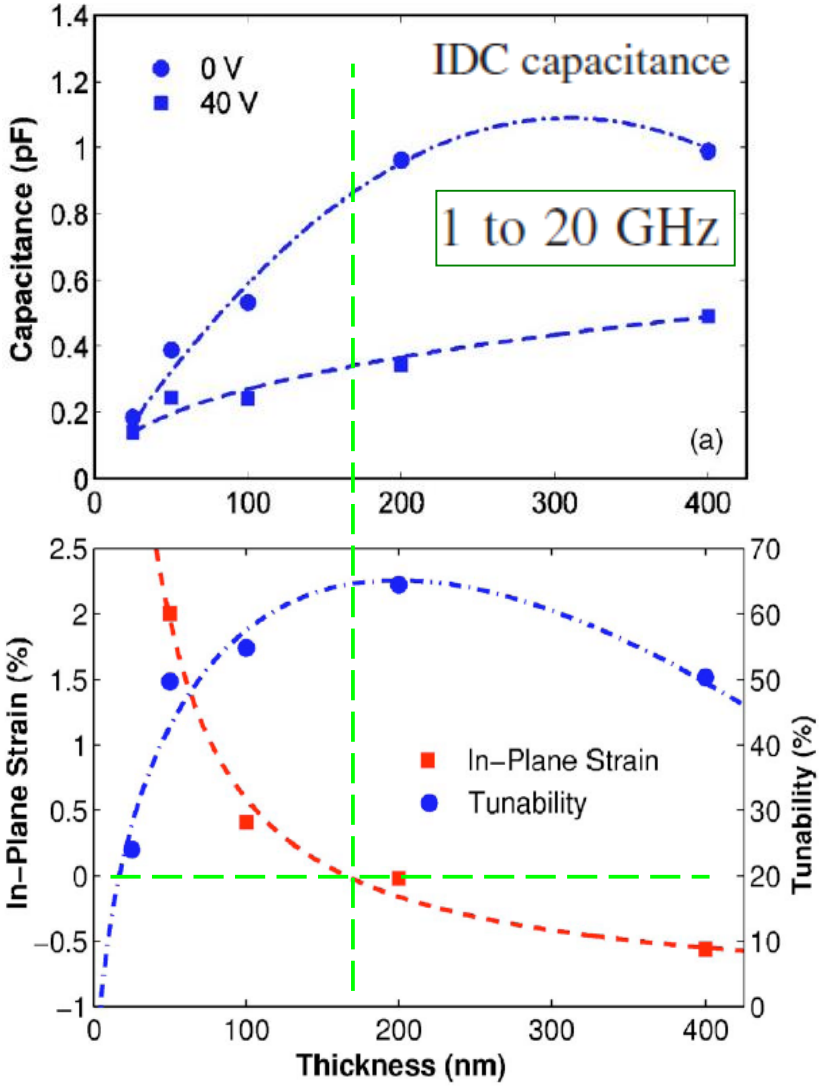
- **Experimental evidences**

$$\text{tunability} = \frac{\epsilon(0\ \text{V}) - \epsilon(V_{dc})}{\epsilon(0\ \text{V})}$$



$BaTiO_3$ on (001) MgO at *f*=10GHz

from L.M.B.Alldredge *et al*, JAP 106, 034108 (2009)



$Ba_{0.6}Sr_{0.4}TiO_3$ on r-sapphire at *f*=1-20GHz

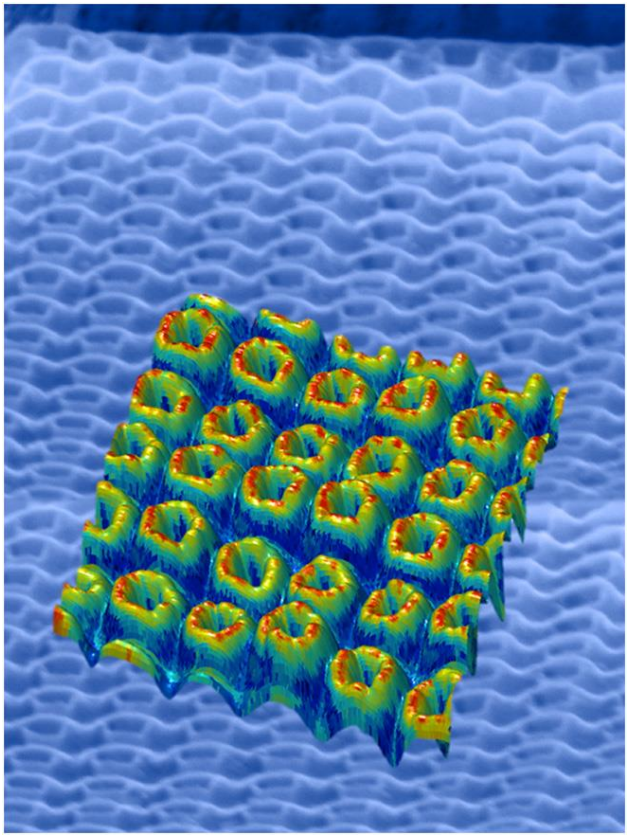
from E.A.Fardin *et al*, APL 89, 182907 (2006)

Work 2: domain antidot structure

- Seriously strained 90^{o} domains & suppressed piezoelectricity
- How to enhance the piezoelectricity?

Background: domain

- **Ferroelectric nanostructures**

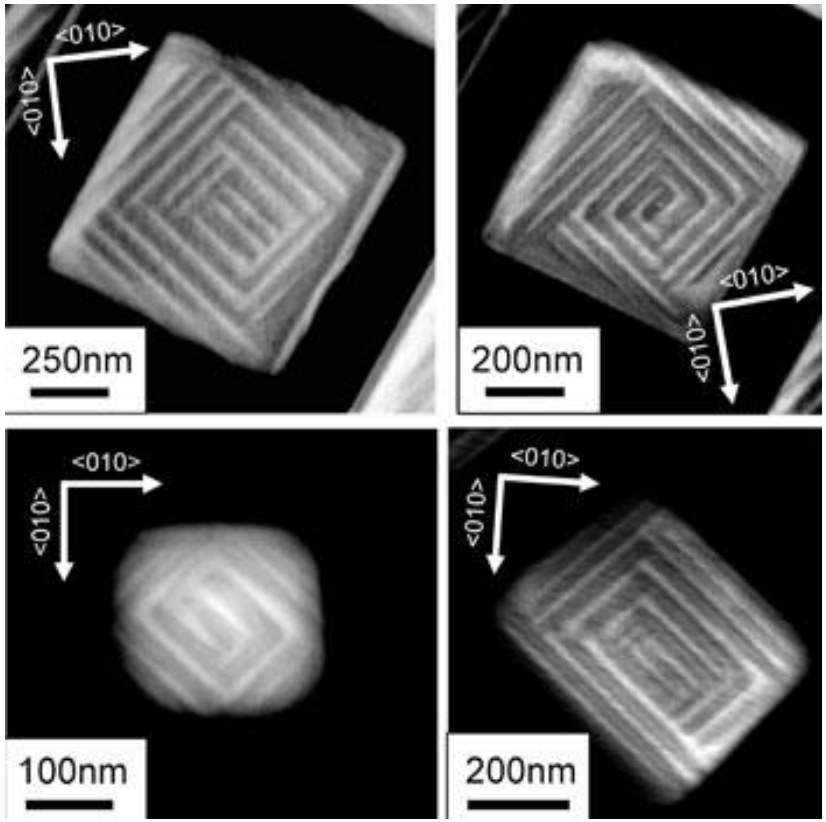


GeorgiaTech

Composite scanning electron microscope (SEM) image of PZT nanotube arrays and their piezoelectric response as measured by band-excitation PFM (BE-PFM)

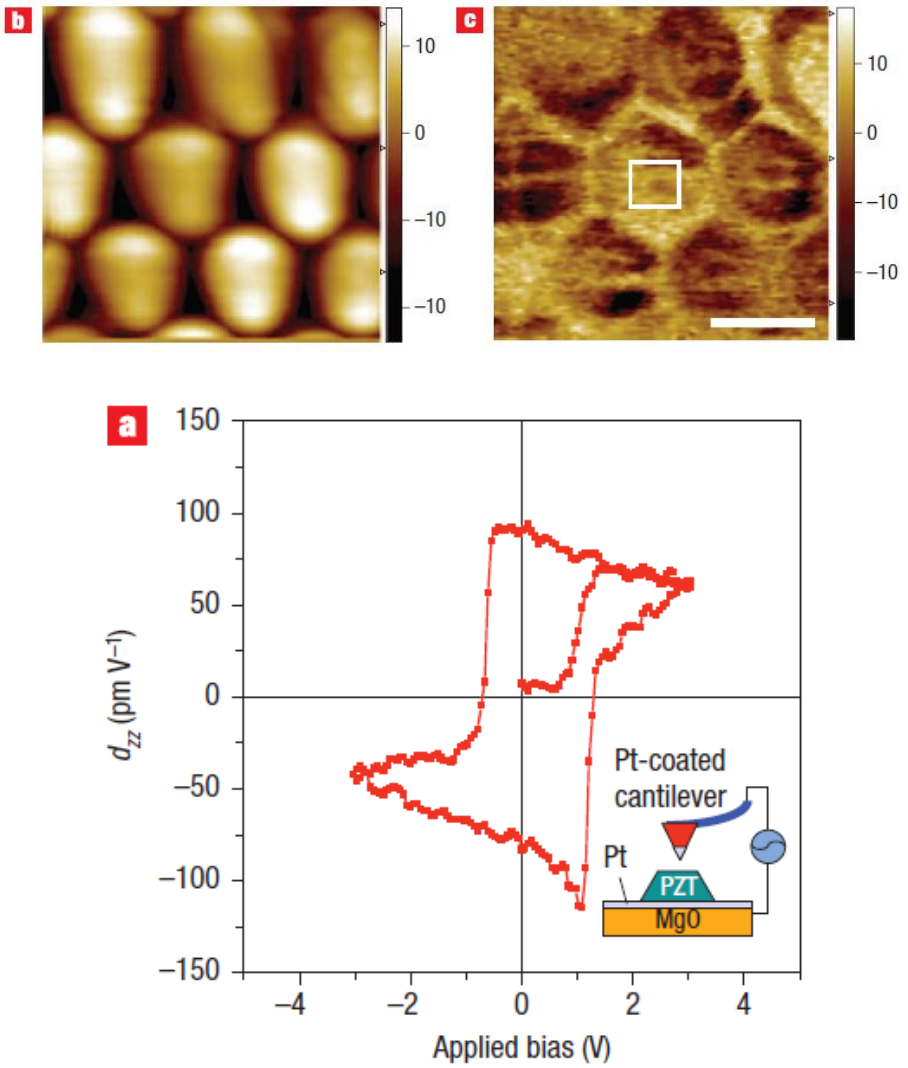
Background: domain

- **Ferroelectric nanostructures**



$BaTiO_3$ nanodot

A.Schilling et al, Nano Lett, 2009, DOI: 10.1021/nl901661a

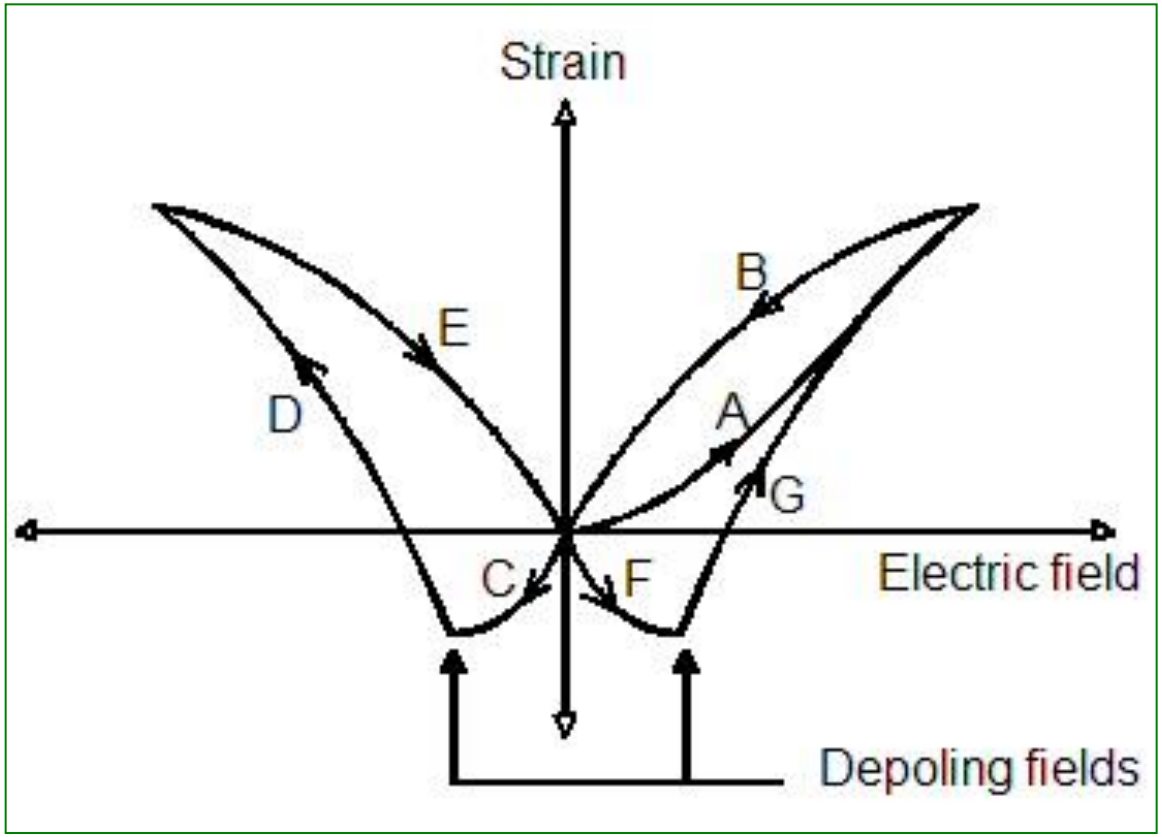


PZT nanodots/(100)MgO

W.Lee et al, Nature Nanotech. 3, 402 (2008)

Motivations: domain structure

- **Enhancing the piezoelectricity**



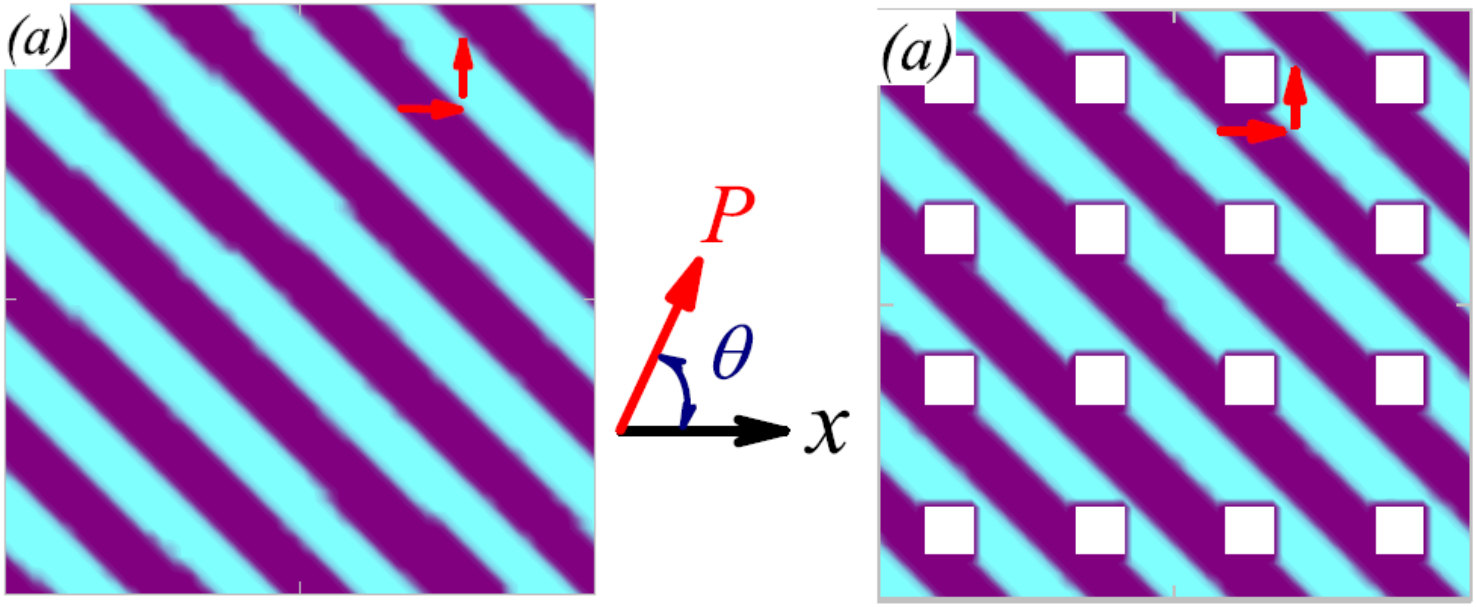
$$\left.\begin{array}{l}\eta - strain\\ E - field\end{array}\right\}$$

$$\left\{\begin{array}{l} piezoelectric\ coefficient \\ d_{ij} \sim \dfrac{\partial \eta_i}{\partial E_j}\end{array}\right.$$

Noliac homepage

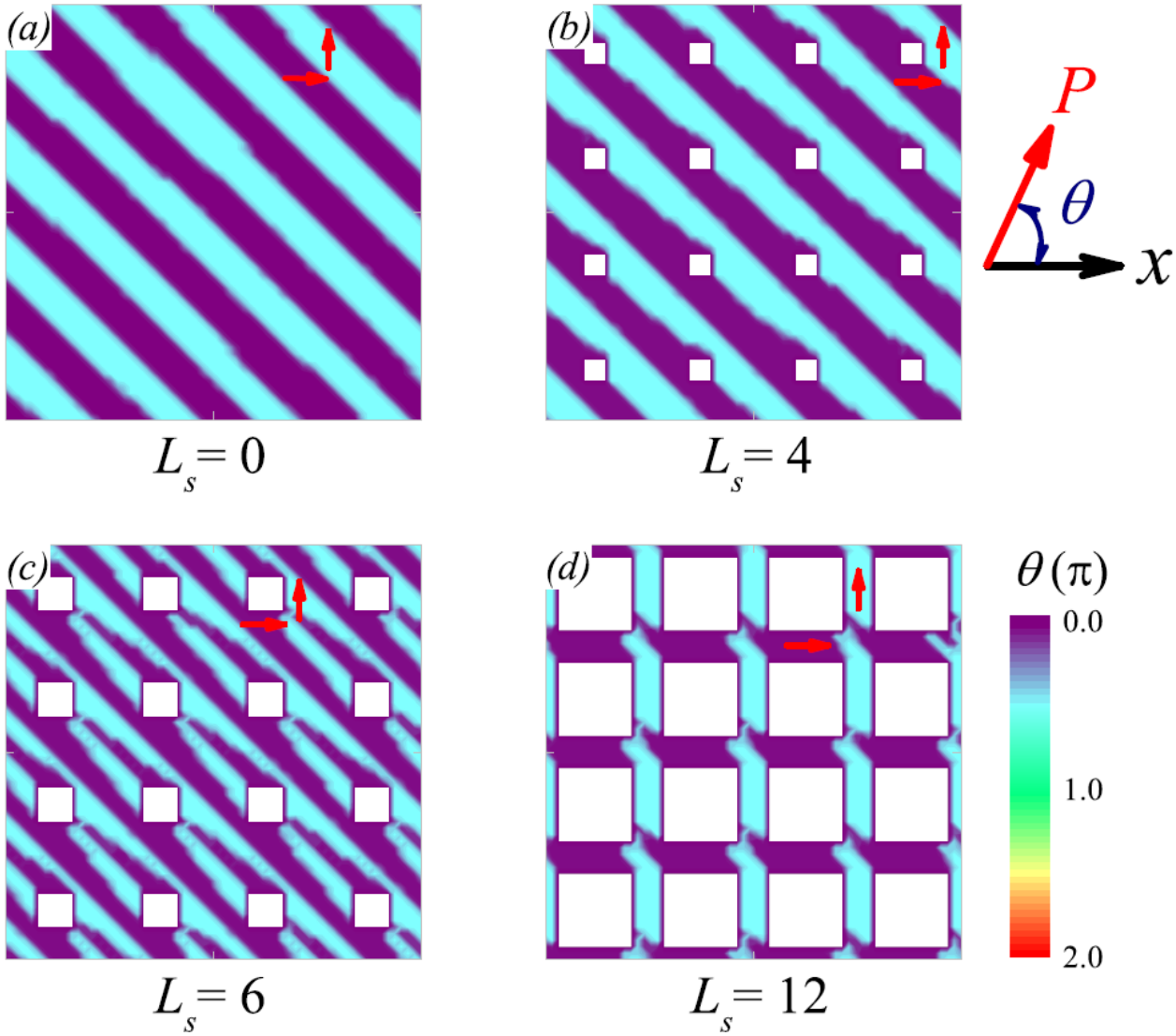
Work 2: domained antidots

- **Strategy: Monte Carlo simulations**



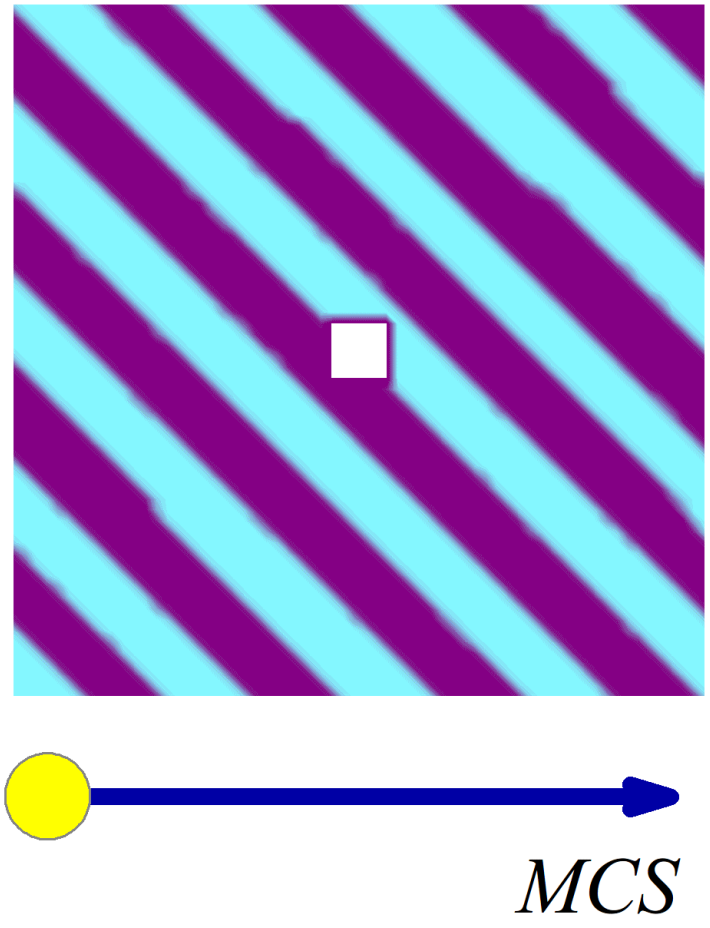
Work 2: domained antidots

- **Effect of domain gridding**

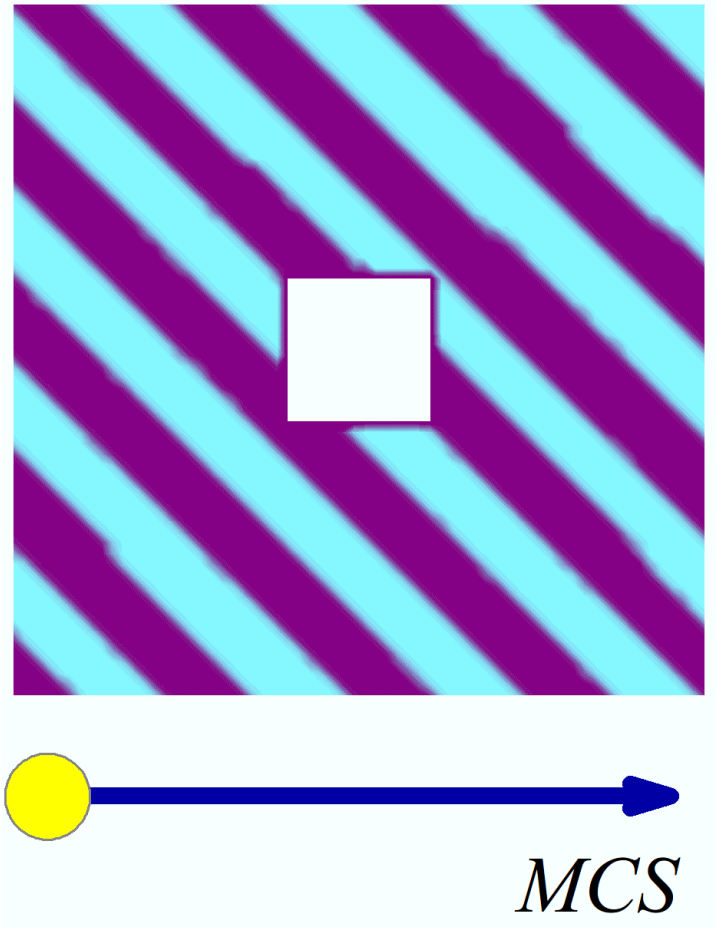


Work 2: domained antidots

- **Domain evolution**



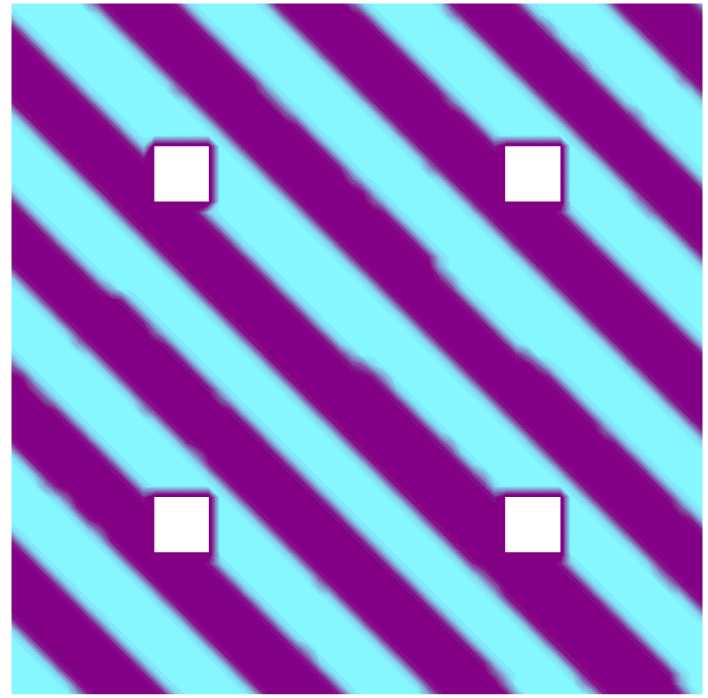
L_s=6



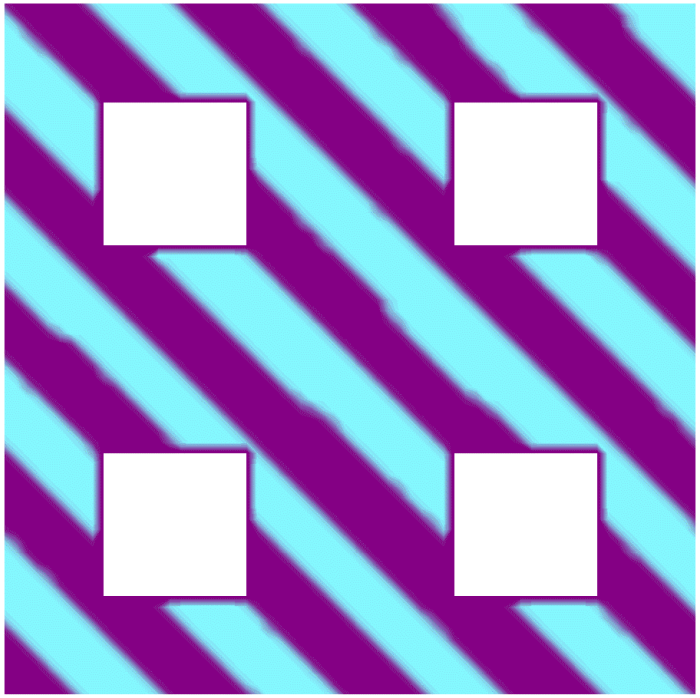
L_s=14

Work 2: domained antidots

- **Domain evolution**



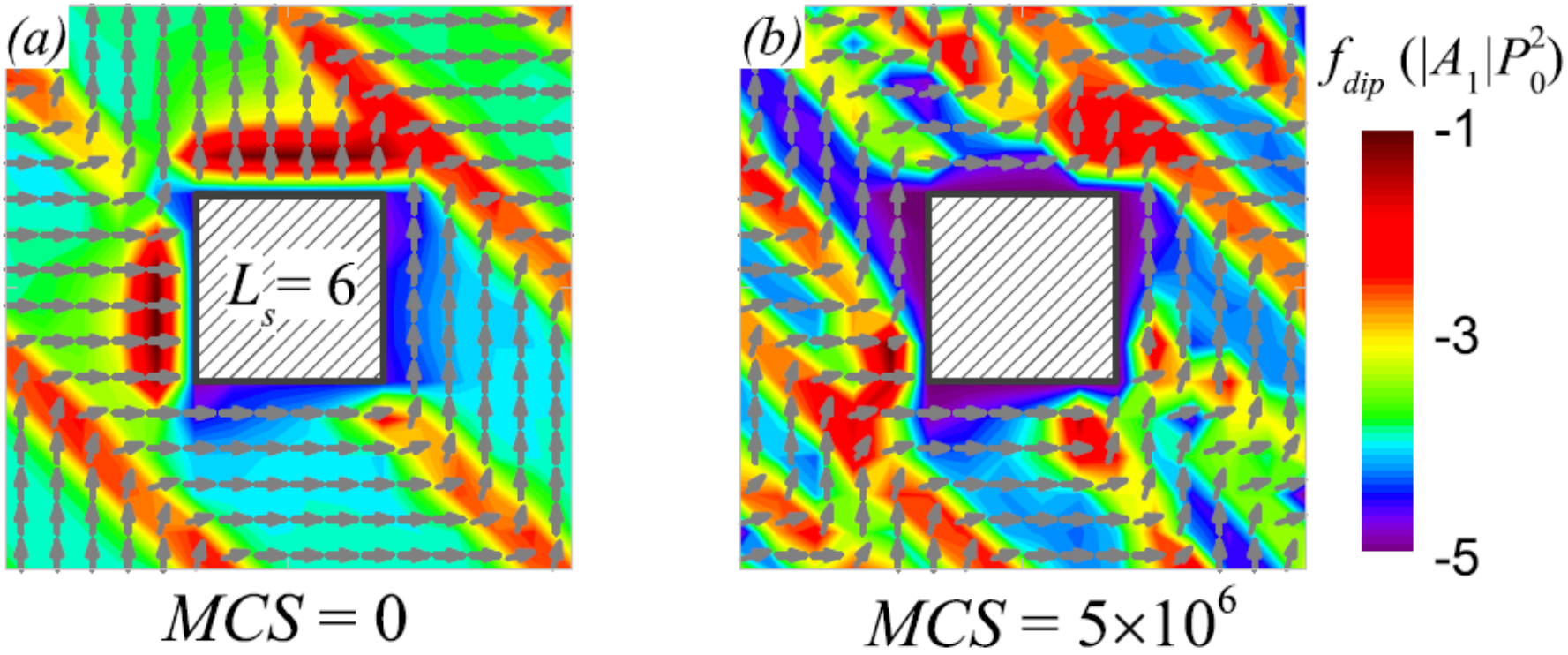
2×2 L_s=6



2×2 L_s=14

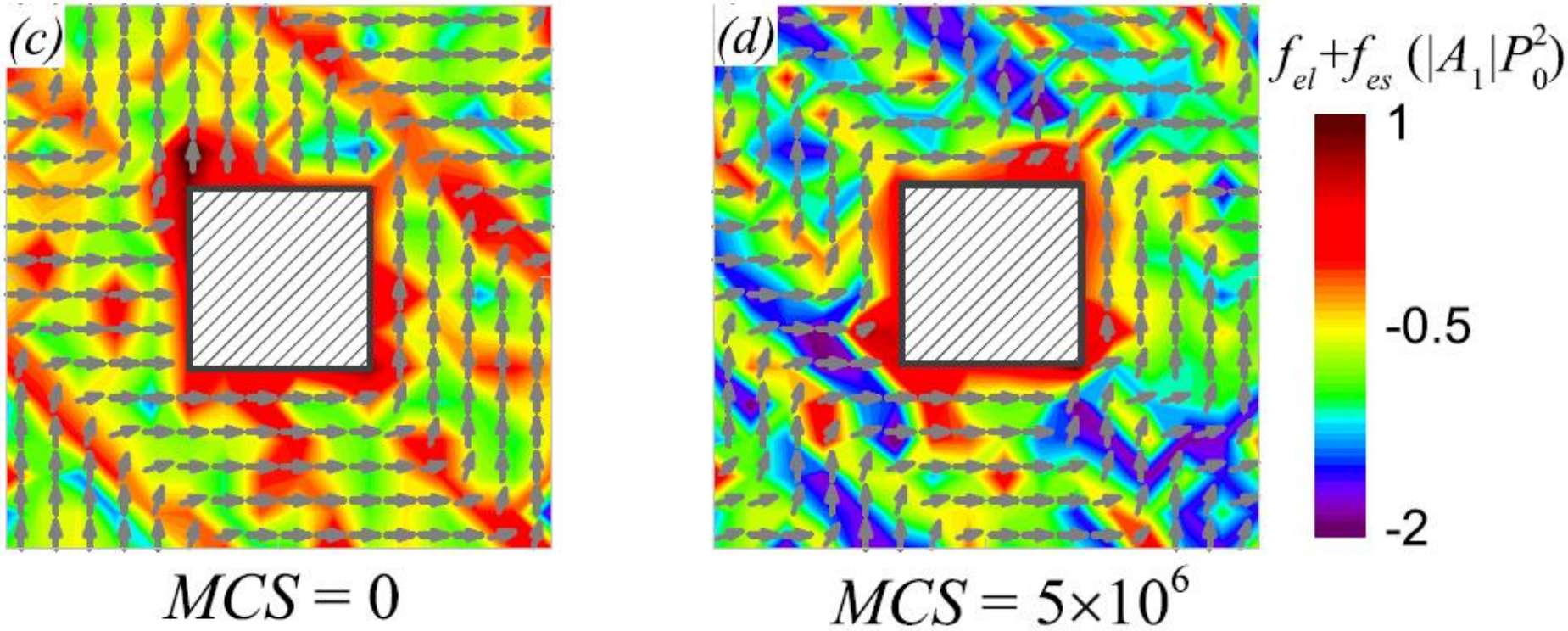
Work 2: domained antidots

- **Energy Landscape**



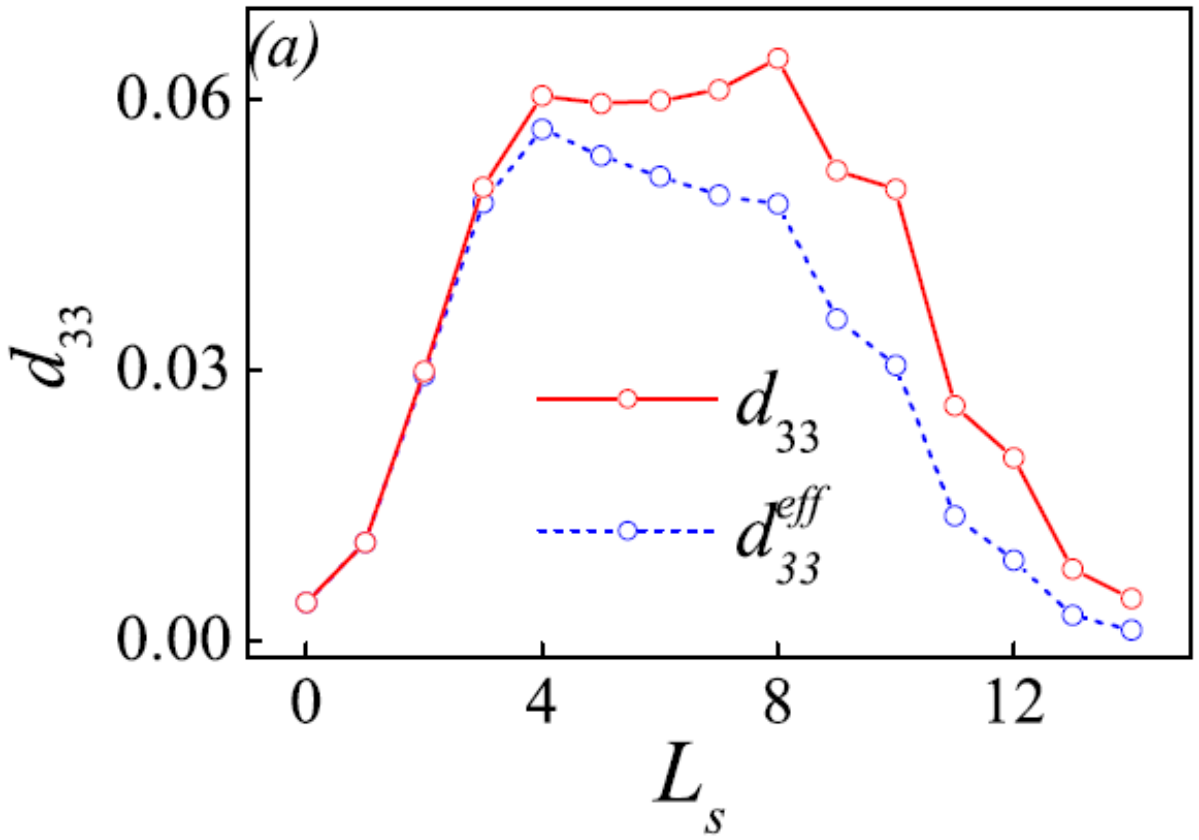
Work 2: domained antidots

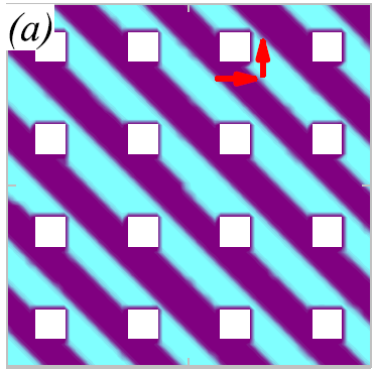
- **Energy Landscape**



Work 2: domained antidots

- **Piezoelectricity enhancement**

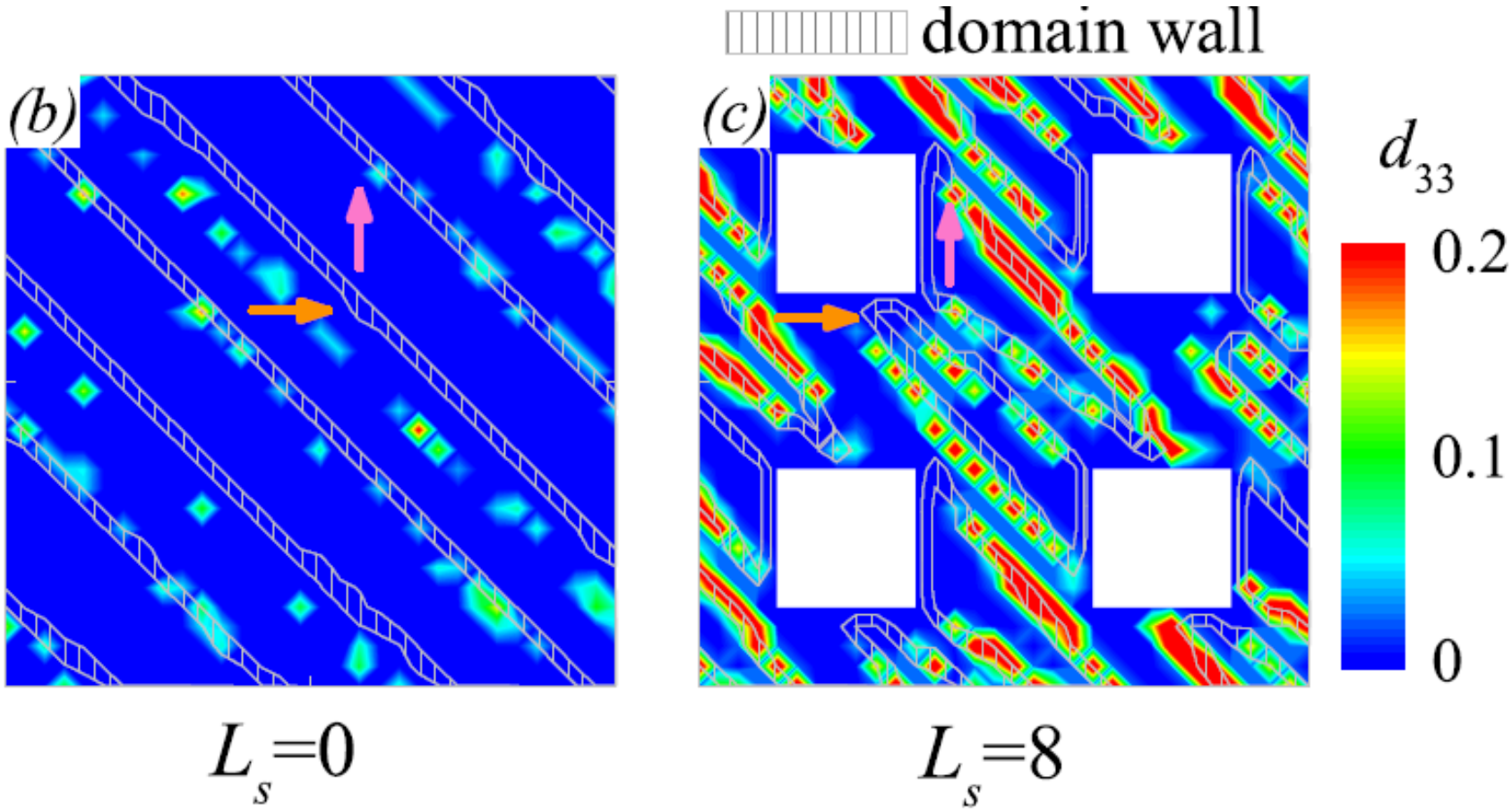




4×4

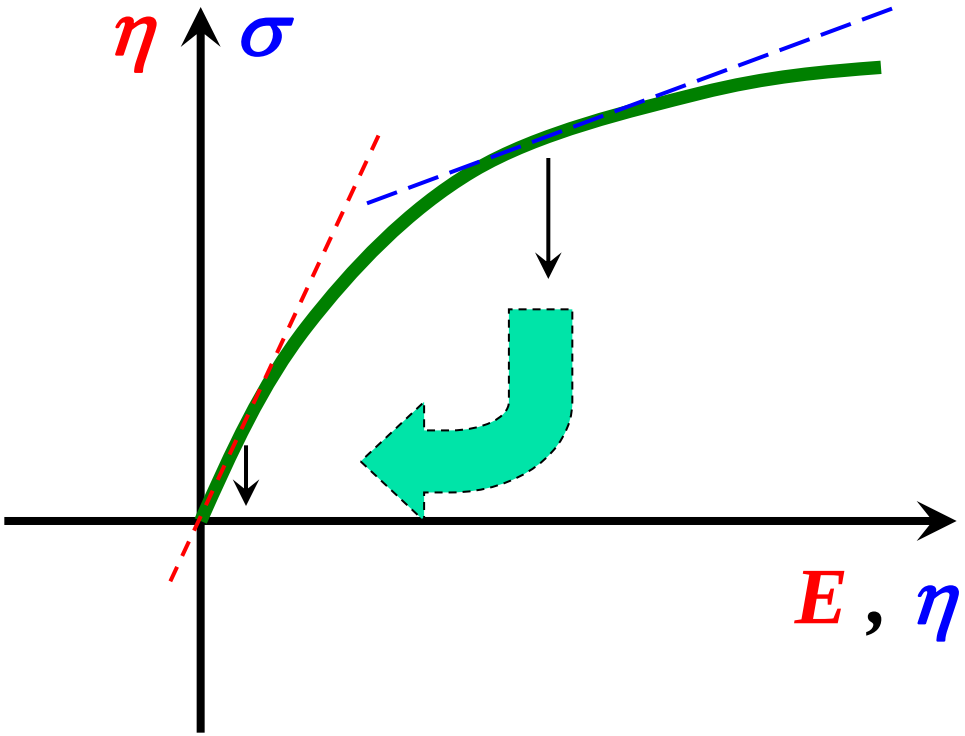
Work 2: domained antidots

- **Piezoelectricity enhancement**



Work 2: domained antidots

- **Piezoelectricity enhancement**

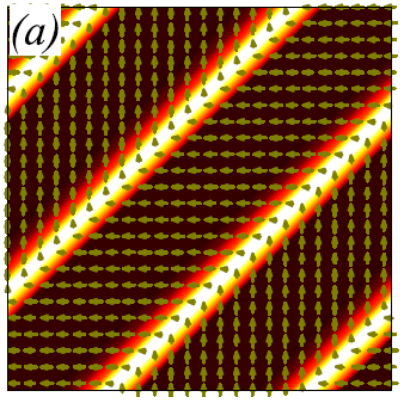


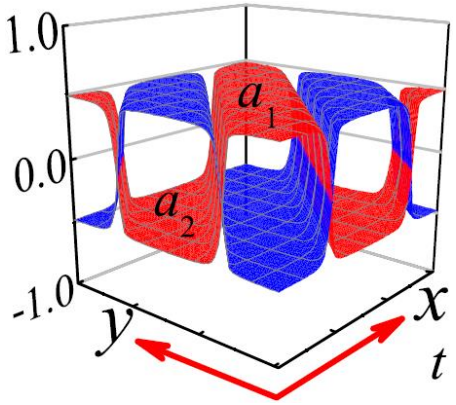
$$\left.\begin{array}{l}\eta - strain\\ E - field\end{array}\right\}$$

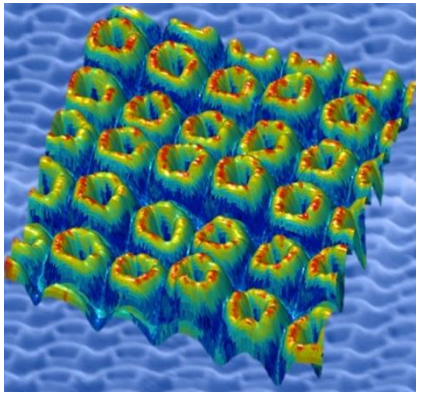
$$\begin{cases} piezoelectric\ coefficient \\ d_{ij} \sim \dfrac{\partial \eta_i}{\partial E_j} \end{cases}$$

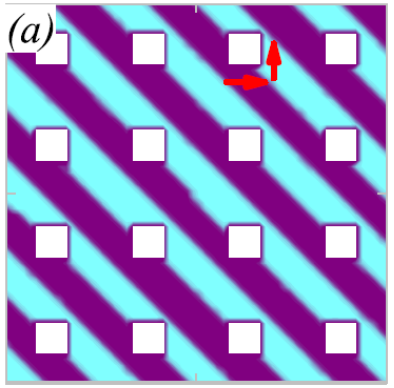
Release the pre-strained lattice but keeping the domain twins

Summary: 90º FE domain structures









- **Phase-field simulation of the high-*f* dielectric response**
- **Consequence of normal tensile and compressive strains**

- **Domain evolution with the lattice gridding**
- **Piezoelectricity enhancement**

Thank you for your attentions