THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 11: Multiphysics PDEs and Order Parameters

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Partial Differential Equations

Describe functions of more than one variable

In physics, this commonly corresponds to fields $\phi(x, y, z)$

Examples:

- Electrostatic potential $\phi(x, y, z)$ (Poisson's equation)

$$\Delta\phi(x, y, z) = -\frac{\rho(x, y, z)}{\epsilon_0}$$

- Density or temperature profiles (diffusion/heat equation)

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} = D\Delta u(\mathbf{x}, t)$$

- Displacement (amplitude) profile (wave equation)

$$\frac{\partial^2 u(\mathbf{x}, t)}{\partial t^2} = c^2\Delta u(\mathbf{x}, t)$$

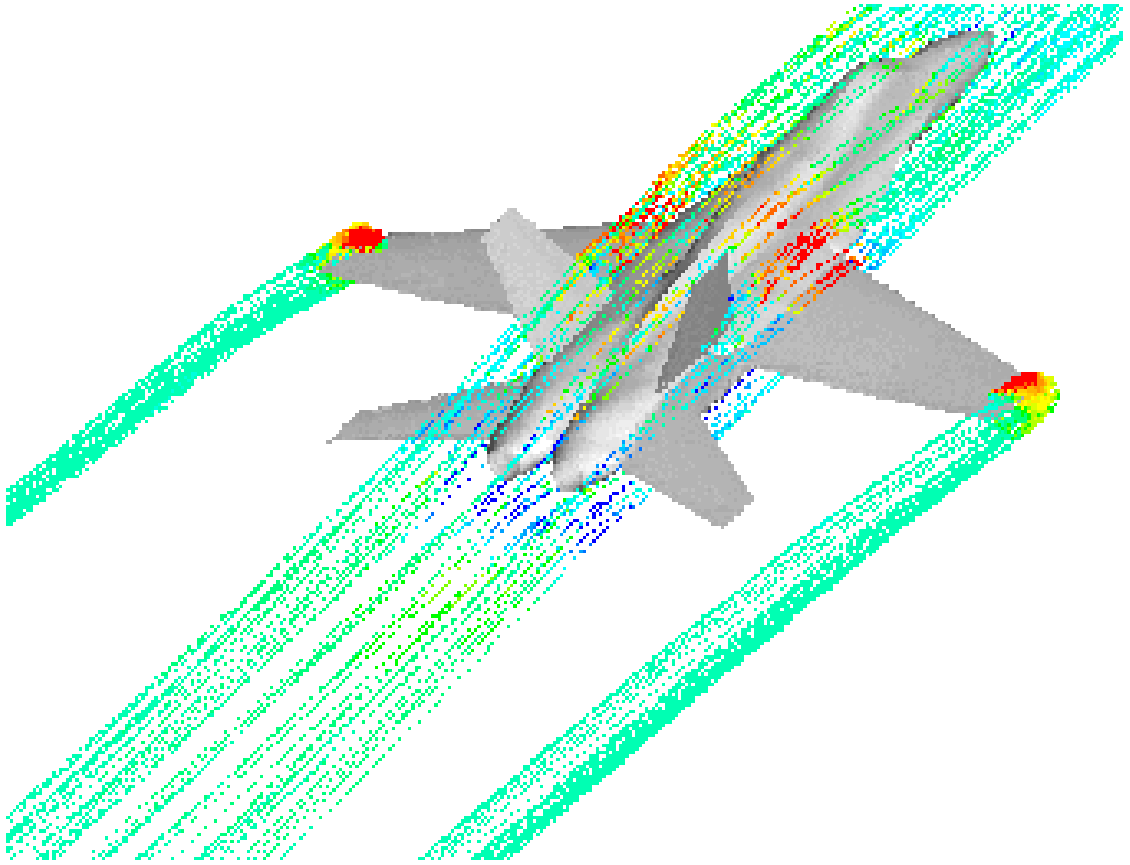
- Fluid dynamical fields (flow velocity) -- e.g. Navier-Stokes equations

$$\frac{\partial}{\partial t}(\rho\,\mathbf{u}) + \nabla\cdot(\rho\,\mathbf{u}\otimes\mathbf{u}) = -\nabla p + \nabla\cdot\boldsymbol{\tau} + \rho\,\mathbf{g}$$

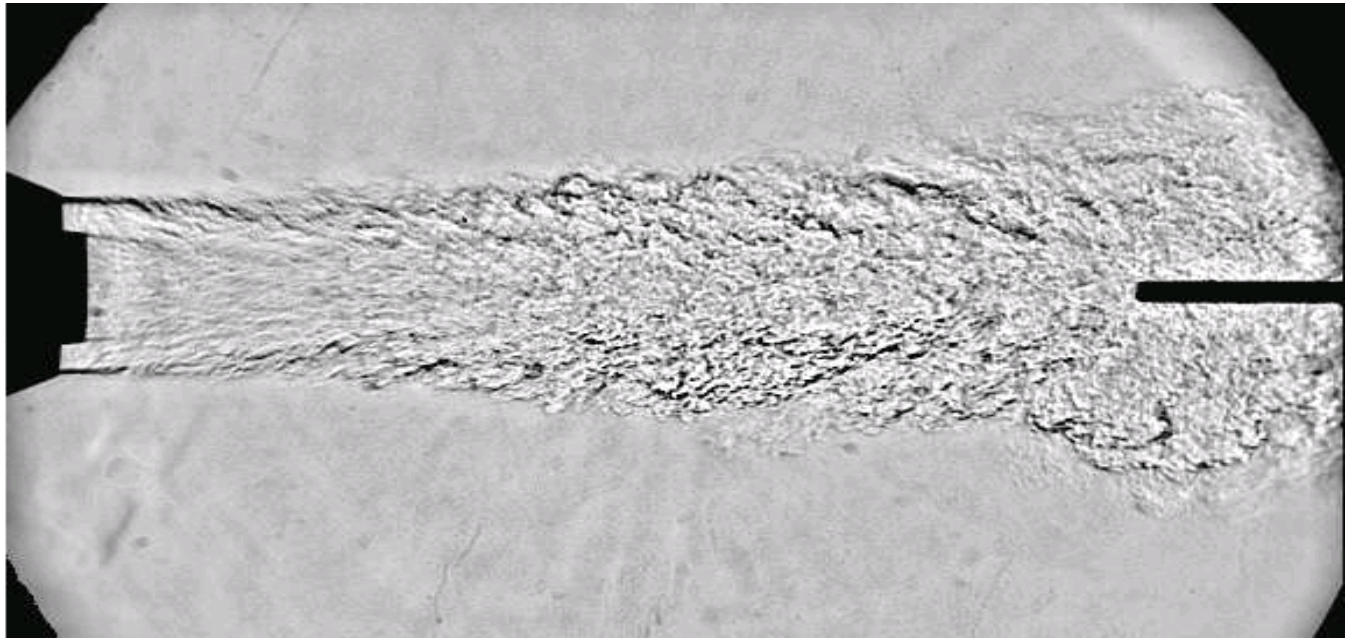
Navier-Stokes Equations

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g}$$

- Fluid flows:
- Airplanes
- Cavitation
- Climate
- And so on



Instabilities

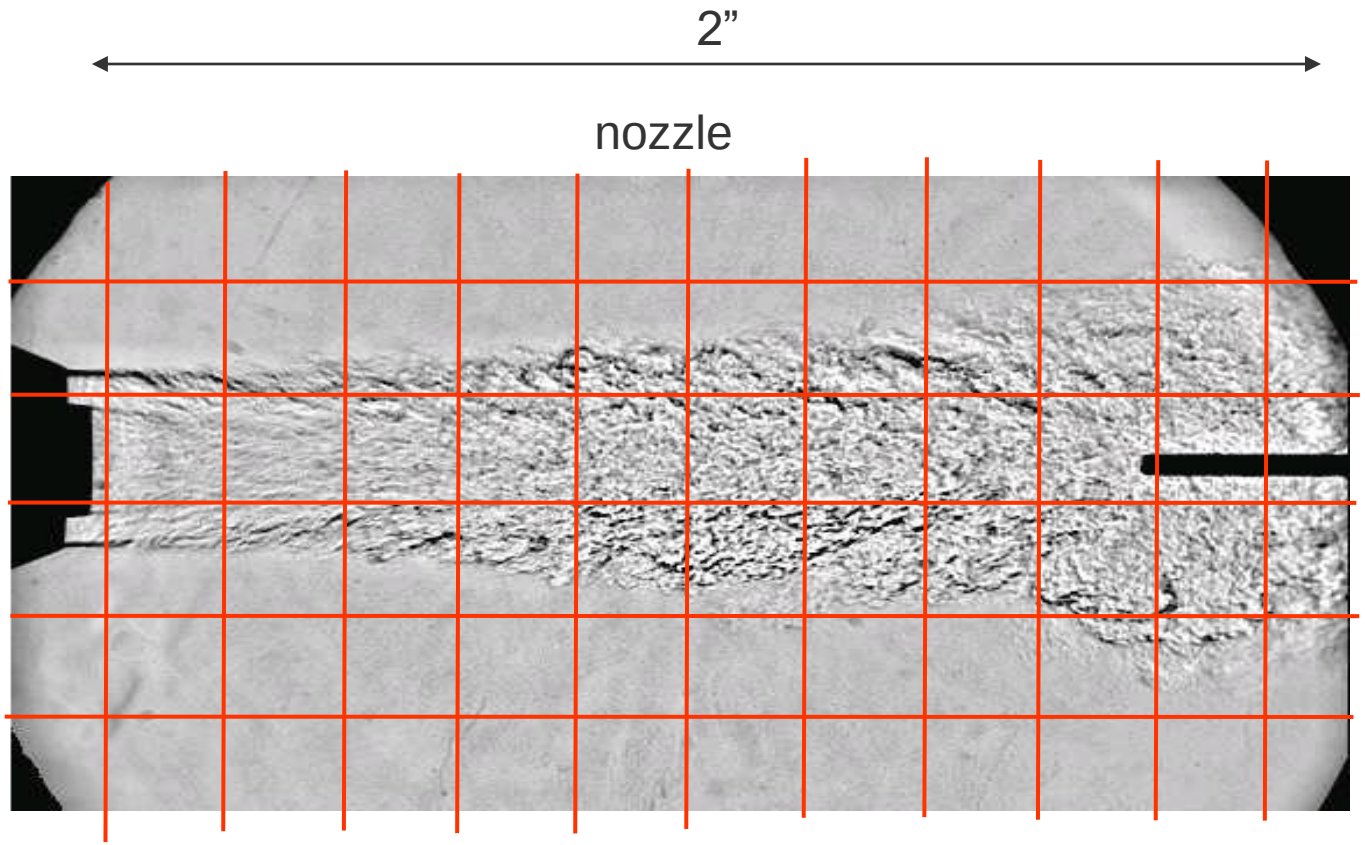


~1000

~2000 cells

For 2D wee need ~ 2 million cells

Instabilities



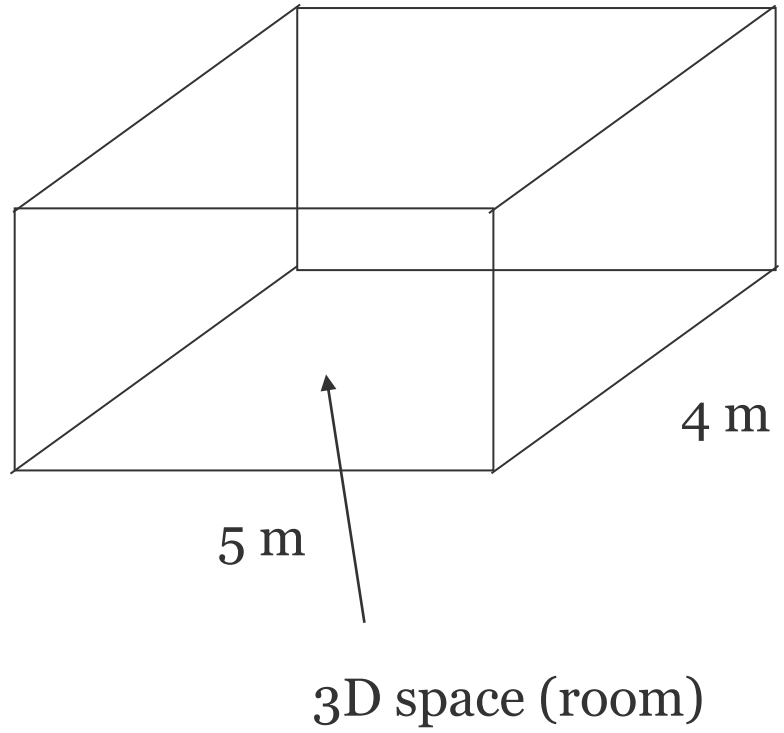
Eddy ~ 1/100 in

Mesh (volume) should be smaller than eddies ！

(approximately order of value)

Mesh Size

- For 3D simulation domain



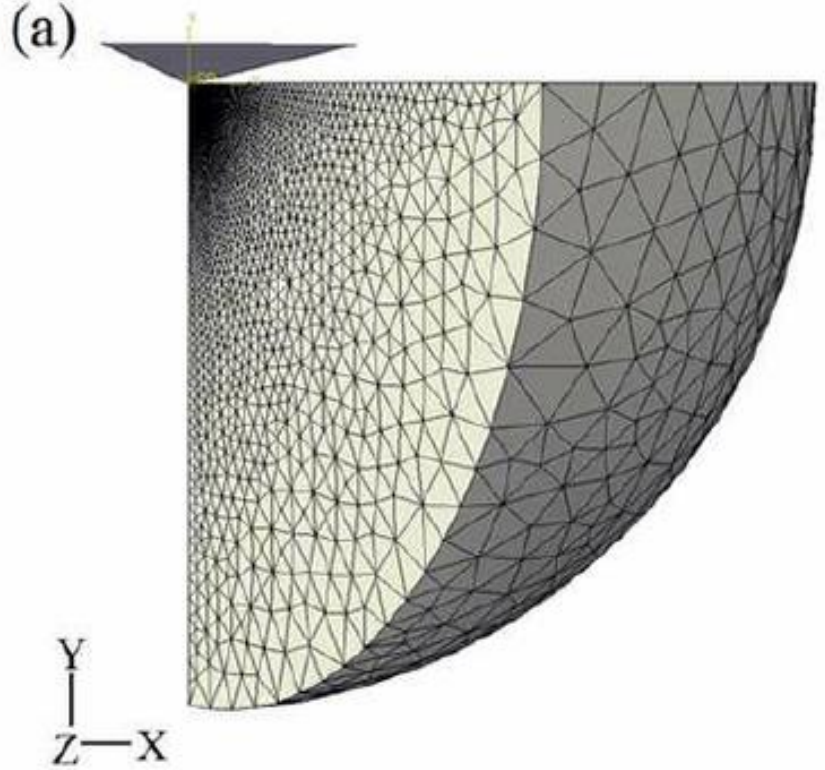
Mesh size 0.1m → 50,000 nodes

Mesh size 0.01m → 50,000,000 nodes

Mesh size 0.001m → $5 \cdot 10^{10}$ nodes

Mesh size 0.0001m → $5 \cdot 10^{13}$ nodes

Finite Element Simulations



- **Basic Concept:** A numerical technique for finding approximate solutions to boundary value problems for partial differential equations.
- **Discretization:** Divides a large problem into smaller, simpler parts called finite elements.
- **Element Assembly:** The individual elements are assembled into a larger system that models the entire problem.
- **Solution Approximation:** Within each element, the solution is approximated by a simple function that satisfies the boundary conditions.
- **Matrix Equation Formation:** Transforms the problem into a set of algebraic equations using matrices.
- **Types of Elements:** Uses various shapes of elements like line segments in 1D, triangles or quadrilaterals in 2D, and tetrahedra or hexahedra in 3D.

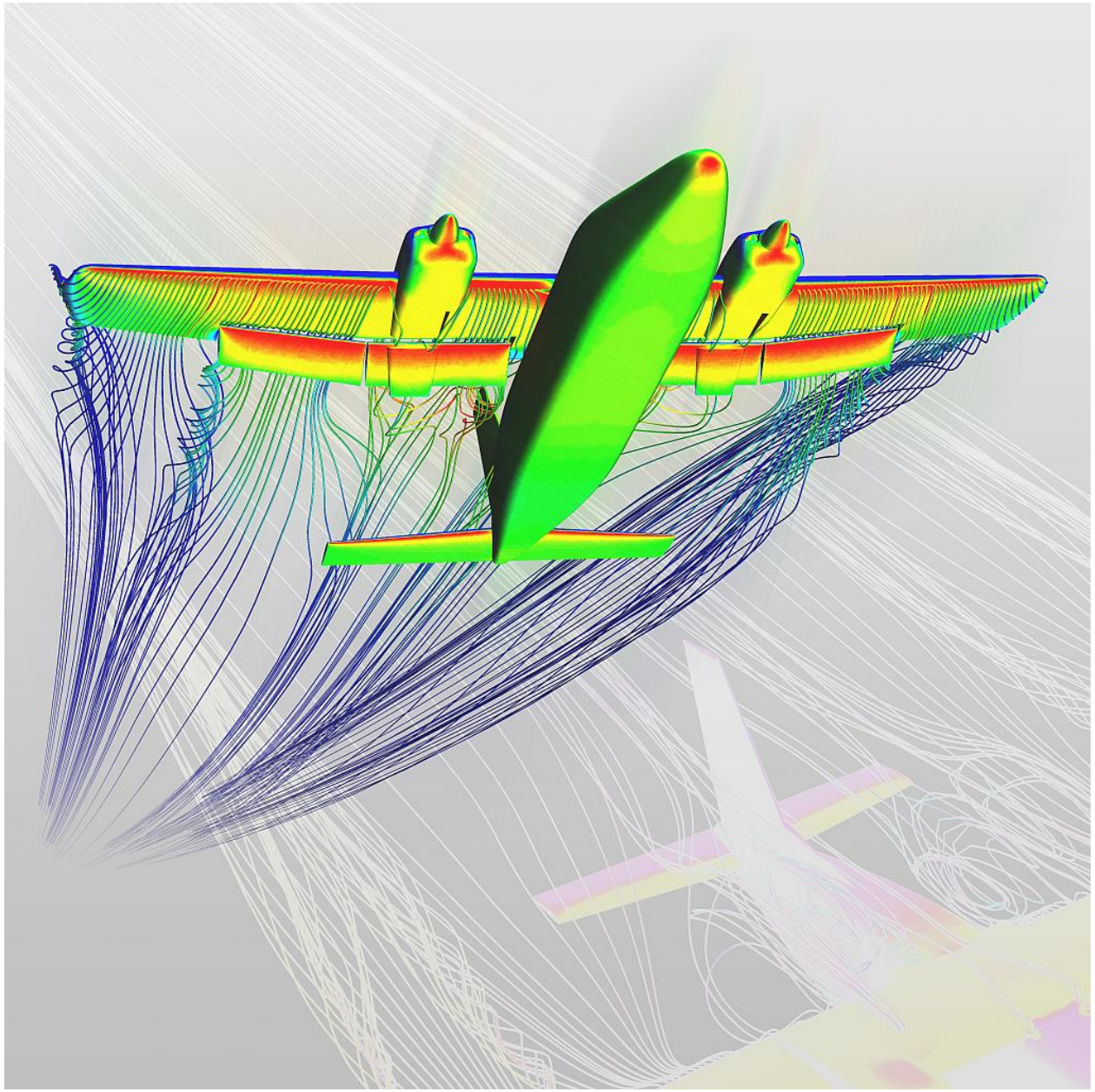
https://www.researchgate.net/publication/277822913_Mechanics_of_Granular_Materials_Experimentation_and_Simulations_for_Determining_the_Compressive_and_Shear_Behaviors_of_Sand_at_Granular_and_Meso_Scales/figures?lo=1

Multiphysics simulations

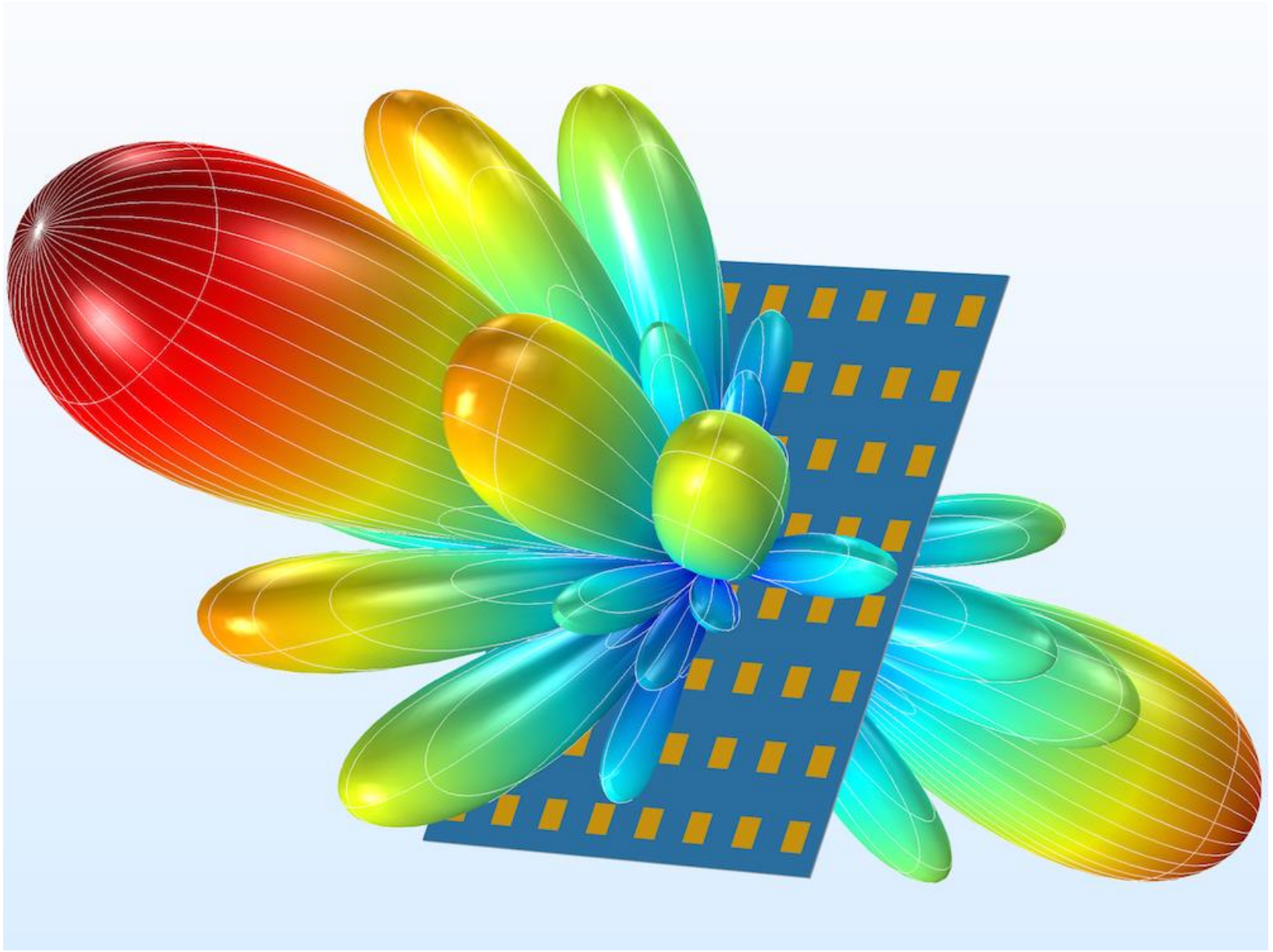
Multiphysics simulations involve the integrated computational modeling of complex systems where multiple physical processes interact simultaneously. These simulations are grounded in the principle that real-world phenomena often encompass interactions across different physical domains, such as

- Thermal,
- Structural,
- Fluid dynamics, and
- Electromagnetic fields.

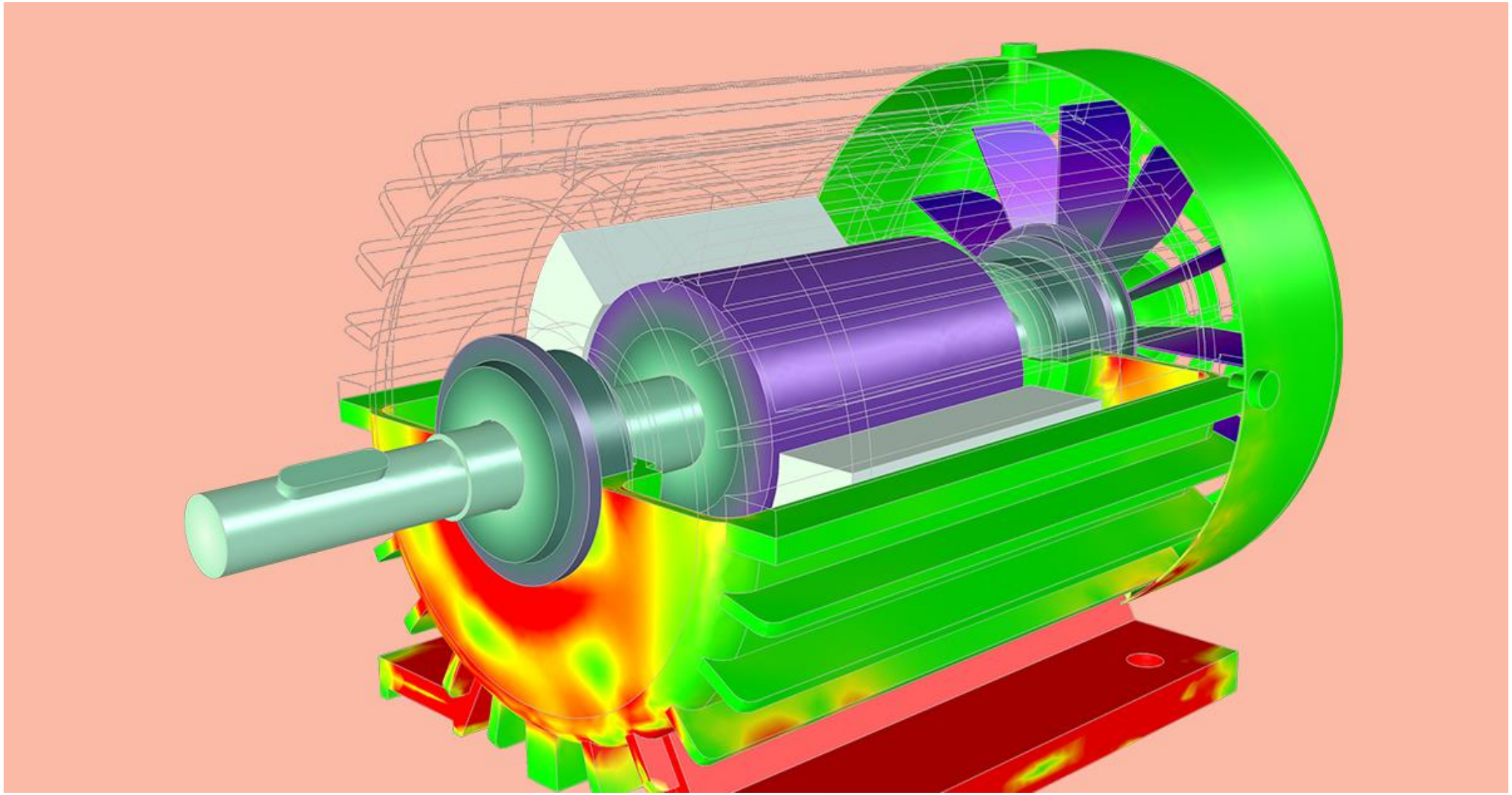
By combining models from these various domains into a single simulation environment, multiphysics simulations enable the accurate prediction and analysis of the behavior of systems under a wide range of conditions.



https://blogs.sw.siemens.com/simcenter/aerospace-aerodynamics-cfd-simulation/

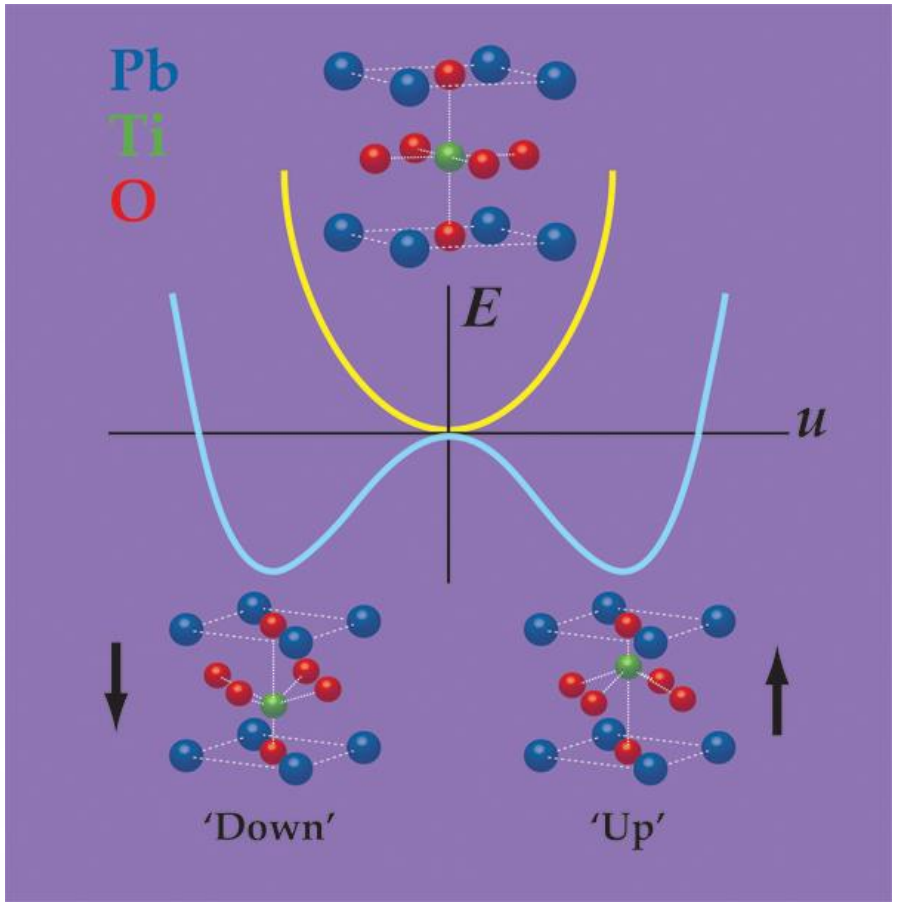


https://www.comsol.com/blogs/introduction-to-efficiently-modeling-antennas-in-comsol-multiphysics/



https://www.comsol.com/blogs/analyzing-the-structural-integrity-of-an-induction-motor-with-simulation/

Order parameters

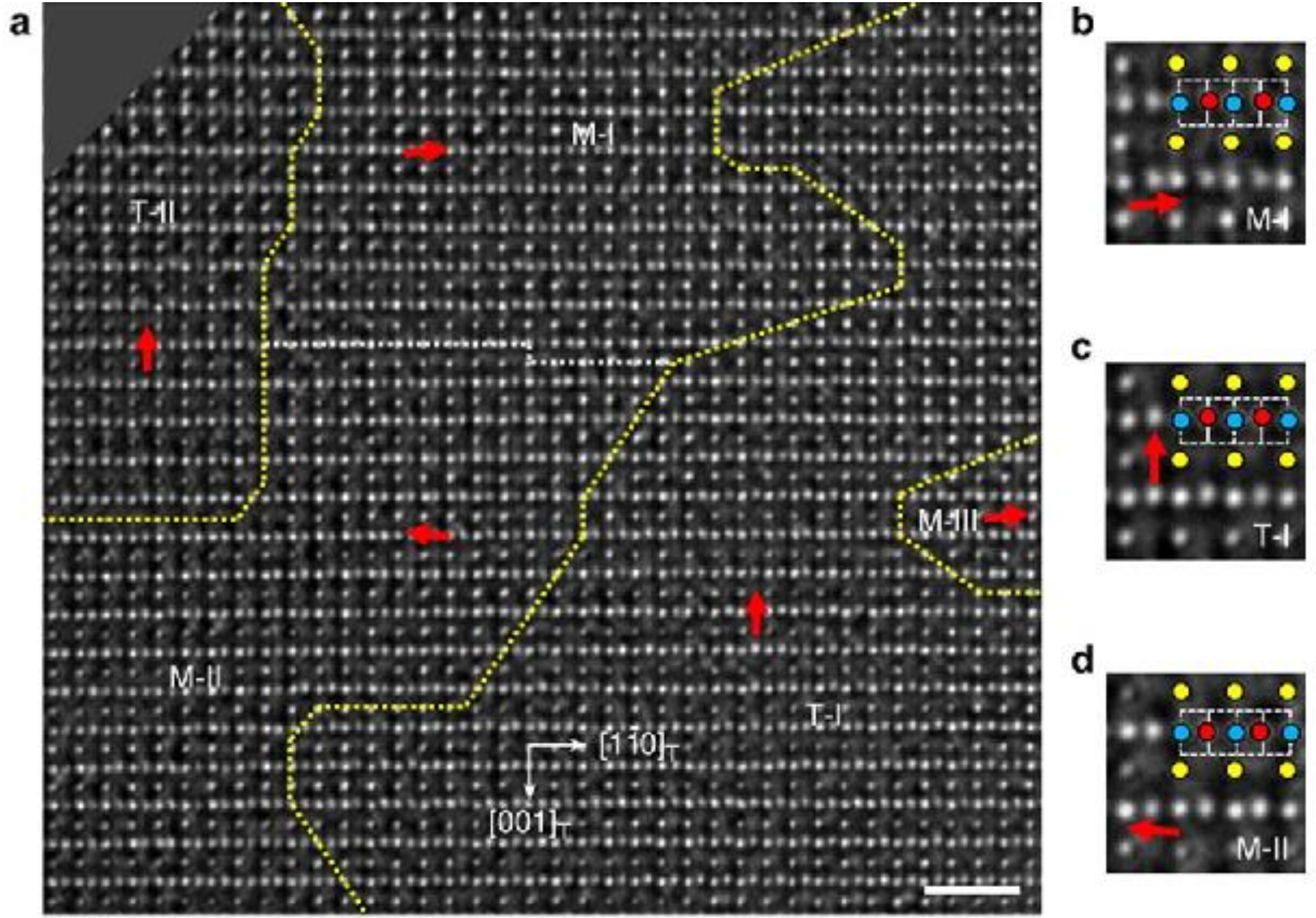


https://physics.aps.org/articles/v7/32

•**Magnetization in Magnetic Systems**: Measures the average magnetic moment per atom or molecule, indicating the degree of alignment of magnetic moments in a material. Used to describe transitions between ferromagnetic and paramagnetic phases.

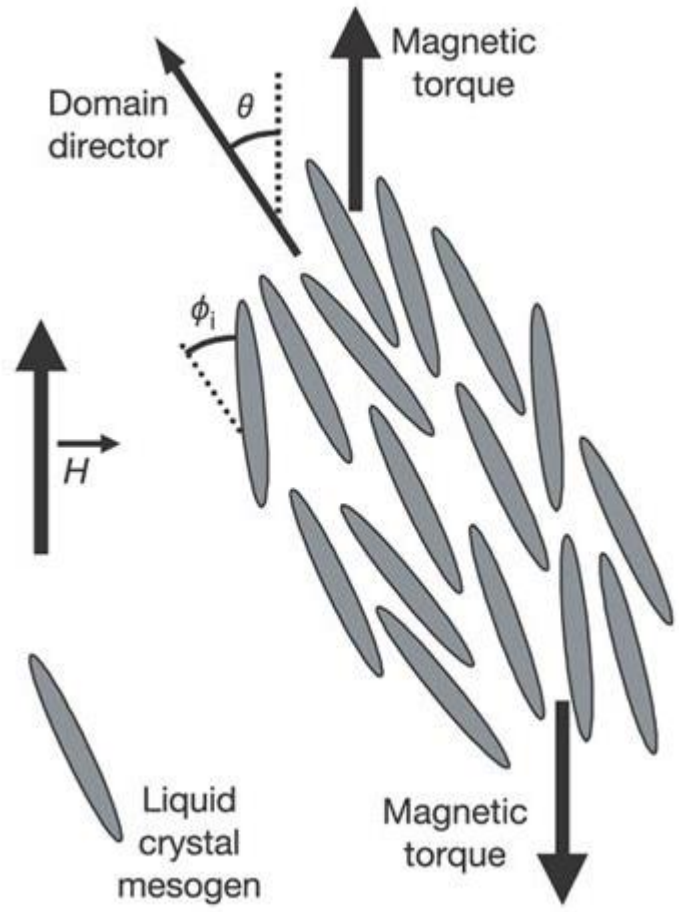
•**Polarization in Ferroelectric Materials**: Quantifies the electric polarization, or the separation of positive and negative charges within a material. It's critical for understanding the ferroelectric phase transition, where a non-polar material becomes polarized under certain conditions.

•**Density in Liquid-Gas Transitions**: The difference in density between the liquid and gas phases serves as an order parameter for liquid-gas phase transitions, distinguishing between the more ordered liquid phase and the less ordered gas phase.



https://www.semanticscholar.org/paper/Aberration-corrected-STEM-techniques-to-investigate-Moore-Bangert/8733b871d206f83397622ef3fa40f9ab647e4818

Order parameters



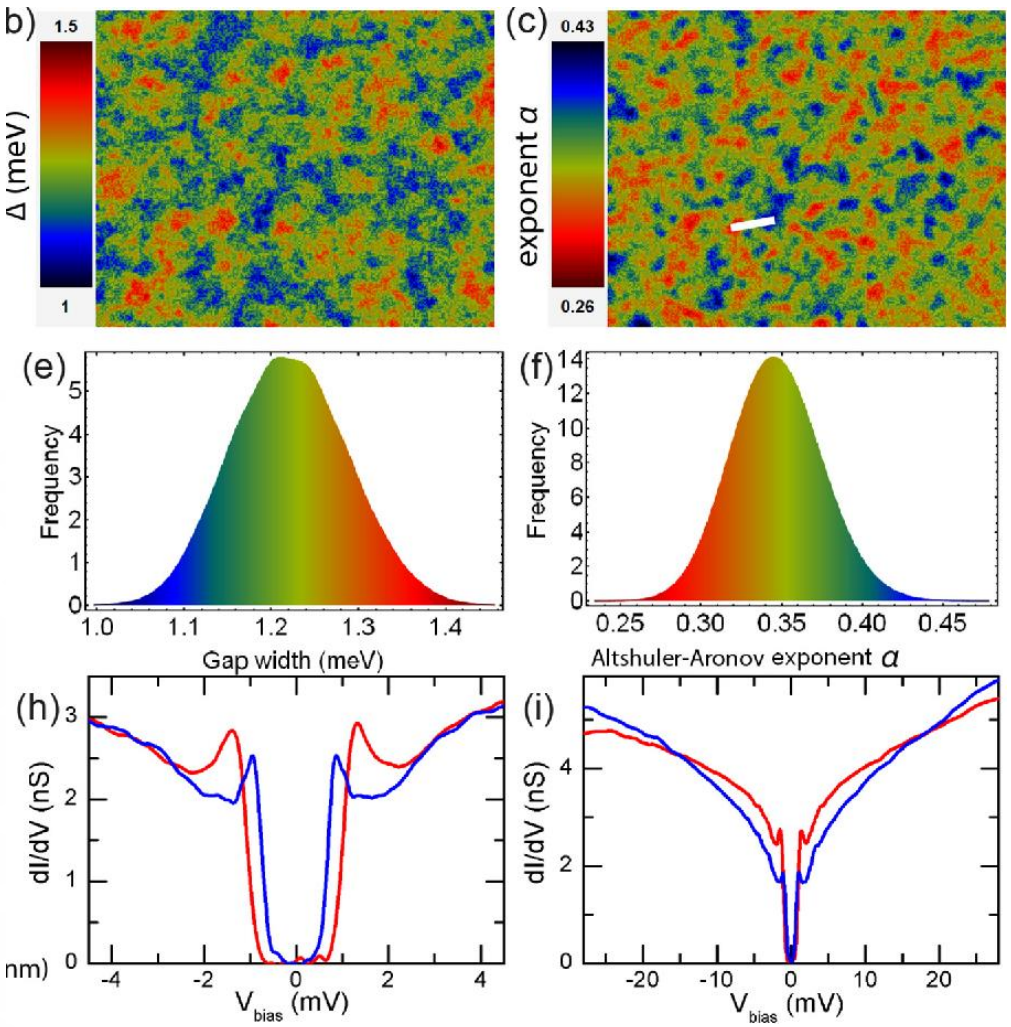
https://www.nature.com/articles/nature01331

• **Concentration in Binary Mixtures**: In alloys or binary mixtures, the concentration of one component can act as an order parameter, especially in phase separation phenomena where the mixture segregates into phases with different concentrations.

• **Superfluid Order Parameter**: In the context of superfluidity, it represents the macroscopic wave function of the superfluid component. The phase transition from normal fluid to superfluid is characterized by the onset of a non-zero value of this parameter.

• **Director in Liquid Crystals**: For liquid crystal phases, the average orientation of the anisotropic molecules, described by the director, acts as an order parameter. It measures the degree of molecular alignment, distinguishing between different liquid crystalline phases (e.g., nematic, smectic).

Order parameters



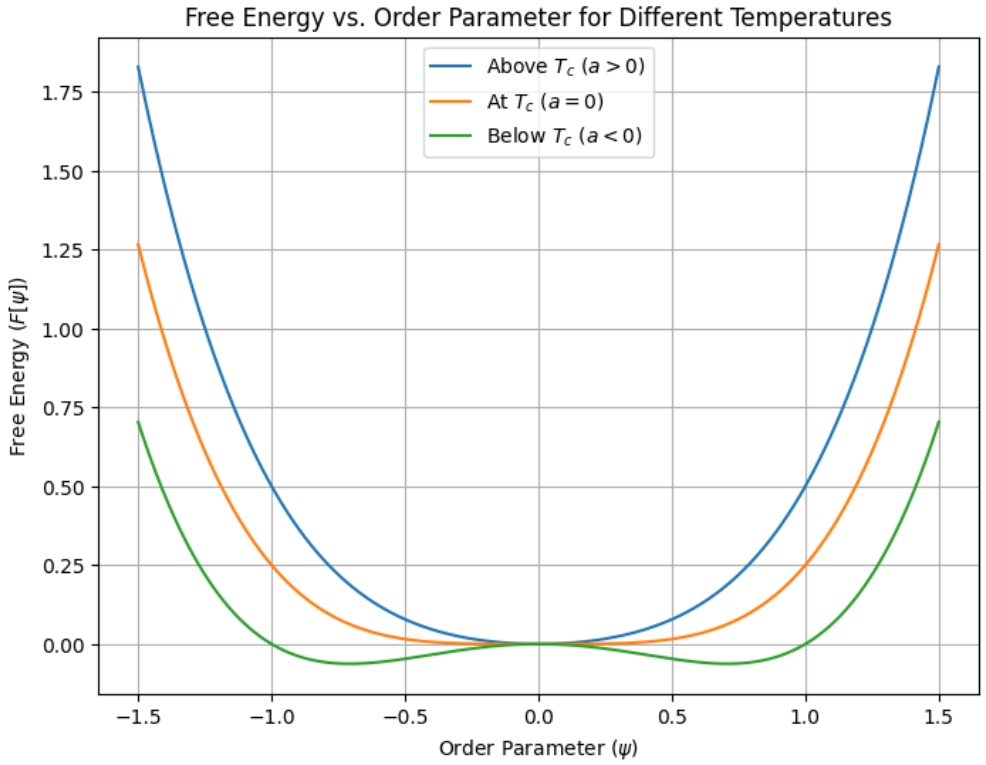
https://www.semanticscholar.org/paper/Spectroscopic-evidence-for-strong-correlations-gap-Carbillet-Cherkez/55c7a53f296608d92734def00e3e440bed385c93

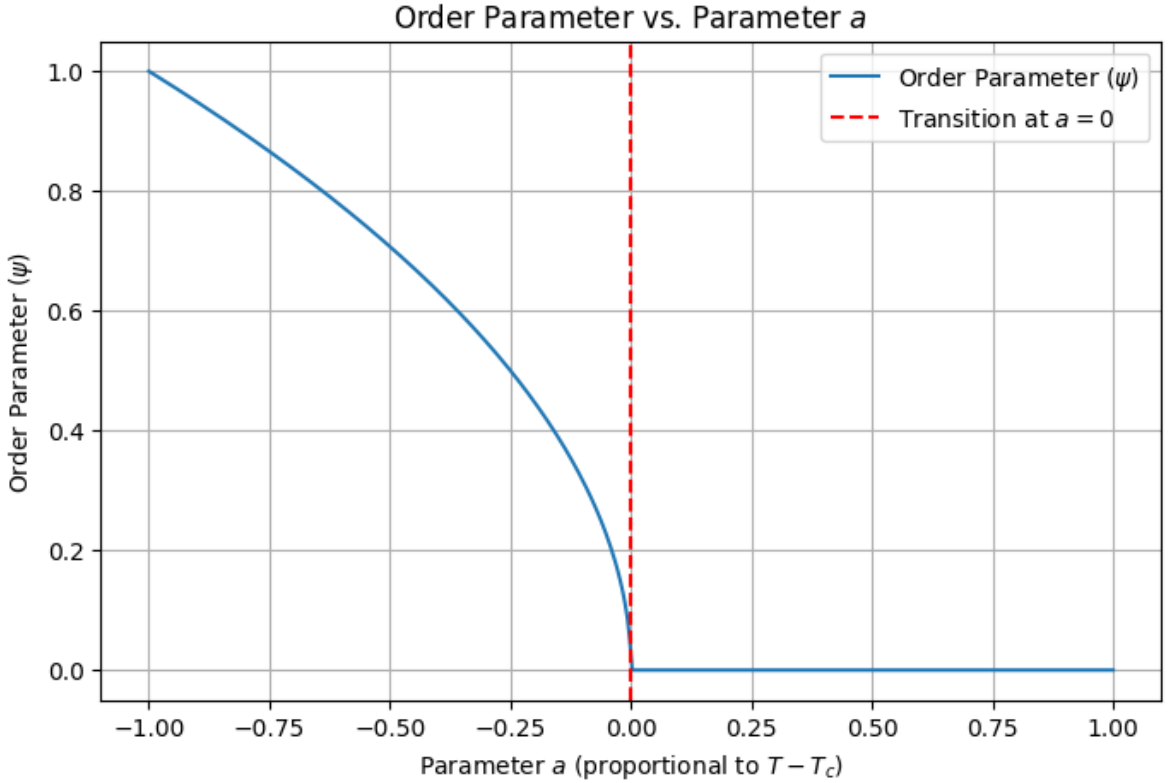
- **Gap Parameter in Superconductivity**: In superconductors, the energy gap that develops at the Fermi surface below the critical temperature serves as an order parameter. It indicates the transition from a normal conducting state to a superconducting state, where electrons form Cooper pairs.

- **Structural Order Parameter**: In materials science, this can refer to the degree of crystallinity in polymers or the long-range order in alloys, indicating transitions between amorphous and crystalline phases.

- **Opinion Polarization in Social Dynamics Models**: In theoretical models of social dynamics, the average opinion or consensus can serve as an order parameter, indicating the degree of agreement or polarization within a population.

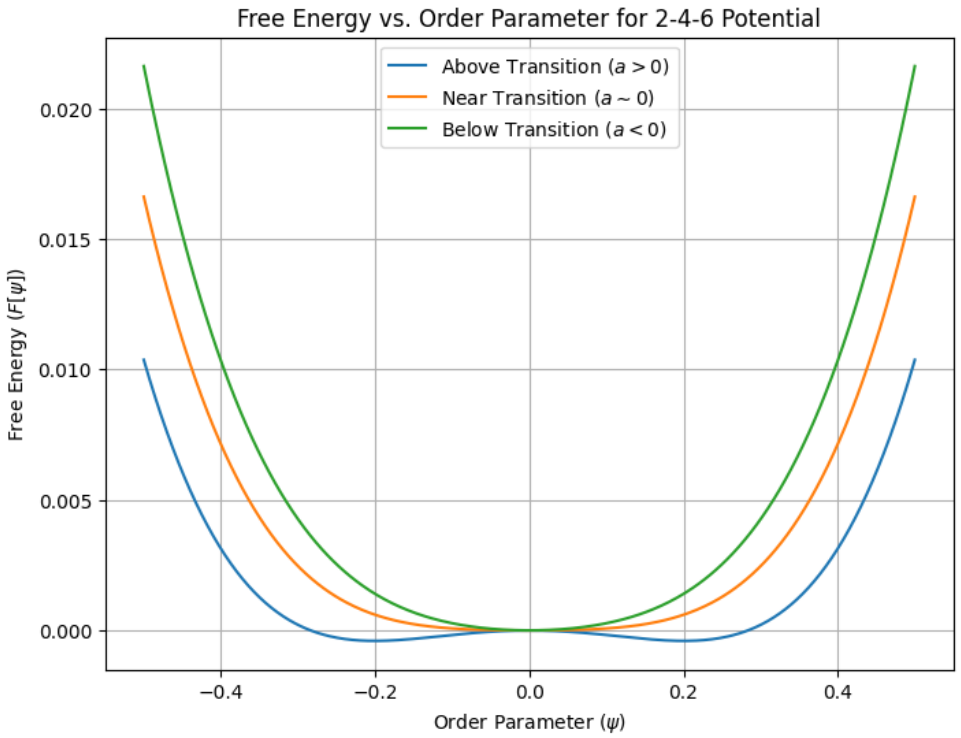
Ginzburg-Landau Theory

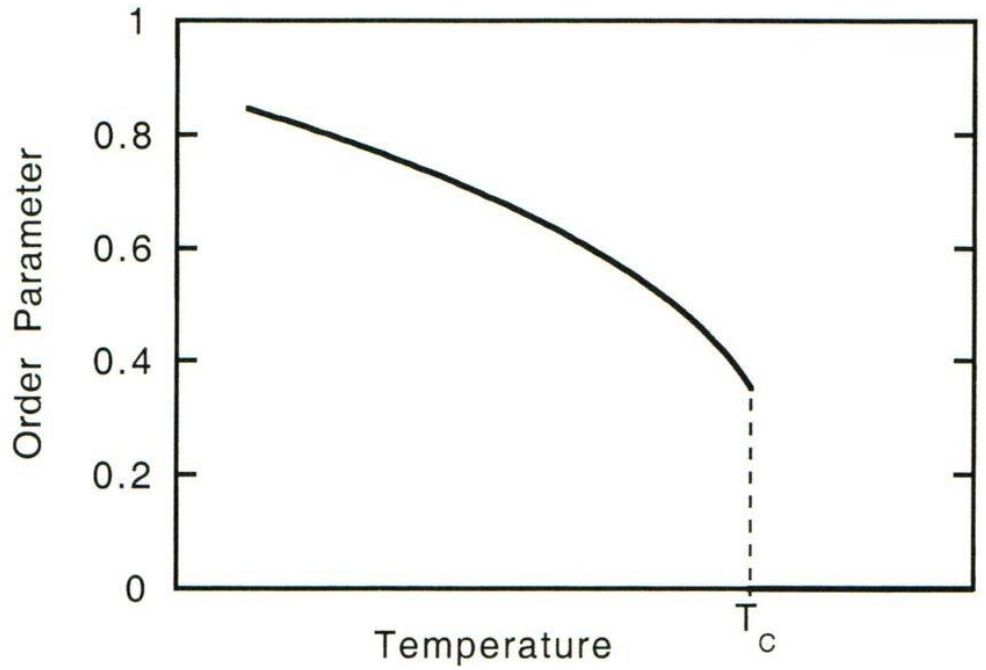




$$F = a(T\text{-}Tc)\, x^2 + b\, x^4$$

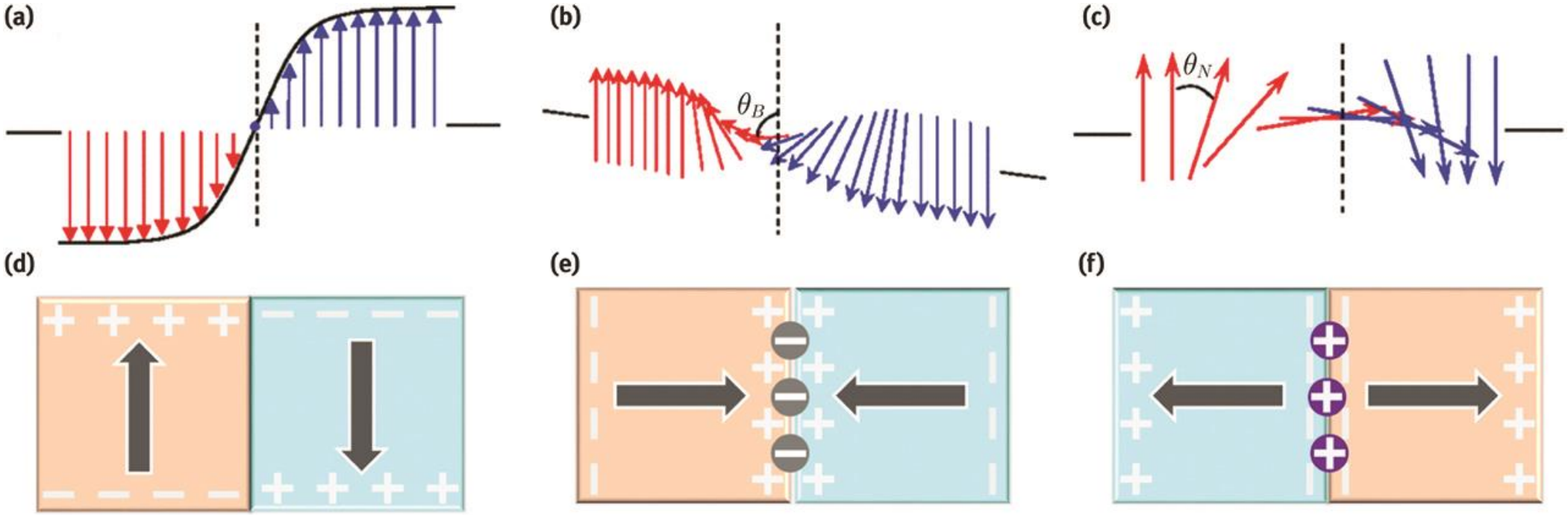
Ginzburg-Landau Theory





$$F = a(T\text{-}Tc)\, x^2 + b\, x^4 + c\, x^6$$

Topological defects and gradient terms



Energy ~ gradient of order parameter

https://www.degruyter.com/document/doi/10.1515/psr-2019-0067/html

Multiple order parameters

$$G = G_{Landau} + G_{grad} + G_{el} + G_{es+flexo} + G_S,$$

$$G_{Landau} = \int_{V_f} d^3r \left[a_i P_i^2 + a_{ij} P_i^2 P_j^2 + a_{ijk} P_i^2 P_j^2 P_k^2 \right],$$

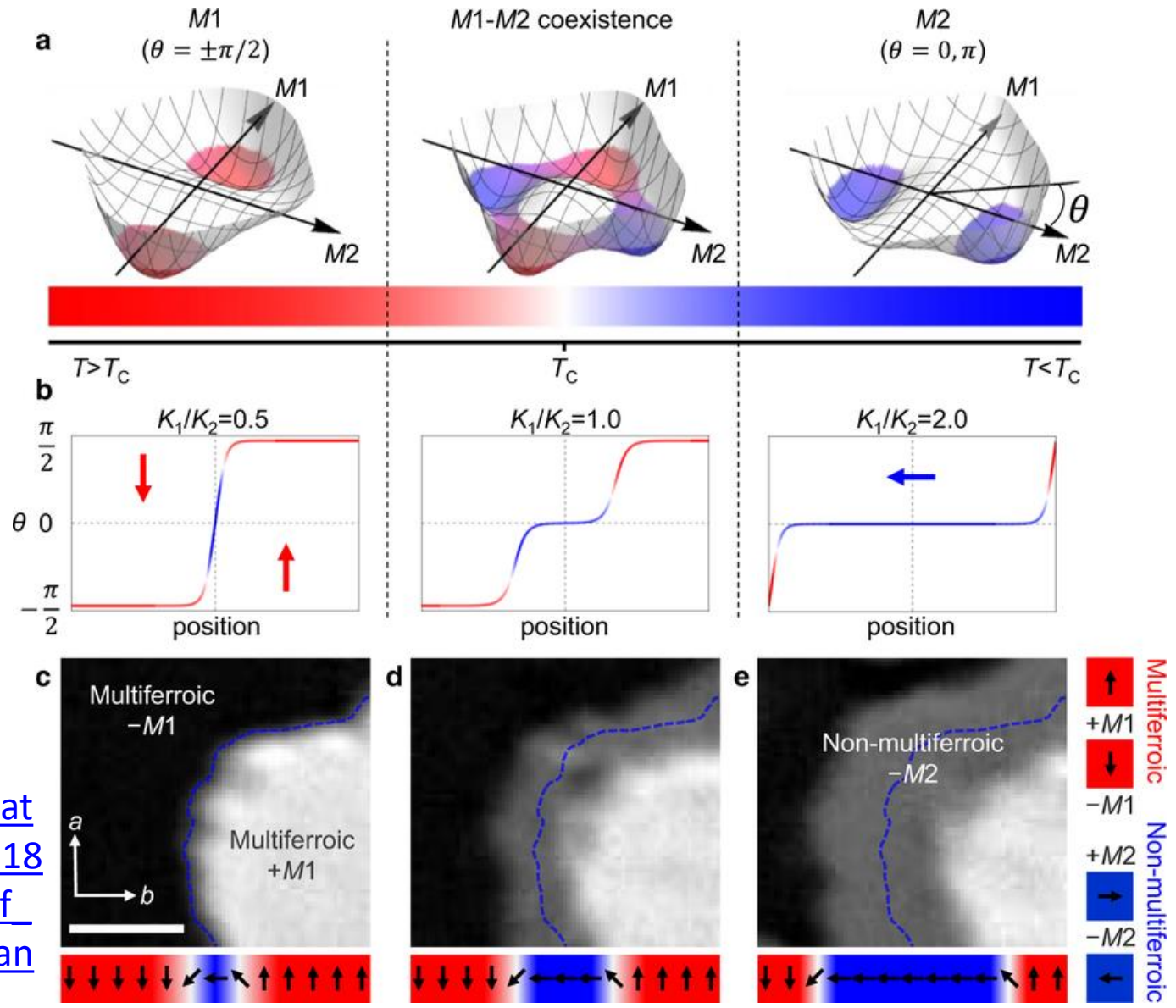
$$G_{grad} = \int_{V_f} d^3r \frac{g_{ijkl}}{2} \frac{\partial P_i}{\partial x_j} \frac{\partial P_k}{\partial x_l},$$

$$G_{el} = -\int_{V_f} d^3r \left(P_i E_i + \frac{\varepsilon_0 \varepsilon_b}{2} E_i E_i \right) - \frac{\varepsilon_0}{2} \int_{Vd} \varepsilon_{ij}^d E_i E_j d^3r,$$

$$G_{es+flexo} = -\int_{V_f} d^3r \left[\frac{s_{ijkl}}{2} \sigma_{ij} \sigma_{kl} + Q_{ijkl} \sigma_{ij} P_k P_l + F_{ijkl} \left(\sigma_{ij} \frac{\partial P_k}{\partial x_l} - P_k \frac{\partial \sigma_{ij}}{\partial x_l} \right) \right]$$

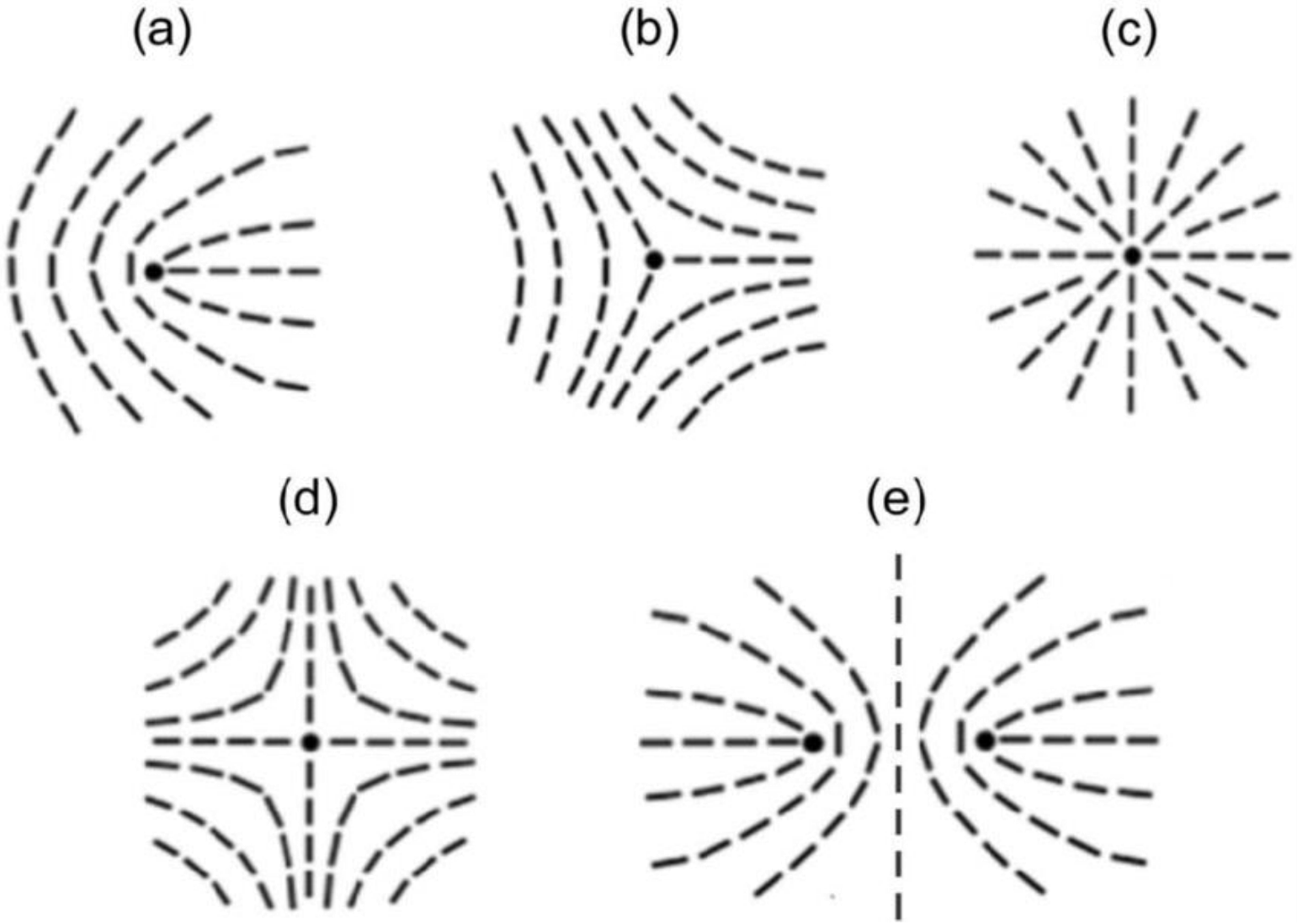
$$G_S = \frac{1}{2} \int_S d^2r \, a_{ij}^{(S)} P_i P_j.$$

Topological defects and gradient terms



https://www.researchgate.net/publication/351518160_Interconversion_of_multiferroic_domains_and_domain_walls

Topological defects and gradient terms



https://www.researchgate.net/publication/322539266_Topological_Defects_from_Simplicity_to_Complexity_Topological_Defects_From_Simplicity_to_Complexity

Cahn – Hilliard Equations

The chemical potential relative to the final equilibrium state

$$\mu_i' = \frac{\delta F}{\delta c_i} = \frac{\partial f(c_i)}{\partial c_i} - \kappa_{c_i}\nabla^2 c_i$$

assume linear kinetics

$$\vec{J}_i = -M_{ij}\nabla\mu_j' = -M_{ij}\frac{\delta F}{\delta c_j} = -M_{ij}\left[\frac{\partial f(c_j)}{\partial c_j} - \kappa_{c_j}\nabla^2 c_j\right]$$

M_i is the diffusional mobility of species i

The mass conservation leads to the Cahn-Hillard equation,

$$\frac{dc_i}{dt} = -\nabla\cdot\vec{J}_i, \qquad \frac{dc_i}{dt} = -\nabla\cdot\vec{J}_i = \nabla\cdot M_{ij}\nabla\frac{\delta F}{\delta c_j} = \nabla\cdot M_{ij}\nabla\left(\frac{\partial f}{\partial c_j} - \kappa_{c_j}\nabla^2 c_j\right)$$

Cahn and Hilliard, J. of Chem. Phys. **28**, 258-267 (1958); Cahn and Hilliard, J. of Chem. Phys. **31**, 688-699 (1959);Cahn, Acta Metall. 9, 795-801 (1961); Cahn, 1967 Institute of Metals Lecture

Slide by L.Q. Chen, Penn State

Coupled Allen-Cahn and Cahn–Hilliard Eqns

Consider both composition and order parameter and their gradients

$$F = \int \left[f(c_i, \xi) + f_{grad}(\nabla c_i, \nabla \xi) \right] dV$$

Approximate gradient energy contributions up to the second order

$$F = \int \left[f(c_i, \xi) + \frac{1}{2}\kappa_{c_i}(\nabla c_i)^2 + \frac{1}{2}\kappa_\xi(\nabla \xi)^2 \right] dV$$

$$\frac{d\xi}{dt} = -L_\xi \frac{\delta F}{\delta \xi} = -L_\xi \left(\frac{\partial f}{\partial \xi} - \kappa_\xi \nabla^2 \xi \right)$$

$$\frac{dc_i}{dt} = \nabla \cdot M_i \nabla \frac{\delta F}{\delta c_i} = \nabla \cdot M_i \nabla \left(\frac{\partial f}{\partial c_i} - \kappa_{c_i} \nabla^2 c_i \right)$$

$$\gamma = \int_{-\infty}^{+\infty} \left[f[c_i, \xi] - f\left[c_i^{eq}, \xi^{eq}\right] + \frac{1}{2}\kappa_{c_i}(\nabla c_i)^2 + \frac{1}{2}\kappa_\xi(\nabla \xi)^2 \right] dx$$

Slide by L.Q. Chen, Penn State

Thermodynamics

$$F = \int_V f\left(c_1, c_2, \ldots, c_N, \eta_1, \eta_2, \ldots, \eta_p, T\right) dV$$

Bulk chemical free energy

$$+ \int_V \left[\sum_{n=1}^{N} \alpha_n (\nabla c_n)^2 + \sum_{p=1}^{P} \beta_{ij} \frac{\partial \eta_p}{\partial r_i} \frac{\partial \eta_p}{\partial r_j} \right] dV$$

Gradient energy

$$+ \int_V \int_{V'} G(\mathbf{r} - \mathbf{r}') dV dV' - \int_V XH dV$$

Long-range interactions

External field

Conserved variables:

$$c_1, c_2, \ldots, c_N$$

Non-conserved variables:

$$\eta_1, \eta_2, \ldots, \eta_p$$

Gradient energy coefficients:

$$\alpha_n \,,\ \beta_{ij}$$

L. Q. Chen, *Phase-Field Models for Microstructure Evolution*, Annual Review of Materials Research **32**, 113 (2002)

Slide by L.Q. Chen, Penn State

Evolution Equations

Cahn-Hilliard equation for a conserved field (concentration)

$$\frac{\partial c_i(r,t)}{\partial t} = \nabla M_{ij} \nabla \frac{\delta F}{\delta c_j(r,t)} + \xi_i(r,t)$$

Allen-Cahn equation for a non-conserved field (order parameter)

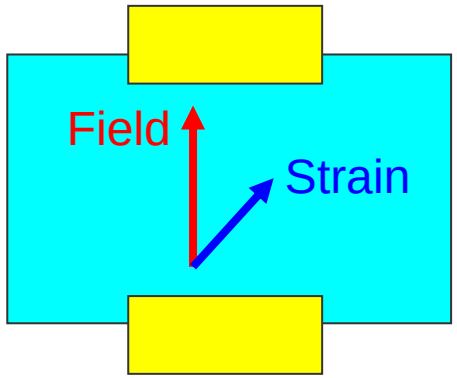
$$\frac{\partial \eta_p(r,t)}{\partial t} = -L_{pq} \frac{\delta F}{\delta \eta_q(r,t)} + \zeta_p(r,t)$$

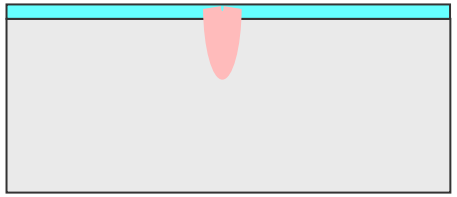
L. Q. Chen, *Phase-Field Models for Microstructure Evolution*, Annual Review of Materials Research **32**, 113 (2002)

Slide by L.Q. Chen, Penn State

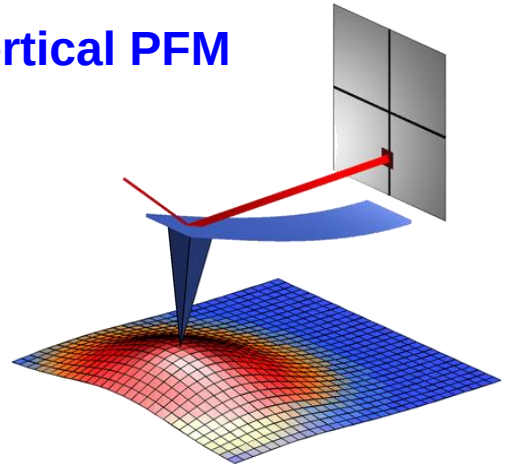
Electromechanics of nanoscale systems

In macroscopic systems, we measure response to the uniform external field (interferometry, etc)

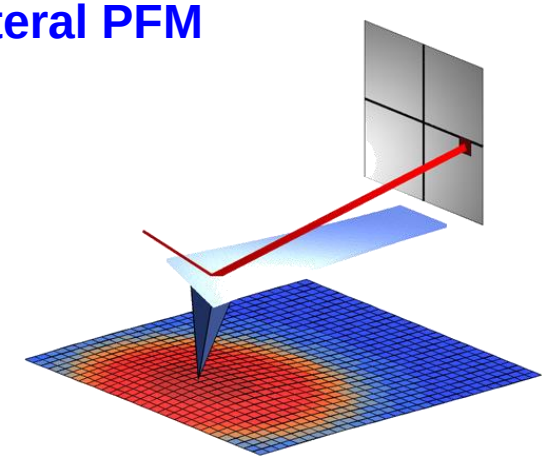




Vertical PFM



Lateral PFM



In nanoscale systems, we need

- Displacements of order of ~pm
- Currents of order of ~fA
- Length scales of ~1-10 nm

Piezoresponse Force Microscopy

Application of AC bias to the tip

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

results in cantilever deflection

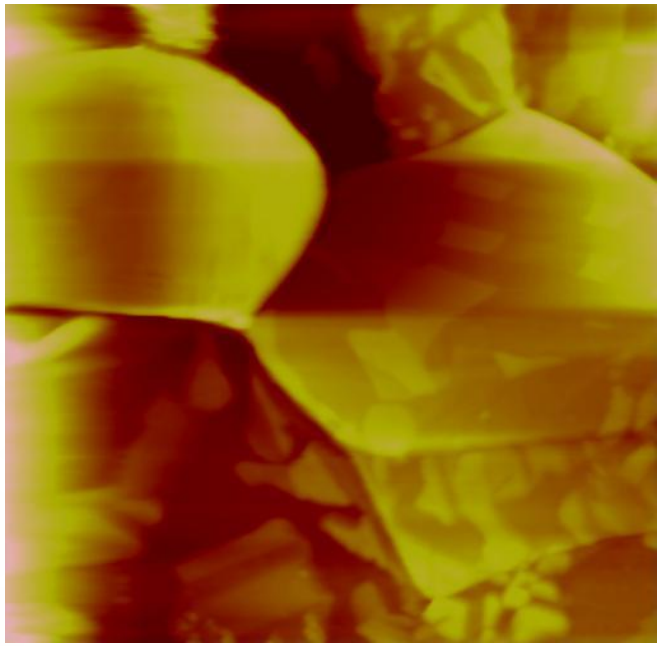
$d = d_0+A(\omega,V_{dc})V_{ac}\cos(\omega t+\varphi)$

due to piezoelectric effect

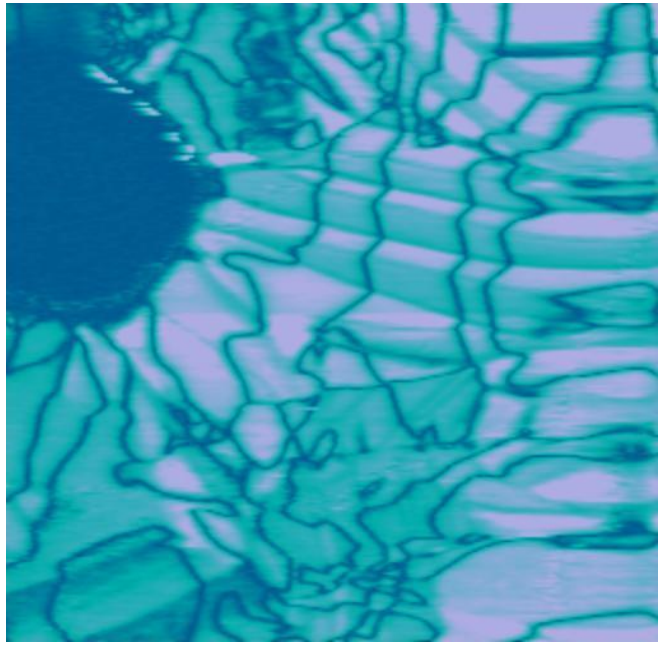
PFM = Nanoelectromechanics

Examples of PFM imaging

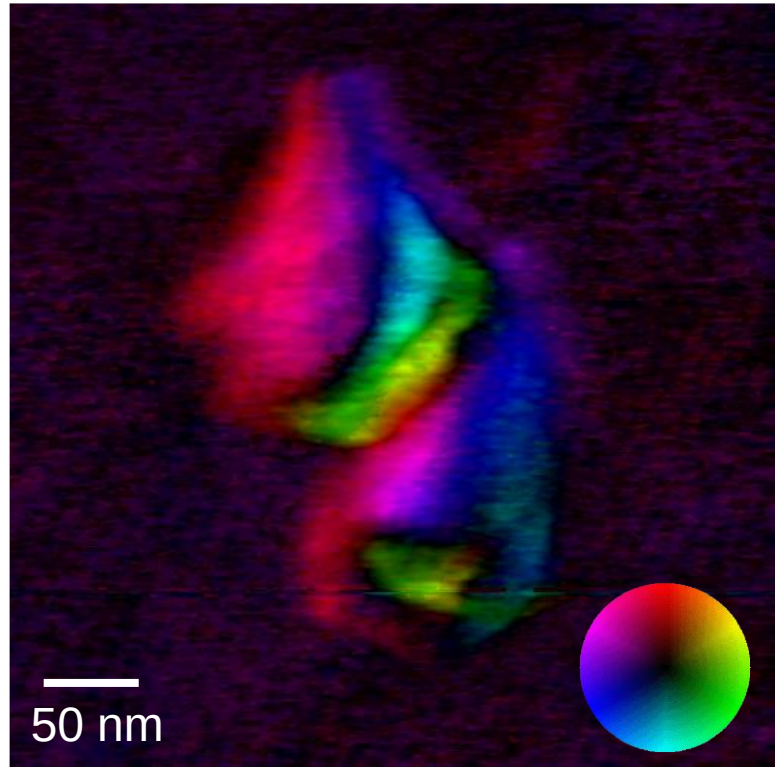
Topography



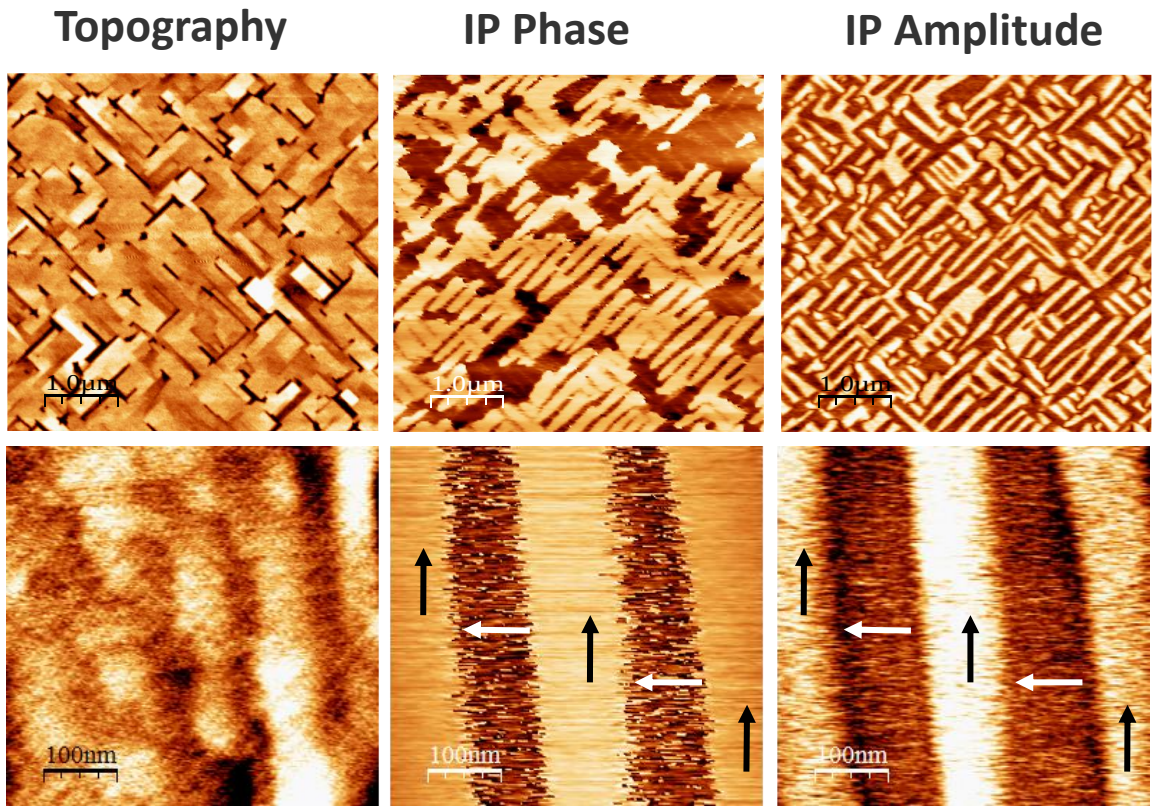
Vertical PFM amplitude

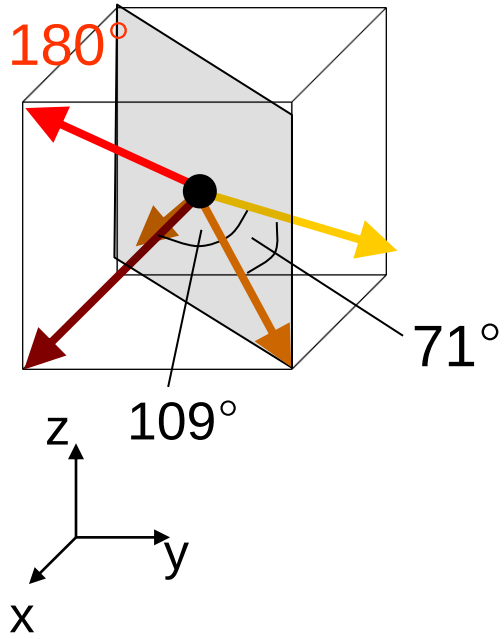


2D Electromechanical Map



PFM of Material with Multiple Order Parameters

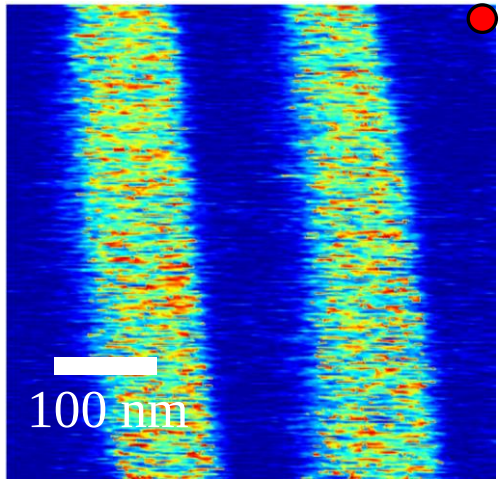




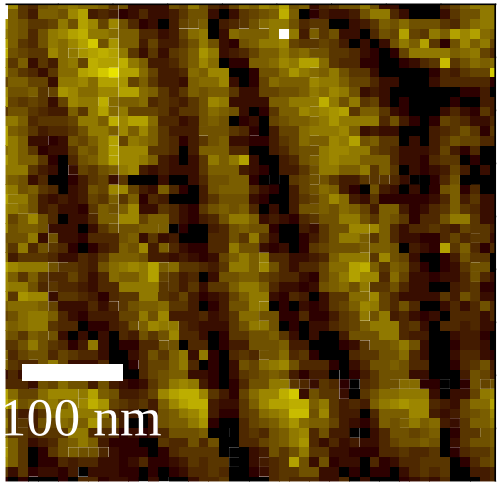
- The out-of-plane polarization is uniformly negative (all domains are [nm-1])
- A number of visible ferroelastic walls
- The ferroelastic walls are not affected by switching (same pattern after SSPFM)

Switching at the Wall

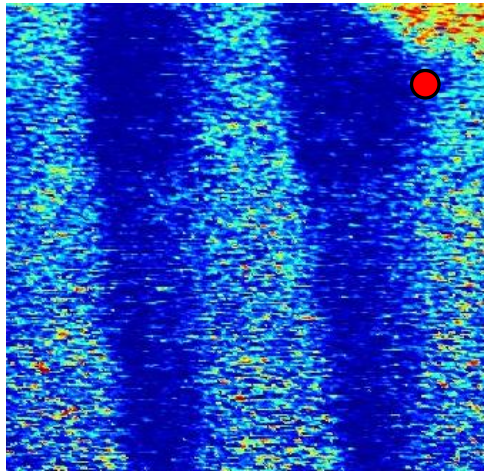
IP PFM before



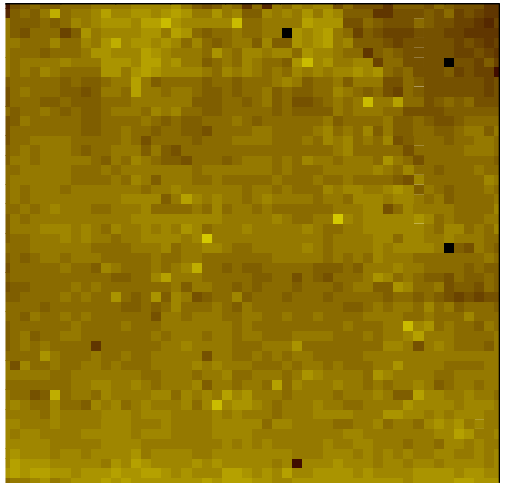
Positive nucleation bias

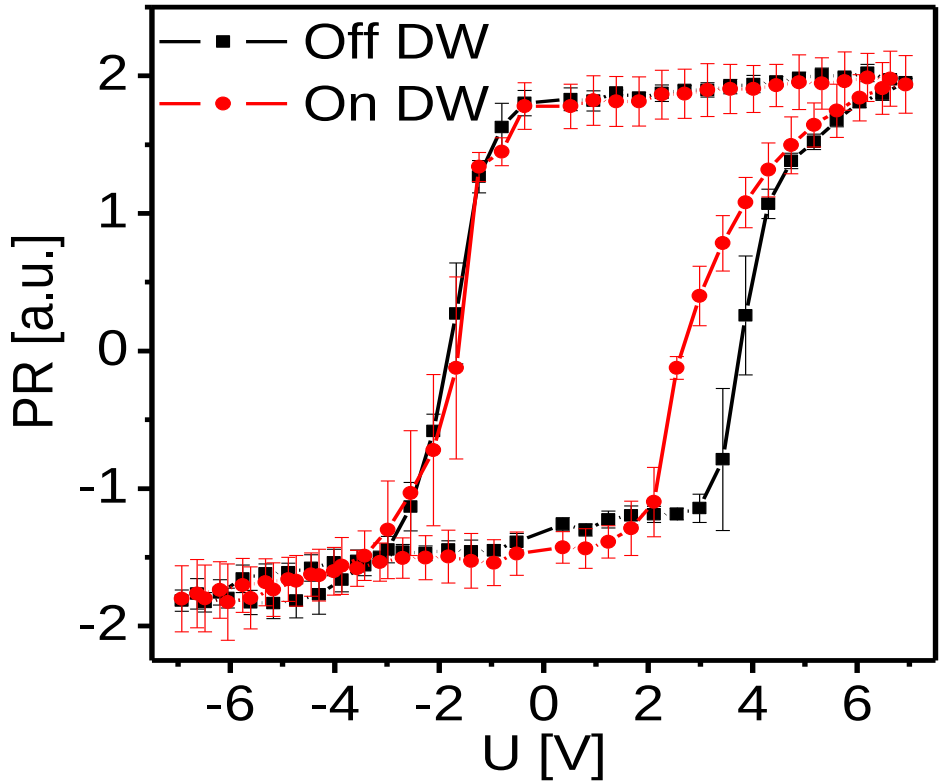


IP PFM after



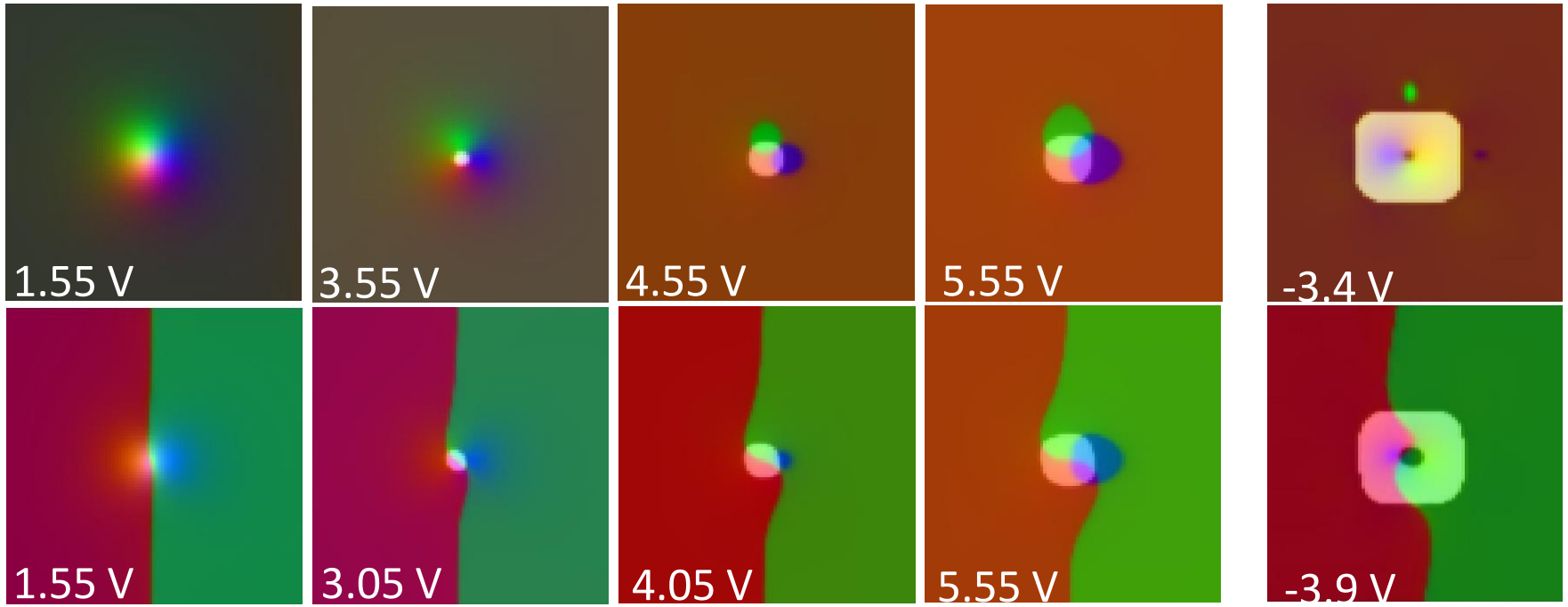
Negative nucleation bias

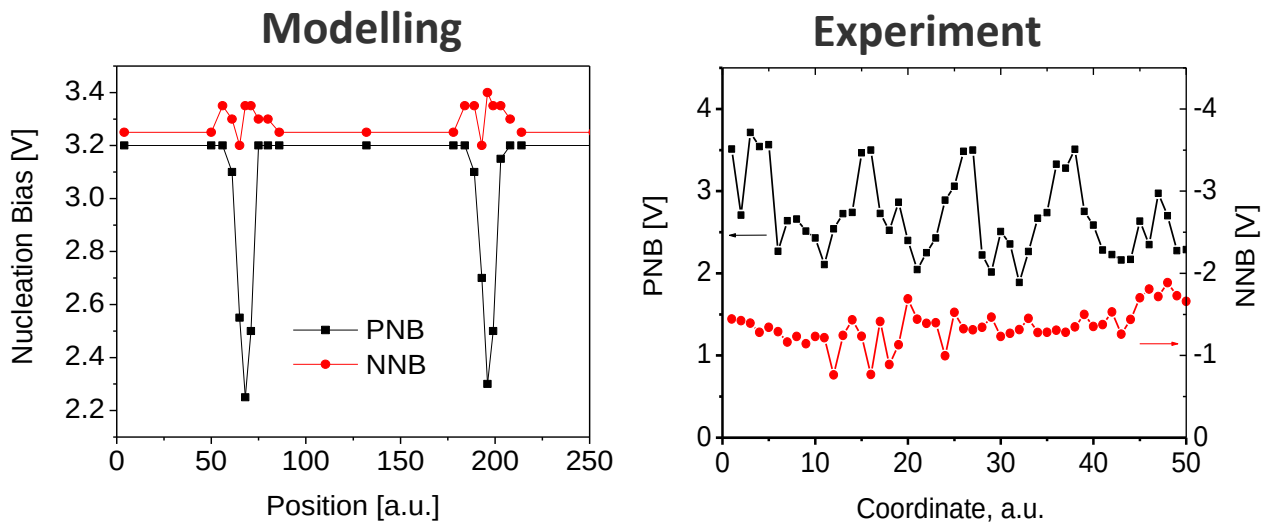




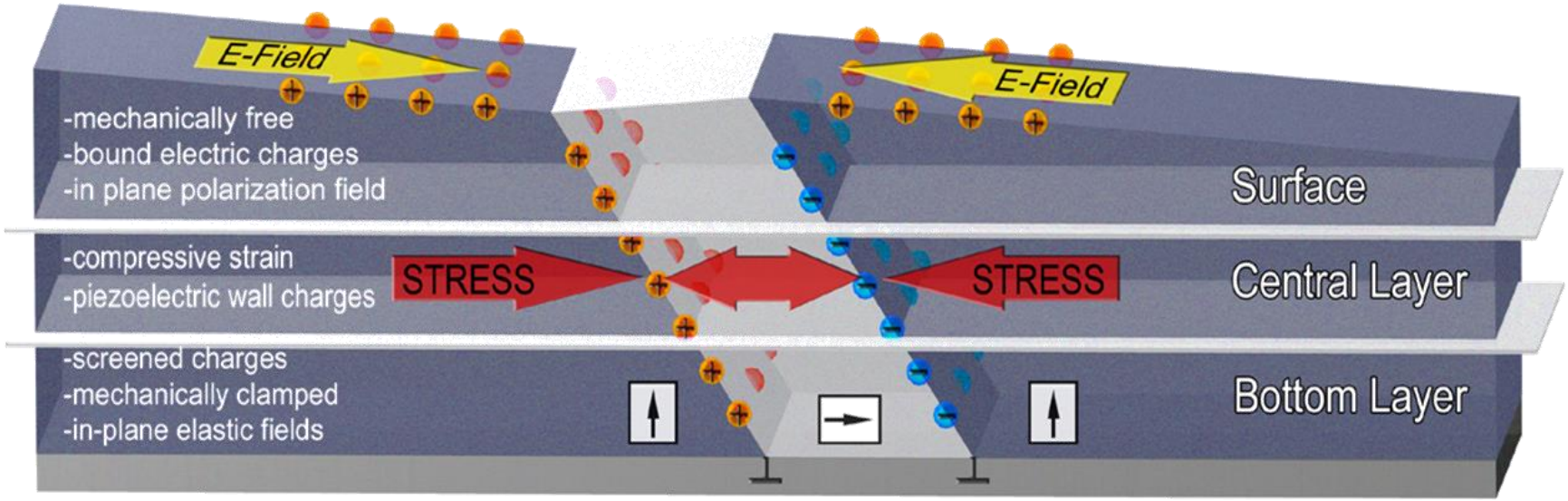
Ferroelastic wall affects ferroelectric switching!

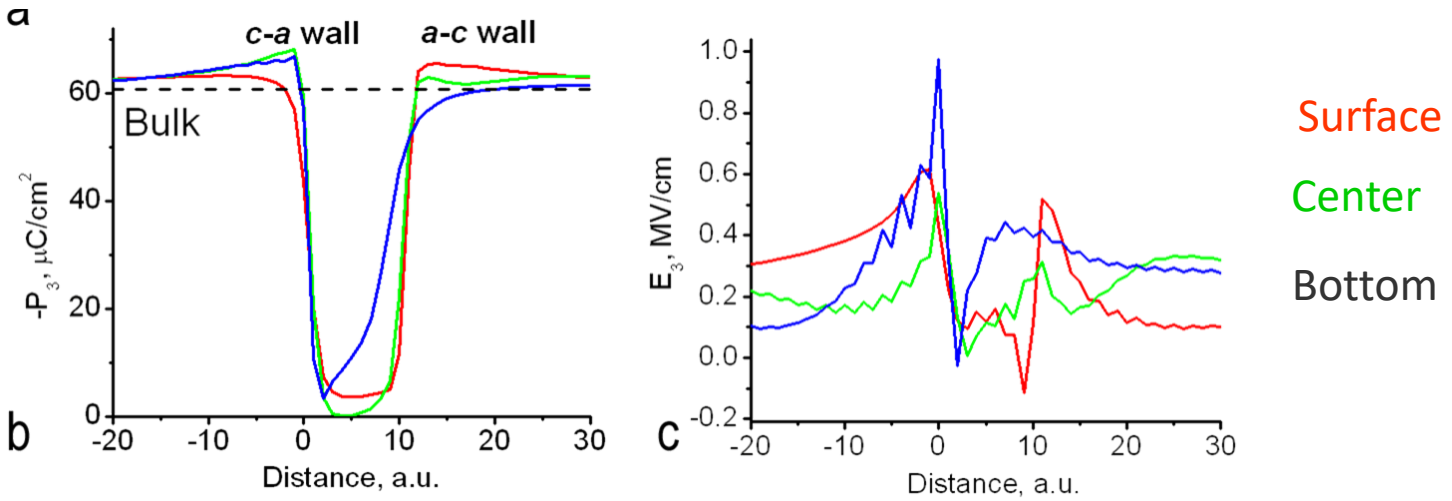
Phase Field Modelling





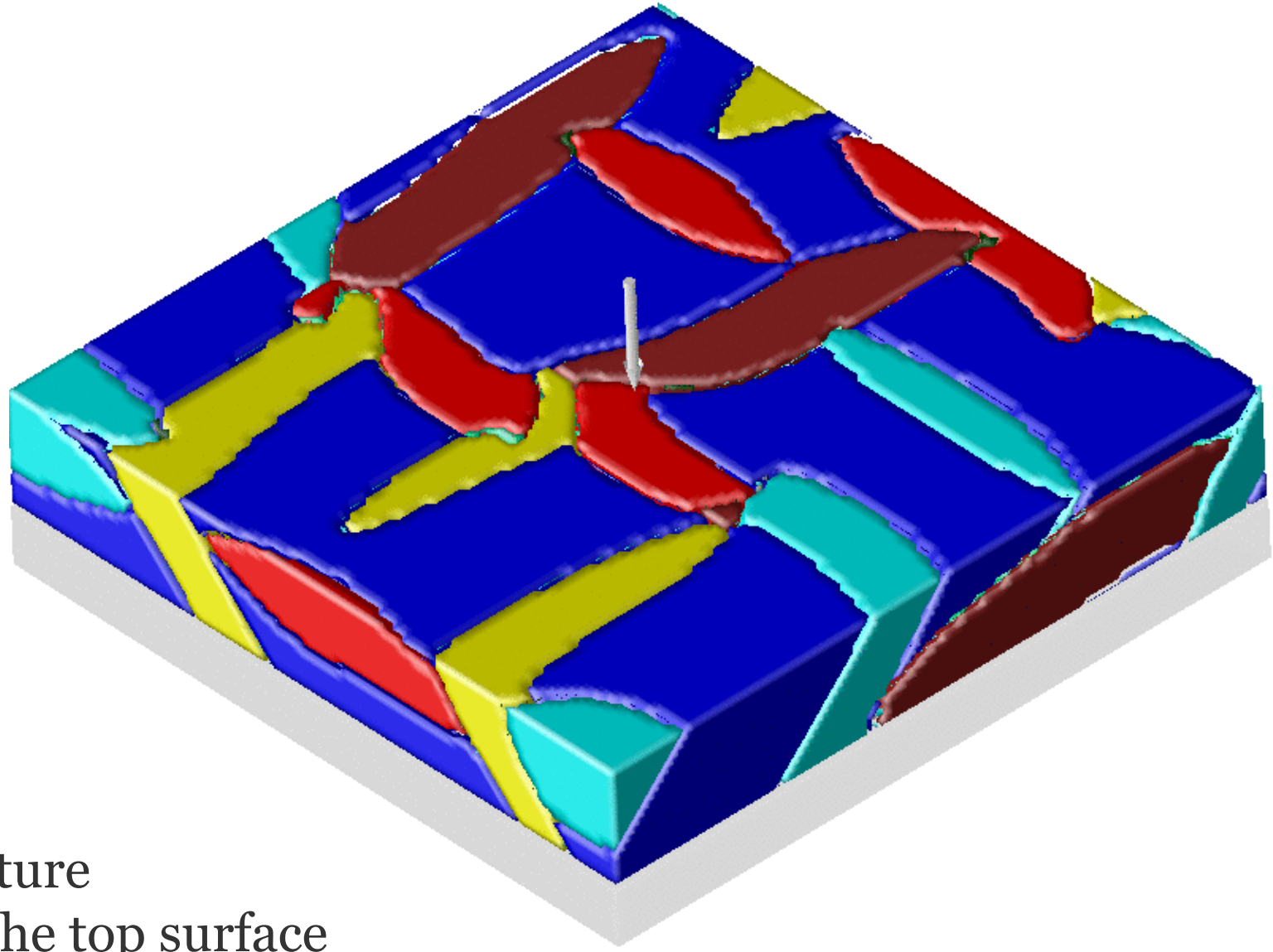
Phase field modeling





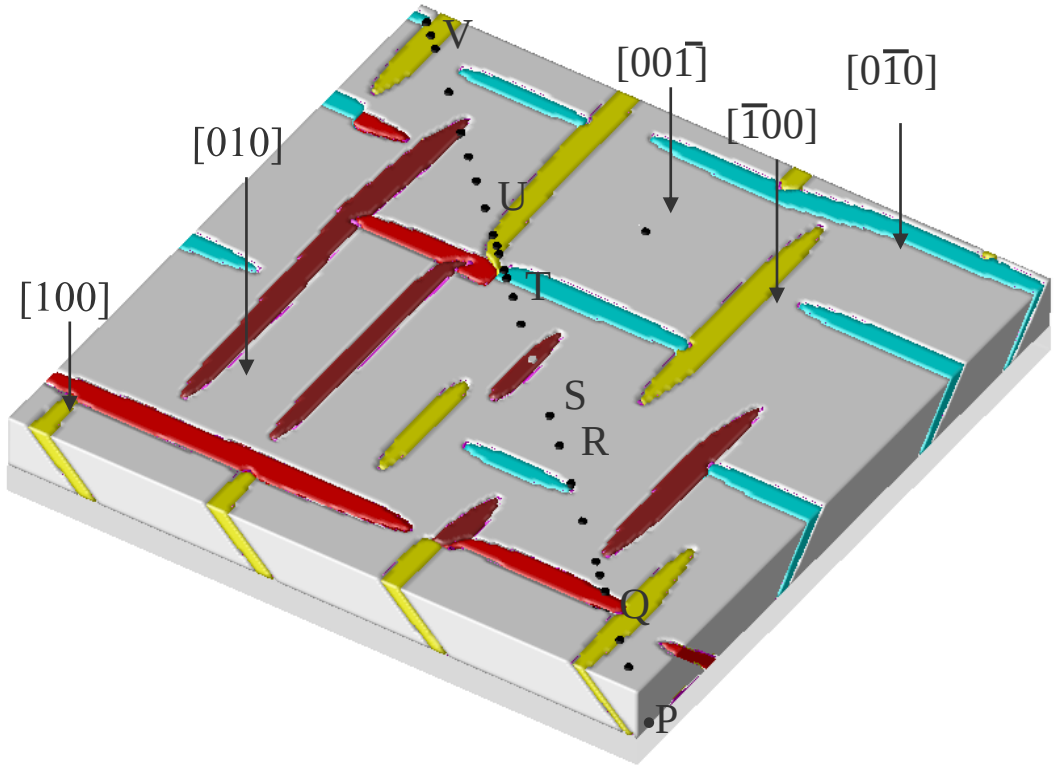
- Phase field modeling provides the information on the electrostatic field structure and polarization distribution within the field: strain, interface, and surface effects at once.
- Area with highest E_3 act as a nucleation site in a uniform field.

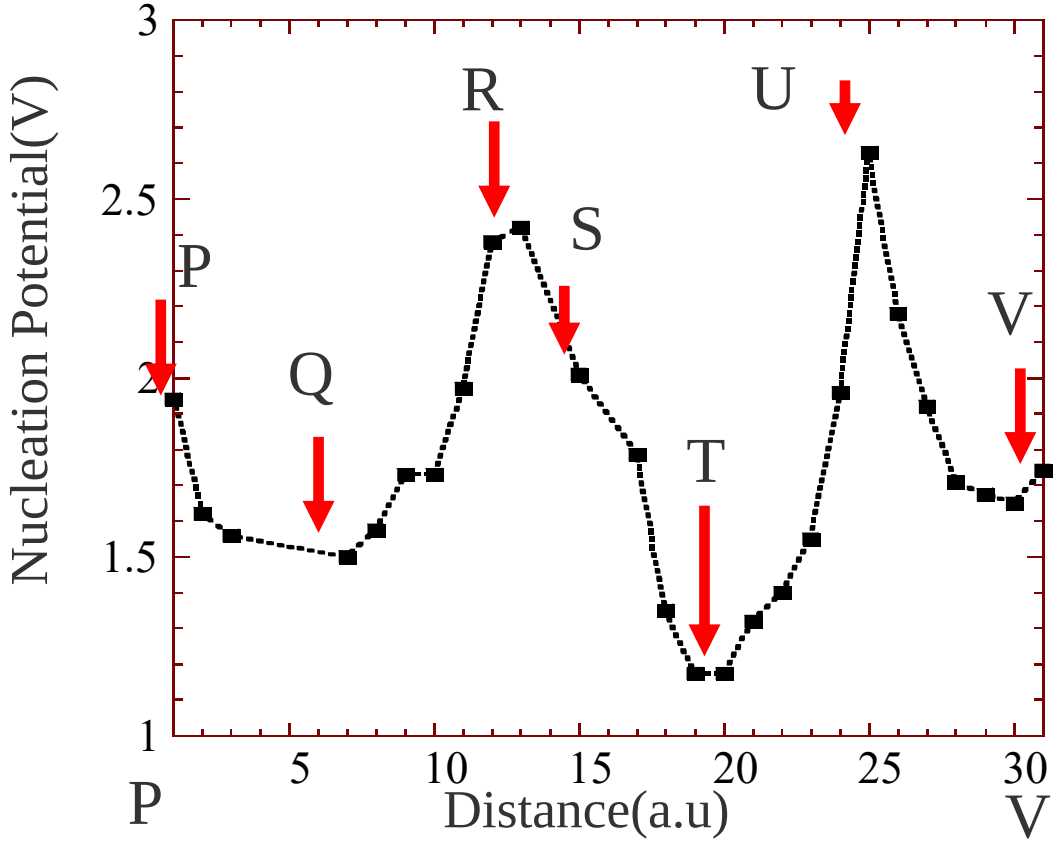
Local ferroelectric switching



- Generate domain structure
- Apply tip potential on the top surface
- Increase potential and observe domain evolution

Local ferroelectric switching





- Domain structure affects nucleation bias
- Realistic model yields 2 V for defect free place (comp. 3 V experimentally)
- And ~ 1 V for a1-a2 domain junction