# INTRODUCTION

Over recent decades, theoretical simulations such as first-principle calculations, atomistic simulations and therrnodynamic models have contributed significantly to the understanding of nanoscale ferroelectric systems. Using proper order parameters, Landau theory can provide a reliable and reasonable description of a system's equilibrium behavior near the phase transition.

Landau free-energy can be expanded near the phase-transition instability in terms of order parameters in the form of the Taylor series, with coefficients that can be fitted to experimental data

# Landau free energy density

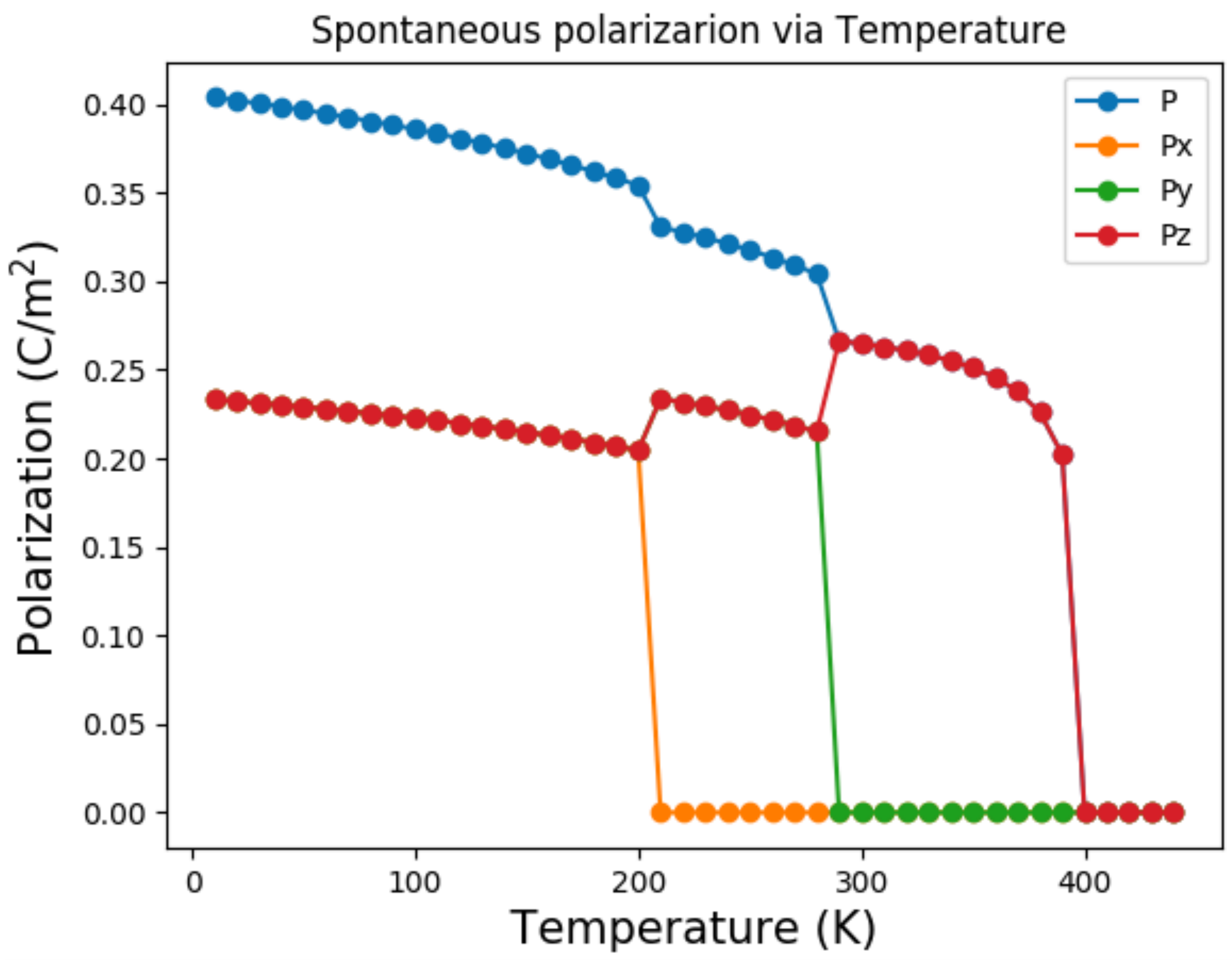
Bulk thermodynamics is characterized by the following Landau free energy density expansion

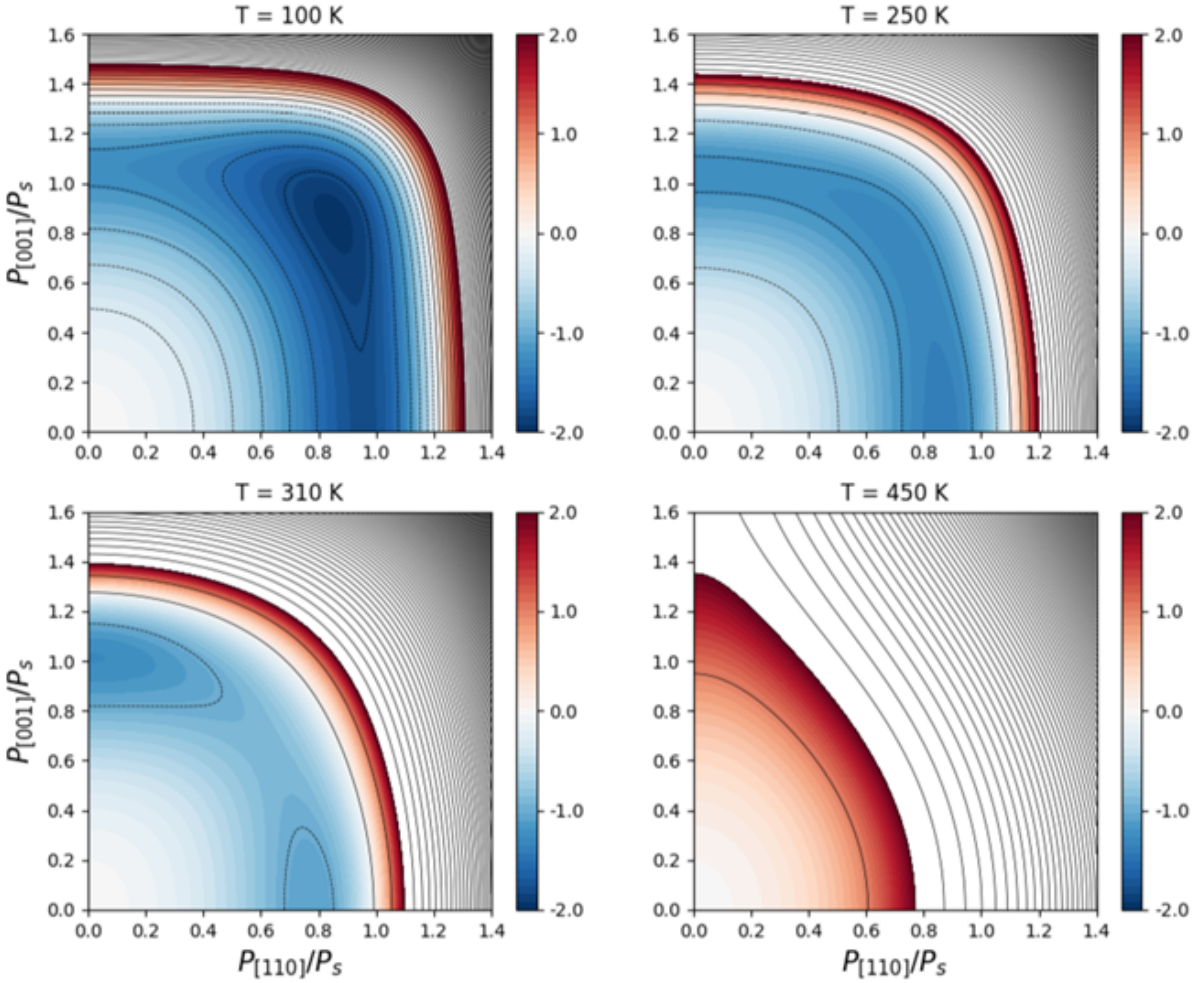
$$
\begin{aligned}
f_L(P_i) &= \alpha_1(P_1^2 + P_2^2 + P_3^2) + \alpha_{11}(P_1^4 + P_2^4 + P_3^4) + \alpha_{12}(P_1^2P_2^2 + P_2^2P_3^2 + P_1^2P_3^2) \\
&\quad + \alpha_{111}(P_1^6 + P_2^6 + P_3^6) \\
&\quad + \alpha_{112}[P_1^4(P_2^2 + P_3^2) + P_2^4(P_1^2 + P_3^2) + P_3^4(P_1^2 + P_2^2)] + \alpha_{123}(P_1^2P_2^2P_3^2),
\end{aligned}
$$

where $\alpha_1, \alpha_{11}, \alpha_{12}, \alpha_{111}, \alpha_{112}, \alpha_{123}$ are the expansion coefficients.

A negative value for $\alpha_1$ corresponds to an unstable parent paraelectric phase with respect to its transition to the ferroelectric state. A positive $\alpha_1$ value indicates a stable parent phase

# Landau free energy density

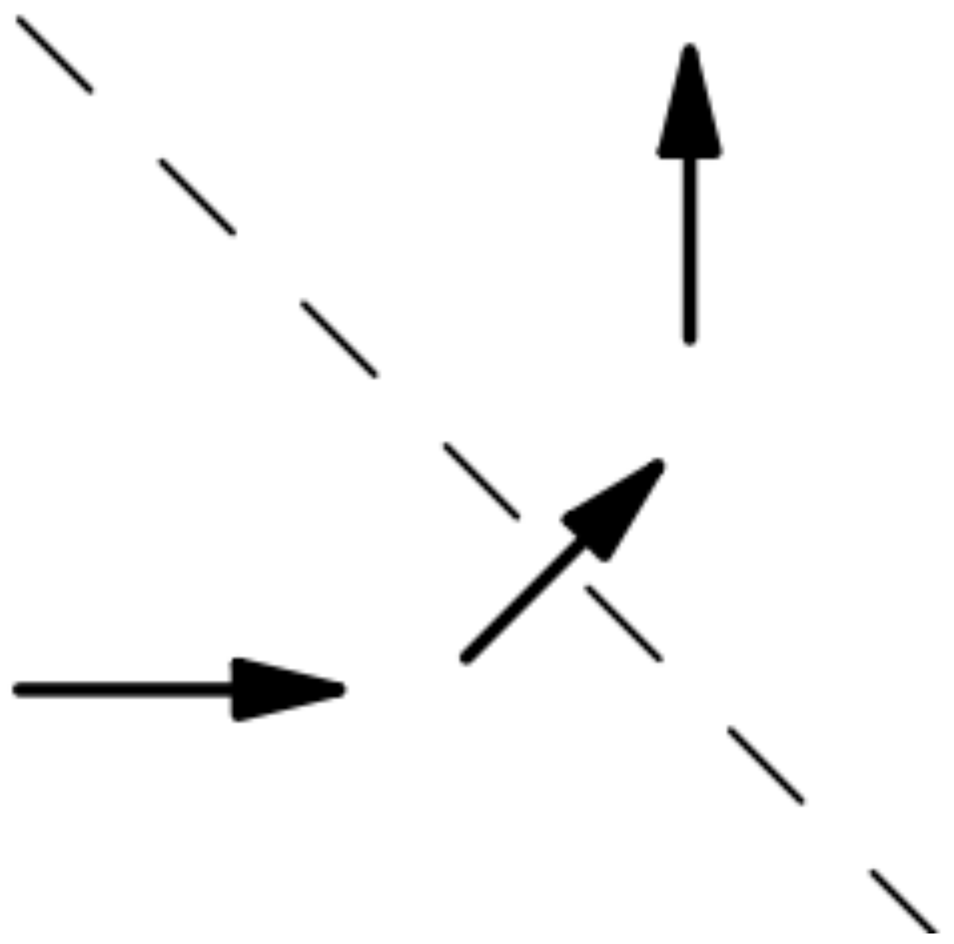


# Gradient energy density

The domain wall energy – the gradient energy contains the lowest-order symmetry-invariant terms in spatial derivatives of polarization

$$f_G = \frac{G_{11}}{2}(P_{1,1}^2 + P_{2,2}^2 + P_{3,3}^2) + G_{14}(P_{1,1}P_{2,2} + P_{2,2}P_{3,3} + P_{1,1}P_{3,3}) + \frac{G_{44}}{2}[P_{1,2}^2 + P_{2,1}^2 + P_{2,3}^2 + P_{3,2}^2 + P_{3,1}^2 + P_{1,3}^2].$$



# Elastic energy density

Involve a change of crystal structure and lattice parameter, elastic strain energy will be generated during the phase transition in order to accommodate the structure change

$$f_C[\{e_{ij}\}] = \frac{1}{2} C_{ijkl} e_{ij} e_{kl}$$

$$f_C[\{e_{ij}\}] = \frac{1}{2} C_{11} \left(e_{11}^2 + e_{22}^2 + e_{33}^2\right) + C_{12} \left(e_{11}e_{22} + e_{22}e_{33} + e_{11}e_{33}\right) + \frac{1}{2} C_{44} \left(e_{23}^2 + e_{12}^2 + e_{13}^2\right)$$

$$= \frac{1}{2} C_{11} \left[\left(\varepsilon_{11} - \varepsilon_{11}^0\right)^2 + \left(\varepsilon_{22} - \varepsilon_{22}^0\right)^2 + \left(\varepsilon_{33} - \varepsilon_{33}^0\right)^2\right] + C_{12} \left[\left(\varepsilon_{22} - \varepsilon_{22}^0\right)\left(\varepsilon_{33} - \varepsilon_{33}^0\right) + \left(\varepsilon_{11} - \varepsilon_{11}^0\right)\left(\varepsilon_{33} - \varepsilon_{33}^0\right) + \left(\varepsilon_{11} - \varepsilon_{11}^0\right)\left(\varepsilon_{22} - \varepsilon_{22}^0\right)\right]$$

$$+2C_{44} \left[\left(\varepsilon_{23} - \varepsilon_{23}^0\right)^2 + \left(\varepsilon_{12} - \varepsilon_{12}^0\right)^2 + \left(\varepsilon_{13} - \varepsilon_{13}^0\right)^2\right]$$

where $C$ represents the elastic stiffness tensor, and $e$, $\varepsilon$, and $\varepsilon^0$ denote the elastic, total, and spontaneous strain tensors, respectively. The spontaneous strain tensor $\varepsilon^0$ is related to the polarization $\vec{P}$ and the electrostriction tensor $Q$:

**Eigenstrain** : In continuum mechanics an **eigenstrain** is any mechanical deformation in a material that is not caused by an external mechanical stress, with thermal expansion often given as a familiar example. A non-uniform distribution of eigenstrains in a material (e.g., in a composite material) leads to corresponding eigenstresses, which affect the mechanical properties of the material. (Toshio Mura)

Many distinct physical causes for eigenstrains exist, such as crystallographic defects, thermal expansion, the inclusion of additional phases in a material, and previous plastic strains. As such, eigenstrains have also been referred to as **"stress-free strains"**[4] and "inherent strains".

Eigenstrain analysis usually relies on the assumption of linear elasticity, such that different contributions to the total strain are additive. In this case, the total strain of a material is divided into the elastic strain and the inelastic eigenstrain :

$$\epsilon_{ij} = e_{ij} + \epsilon^*_{ij}$$

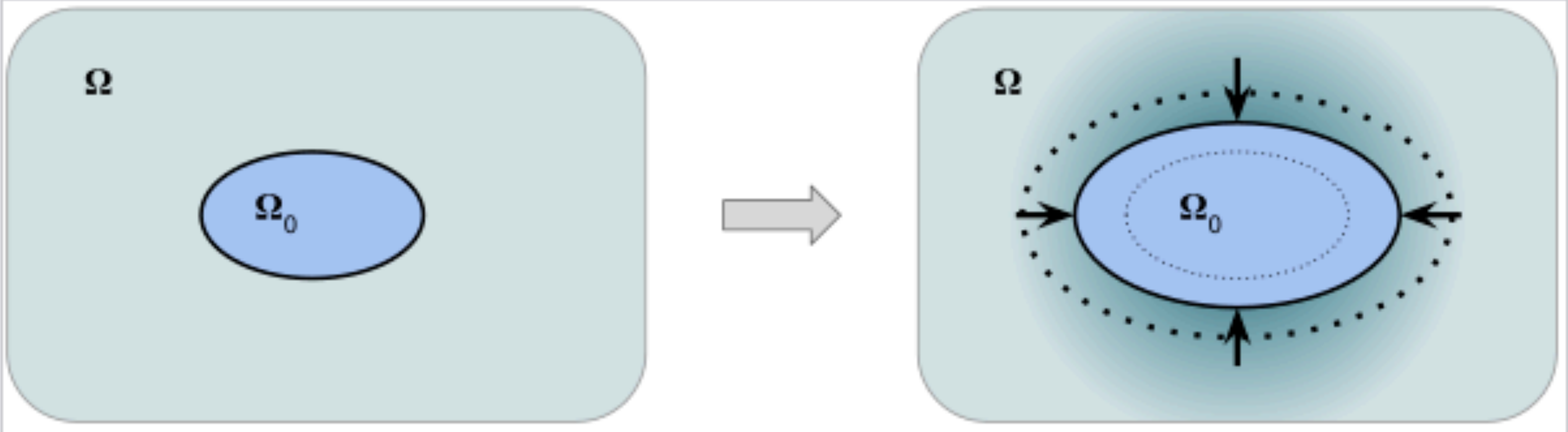
Another assumption of linear elasticity is that the stress can be linearly related to the elastic strain and the stiffness by Hooke's Law:

$$\sigma_{ij} = C_{ijkl} e_{kl}$$

In this form, the eigenstrain is not in the equation for stress, hence the term "stress-free strain". However, a non-uniform distribution of eigenstrain alone will cause elastic strains to form in response, and therefore a corresponding elastic stress.

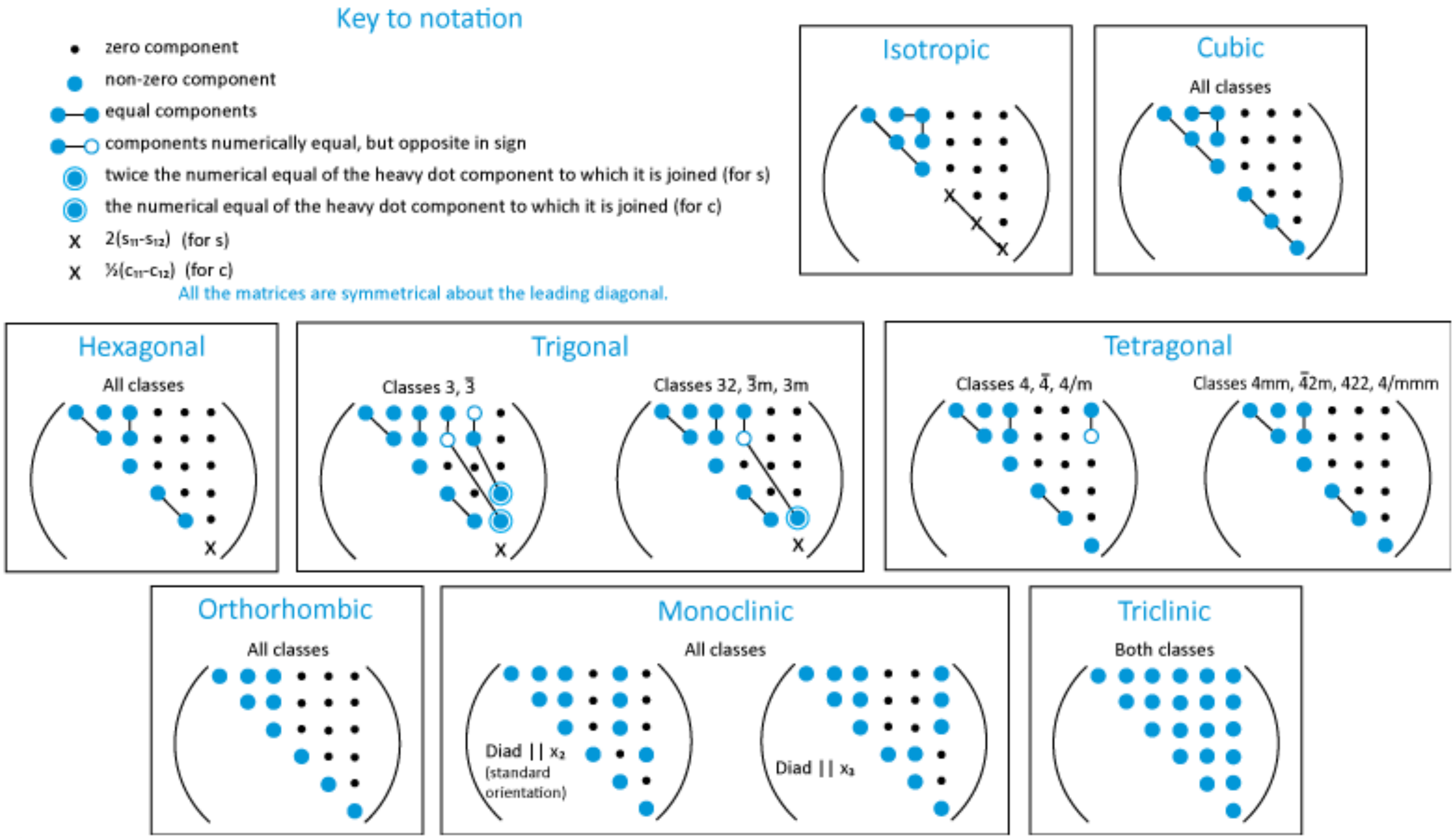
## Ellipsoidal inclusion in an infinite medium [ edit ]

One of the earliest examples providing such a closed-form solution analyzed a ellipsoidal inclusion of material $\Omega_0$ with a uniform eigenstrain, constrained by an infinite medium $\Omega$ with the same elastic properties.[6] This can be imagined with the figure on the right. The inner ellipse represents the region $\Omega_0$. The outer region represents the extent of $\Omega_0$ if it fully expanded to the eigenstrain without being constrained by the surrounding $\Omega$. Because the total strain, shown by the solid outlined ellipse, is the sum of the elastic and eigenstrains, it follows that in this example the elastic strain in the region $\Omega_0$ is negative, corresponding to a compression by $\Omega$ on the region $\Omega_0$.



Ellipsoidal eigenstrain inclusion

# Form of the ($s_{ij}$) and ($c_{ij}$) matrices




After Nye, 1959

For cubic

$$C_{ijkl} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & 0 & 0 & 0 \\ C_{2211} & C_{2222} & C_{2233} & 0 & 0 & 0 \\ C_{3311} & C_{3322} & C_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{1313} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{1212} \end{bmatrix}$$

$$= \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}$$

$$\varepsilon_{11}^0 = Q_{11}P_1^2 + Q_{12}P_2^2 + Q_{13}P_3^2 = Q_{11}P_1^2 + Q_{12}P_2^2 + Q_{12}P_3^2$$
$$\varepsilon_{22}^0 = Q_{21}P_1^2 + Q_{22}P_2^2 + Q_{23}P_3^2 = Q_{12}P_1^2 + Q_{11}P_2^2 + Q_{12}P_3^2$$
$$\varepsilon_{33}^0 = Q_{31}P_1^2 + Q_{32}P_2^2 + Q_{33}P_3^2 = Q_{12}P_1^2 + Q_{12}P_2^2 + Q_{11}P_3^2$$
$$\varepsilon_{23}^0 = Q_{44}P_2P_3$$
$$\varepsilon_{13}^0 = Q_{44}P_1P_3$$
$$\varepsilon_{12}^0 = Q_{44}P_1P_2$$

The total strain $\varepsilon_{ij}$ can be written as the sum of the spatially independent homogenous strain, $\bar{\varepsilon}_{ij}$, and a spatially dependent heterogeneous strain,$\delta\varepsilon_{ij}$

$$\varepsilon_{ij} = \bar{\varepsilon}_{ij} + \delta\varepsilon_{ij}$$

The homogenous strain determines the macroscopic shape and volume deformation of the entire model resulting from an applied strain, phase transitions or domain structure changes. If the external boundary of the model is clamped, $\bar{\varepsilon}_{ij}$ is zero. Displacements and strains are linked by the equation:

$$\varepsilon_{ij} = \delta\varepsilon_{ij} = \frac{1}{2}\left(\frac{du_i}{dx_j} + \frac{du_j}{dx_i}\right)$$

The elastic strain $\varepsilon_{kl} - \varepsilon_{kl}^0$ is related to stress $\sigma_{ij}$ by Hooke's law:

$$\sigma_{ij} = C_{ijkl}\left(\varepsilon_{kl} - \varepsilon_{kl}^0\right) = C_{ijkl}\left(u_{k,l} - \varepsilon_{kl}^0\right)$$

The equilibrium condition with material domain is assumed to be free from any external force is

$$\sigma_{ij,j} = 0$$

By substituting

$$C_{ijkl}u_{k,lj} = C_{ijkl}\epsilon_{kl,j}^0$$

## Displacement and strain relation

$$\varepsilon_{11} = \frac{1}{2}\left(\frac{du_1}{dx_1} + \frac{du_1}{dx_1}\right) = \frac{du_1}{dx_1} \qquad \varepsilon_{23} = \frac{1}{2}\left(\frac{du_2}{dx_3} + \frac{du_3}{dx_2}\right)$$

$$\varepsilon_{22} = \frac{1}{2}\left(\frac{du_2}{dx_2} + \frac{du_2}{dx_2}\right) = \frac{du_2}{dx_2} \qquad \varepsilon_{13} = \frac{1}{2}\left(\frac{du_1}{dx_3} + \frac{du_3}{dx_1}\right)$$

$$\varepsilon_{33} = \frac{1}{2}\left(\frac{du_3}{dx_3} + \frac{du_3}{dx_3}\right) = \frac{du_3}{dx_3} \qquad \varepsilon_{12} = \frac{1}{2}\left(\frac{du_1}{dx_2} + \frac{du_2}{dx_1}\right)$$

## Hooke's law

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & 0 & 0 & 0 \\ C_{2211} & C_{2222} & C_{2233} & 0 & 0 & 0 \\ C_{3311} & C_{3322} & C_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{2323} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{1313} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{1212} \end{bmatrix} \begin{bmatrix} e_{11} \\ e_{22} \\ e_{33} \\ 2e_{23} \\ 2e_{13} \\ 2e_{12} \end{bmatrix}$$

$$\begin{aligned}
\sigma_{11} &= C_{1111}e_{11} + C_{1122}e_{22} + C_{1133}e_{33} = C_{1111}\left(u_{1,1} - \varepsilon_{11}^0\right) + C_{1122}\left(u_{2,2} - \varepsilon_{22}^0\right) + C_{1133}\left(u_{3,3} - \varepsilon_{33}^0\right) \\
\sigma_{22} &= C_{2211}e_{11} + C_{2222}e_{22} + C_{2233}e_{33} = C_{2211}\left(u_{1,1} - \varepsilon_{11}^0\right) + C_{2222}\left(u_{2,2} - \varepsilon_{22}^0\right) + C_{2233}\left(u_{3,3} - \varepsilon_{33}^0\right) \\
\sigma_{33} &= C_{3311}e_{11} + C_{3322}e_{22} + C_{3333}e_{33} = C_{3311}\left(u_{1,1} - \varepsilon_{11}^0\right) + C_{3322}\left(u_{2,2} - \varepsilon_{22}^0\right) + C_{3333}\left(u_{3,3} - \varepsilon_{33}^0\right) \\
\sigma_{23} &= 2C_{2323}e_{23} = 2C_{2323}\left(u_{2,3} - \varepsilon_{23}^0\right) \\
\sigma_{13} &= 2C_{1313}e_{13} = 2C_{1313}\left(u_{1,3} - \varepsilon_{13}^0\right) \\
\sigma_{12} &= 2C_{1212}e_{12} = 2C_{1212}\left(u_{1,2} - \varepsilon_{12}^0\right)
\end{aligned}$$

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix} \begin{bmatrix} e_{11} \\ e_{22} \\ e_{33} \\ 2e_{23} \\ 2e_{13} \\ 2e_{12} \end{bmatrix}$$

$$\begin{aligned}
\sigma_{11} &= C_{11}e_{11} + C_{12}e_{22} + C_{12}e_{33} = C_{11}\left(u_{1,1} - \varepsilon_{11}^0\right) + C_{12}\left(u_{2,2} - \varepsilon_{22}^0\right) + C_{12}\left(u_{3,3} - \varepsilon_{33}^0\right) \\
\sigma_{22} &= C_{12}e_{11} + C_{11}e_{22} + C_{12}e_{33} = C_{12}\left(u_{1,1} - \varepsilon_{11}^0\right) + C_{11}\left(u_{2,2} - \varepsilon_{22}^0\right) + C_{12}\left(u_{3,3} - \varepsilon_{33}^0\right) \\
\sigma_{33} &= C_{12}e_{11} + C_{12}e_{22} + C_{11}e_{33} = C_{12}\left(u_{1,1} - \varepsilon_{11}^0\right) + C_{23}\left(u_{2,2} - \varepsilon_{22}^0\right) + C_{11}\left(u_{3,3} - \varepsilon_{33}^0\right) \\
\sigma_{23} &= 2C_{44}e_{23} = 2C_{44}\left(u_{2,3} - \varepsilon_{23}^0\right) \\
\sigma_{13} &= 2C_{44}e_{13} = 2C_{44}\left(u_{1,3} - \varepsilon_{13}^0\right) \\
\sigma_{12} &= 2C_{44}e_{12} = 2C_{44}\left(u_{1,2} - \varepsilon_{12}^0\right)
\end{aligned}$$

Equilibrium condition $\sigma_{ij,j} = 0$

$$\sigma_{11,1} + \sigma_{12,2} + \sigma_{13,3} = 0$$

$$\sigma_{21,1} + \sigma_{22,2} + \sigma_{23,3} = 0$$

$$\sigma_{31,1} + \sigma_{32,2} + \sigma_{33,3} = 0$$

$$\sigma_{11,1} = C_{1111}\left(u_{1,11} - \varepsilon^0_{11,1}\right) + C_{1122}\left(u_{2,21} - \varepsilon^0_{22,1}\right) + C_{1133}\left(u_{3,31} - \varepsilon^0_{33,1}\right)$$

$$\sigma_{12,2} = 2C_{1212}\left(u_{1,22} - \varepsilon^0_{12,2}\right)$$

$$\sigma_{13,3} = 2C_{1313}\left(u_{1,33} - \varepsilon^0_{13,3}\right)$$

$$\Rightarrow C_{1111}u_{1,11} + C_{1122}u_{2,21} + C_{1133}u_{3,31} + 2C_{1212}u_{1,22} + 2C_{1313}u_{1,33} = C_{1111}\varepsilon^0_{11,1} + C_{1122}\varepsilon^0_{22,1} + C_{1133}\varepsilon^0_{33,1} + 2C_{1212}\varepsilon^0_{12,2} + 2C_{1313}\varepsilon^0_{13,3}$$

$$\sigma_{21,1} = 2C_{2121}\left(u_{1,21} - \varepsilon^0_{21,1}\right)$$

$$\sigma_{22,2} = C_{2211}\left(u_{1,12} - \varepsilon^0_{11,2}\right) + C_{2222}\left(u_{2,22} - \varepsilon^0_{22,2}\right) + C_{2233}\left(u_{3,32} - \varepsilon^0_{33,2}\right)$$

$$\sigma_{23,3} = 2C_{2323}\left(u_{2,33} - \varepsilon^0_{23,3}\right)$$

$$\Rightarrow 2C_{2121}u_{2,11} + C_{2211}u_{1,12} + C_{2222}u_{2,22} + C_{2233}u_{3,32} + 2C_{2323}u_{2,33} = 2C_{2121}\varepsilon^0_{12,1} + C_{2211}\varepsilon^0_{11,2} + C_{2222}\varepsilon^0_{22,2} + C_{2233}\varepsilon^0_{33,2} + 2C_{2323}\varepsilon^0_{23,3}$$

$$\sigma_{31,1} = 2C_{3131}\left(u_{1,31} - \varepsilon^0_{13,1}\right)$$

$$\sigma_{32,2} = 2C_{3232}\left(u_{2,32} - \varepsilon^0_{23,2}\right)$$

$$\sigma_{33,3} = C_{3311}\left(u_{1,13} - \varepsilon^0_{11,3}\right) + C_{3322}\left(u_{2,23} - \varepsilon^0_{22,3}\right) + C_{3333}\left(u_{3,33} - \varepsilon^0_{33,3}\right)$$

$$\Rightarrow 2C_{3131}u_{3,11} + 2C_{3232}u_{3,22} + C_{3311}u_{1,13} + C_{3322}u_{2,23} + C_{3333}u_{3,33} = 2C_{3131}\varepsilon^0_{13,1} + 2C_{3232}\varepsilon^0_{23,2} + C_{3311}\varepsilon^0_{11,3} + C_{3322}\varepsilon^0_{22,3} + C_{3333}\varepsilon^0_{33,3}$$

Fourier transforms: https://www.thefouriertransform.com/

Fourier Transform Properties: https://www.thefouriertransform.com/transform/properties.php

Fourier Transform Applied to Differential Equations: https://www.thefouriertransform.com/applications/differentialequations.php

The Fourier Transform of a function f(x) is defined by:

$$\hat{f}(\omega) = \mathcal{F}\left(f(x)\right) = \int_{-\infty}^{\infty} f(x) e^{-i\omega x}\, dx.$$

$$f(x) = \mathcal{F}^{-1}\left(\hat{f}(\omega)\right) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{f}(\omega) e^{i\omega x}\, d\omega$$

Derivative Property of the Fourier Transform (Differentiation)

$$\begin{aligned}
\mathcal{F}\left(\frac{d}{dx}f(x)\right) &= \int_{-\infty}^{\infty} \overbrace{f'(x)}^{dv}\, \overbrace{e^{-i\omega x}}^{u}\, dx \\
&= \Big[\underbrace{f(x)e^{-i\omega x}}_{uv}\Big]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \underbrace{f(x)}_{v} \Big[\underbrace{-i\omega e^{-i\omega x}}_{du}\Big]\, dx \\
&= i\omega \int_{-\infty}^{\infty} f(x) e^{-i\omega x}\, dx \\
&= i\omega \mathcal{F}(f(x)).
\end{aligned}$$

$$\mathcal{F}_{\mathrm{d}}\left[f(\mathbf{r}_{\mathrm{d}})\right](\mathbf{k}_{\mathrm{d}}) = \sum_{x=0}^{R_1-1}\sum_{y=0}^{R_2-1}\sum_{z=0}^{R_3-1} f([x,y,z])exp\left[-2\pi i\left(u\frac{x}{R_1}+v\frac{y}{R_2}+w\frac{z}{R_3}\right)\right]$$
$$\mathcal{F}_{\mathrm{d}}^{-1}\left[f(\mathbf{k}_{\mathrm{d}})\right](\mathbf{r}_{\mathrm{d}}) = \frac{1}{R_1R_2R_3}\sum_{u=0}^{R_1-1}\sum_{v=0}^{R_2-1}\sum_{w=0}^{R_3-1} f([u,v,w])exp\left[2\pi i\left(x\frac{u}{R_1}+y\frac{v}{R_2}+z\frac{w}{R_3}\right)\right], \tag{B.8}$$

where $\mathbf{r}_{\mathrm{d}}, \mathbf{k}_{\mathrm{d}} \in (\{1,2,..,R_1\},\{1,2,..,R_2\},\{1,2,..,R_3\})$ stands for "discrete" point in direct and Fourier space, resp. $\mathbf{r}_{\mathrm{d}} = [x,y,z]$, $\mathbf{k}_{\mathrm{d}} = [u,v,w]$. Here, $R_d$ is the number of discrete points in a particular direction. Normalization of transformed variables is performed for backward transform only. Discrete derivatives in Fourier space are

$$\mathcal{F}_{\mathrm{d}}\left[\frac{\partial f}{\partial x}(\mathbf{r}_{\mathrm{d}})\right](\mathbf{k}_{\mathrm{d}}) = \frac{2\pi k_{dx}}{R_1\Delta}\mathcal{F}_{\mathrm{d}}\left[f(\mathbf{r}_{\mathrm{d}})\right](\mathbf{k}_{\mathrm{d}}), \tag{B.9}$$

where $\Delta$ is regular lattice spacing which we consider equal in all directions. Similarly, second derivatives are computed as

$$\mathcal{F}_{\mathrm{d}}\left[\frac{\partial^2 f}{\partial x^2}(\mathbf{r}_{\mathrm{d}})\right](\mathbf{k}_{\mathrm{d}}) = \frac{4\pi^2k_{dx}^2}{R_1^2\Delta^2}\mathcal{F}_{\mathrm{d}}\left[f(\mathbf{r}_{\mathrm{d}})\right](\mathbf{k}_{\mathrm{d}})$$
$$\mathcal{F}_{\mathrm{d}}\left[\frac{\partial^2 f}{\partial x\partial y}(\mathbf{r}_{\mathrm{d}})\right](\mathbf{k}_{\mathrm{d}}) = \frac{4\pi^2k_{dx}k_{dy}}{R_1R_2\Delta^2}\mathcal{F}_{\mathrm{d}}\left[f(\mathbf{r}_{\mathrm{d}})\right](\mathbf{k}_{\mathrm{d}}). \tag{B.10}$$

Discrete Fourier transformation

$$\mathscr{F}\left[f(r)\right] = \sum_{x=0}^{nx-1}\sum_{y=0}^{ny-1}\sum_{z=0}^{nz-1} f\left(ix, iy, iz\right)\exp\left[-2\pi i\left(\xi_1\frac{x}{nx} + \xi_2\frac{y}{ny} + \xi_3\frac{z}{nz}\right)\right]$$

$$\mathscr{F}^{-1}\left[f(r)\right] = \sum_{\xi_1=0}^{nx-1}\sum_{\xi_2=0}^{ny-1}\sum_{\xi_3=0}^{nz-1} f\left(\xi_1, \xi_2, \xi_3\right)\exp\left[2\pi i\left(x\frac{\xi_1}{nx} + y\frac{\xi_2}{ny} + z\frac{\xi_3}{nz}\right)\right]$$

Derivation Fourier transformation

## Example [ edit ]

Let $N = 4$ and

$$\mathbf{x} = \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 - i \\ -i \\ -1 + 2i \end{pmatrix}$$

Here we demonstrate how to calculate the DFT of $\mathbf{x}$ using **Eq.1**:

$$X_0 = e^{-i2\pi 0\cdot 0/4} \cdot 1 + e^{-i2\pi 0\cdot 1/4} \cdot (2-i) + e^{-i2\pi 0\cdot 2/4} \cdot (-i) + e^{-i2\pi 0\cdot 3/4} \cdot (-1+2i) = 2$$
$$X_1 = e^{-i2\pi 1\cdot 0/4} \cdot 1 + e^{-i2\pi 1\cdot 1/4} \cdot (2-i) + e^{-i2\pi 1\cdot 2/4} \cdot (-i) + e^{-i2\pi 1\cdot 3/4} \cdot (-1+2i) = -2-2i$$
$$X_2 = e^{-i2\pi 2\cdot 0/4} \cdot 1 + e^{-i2\pi 2\cdot 1/4} \cdot (2-i) + e^{-i2\pi 2\cdot 2/4} \cdot (-i) + e^{-i2\pi 2\cdot 3/4} \cdot (-1+2i) = -2i$$
$$X_3 = e^{-i2\pi 3\cdot 0/4} \cdot 1 + e^{-i2\pi 3\cdot 1/4} \cdot (2-i) + e^{-i2\pi 3\cdot 2/4} \cdot (-i) + e^{-i2\pi 3\cdot 3/4} \cdot (-1+2i) = 4+4i$$

$$\mathbf{X} = \begin{pmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \end{pmatrix} = \begin{pmatrix} 2 \\ -2-2i \\ -2i \\ 4+4i \end{pmatrix}$$

```c
fftw_plan p;
fftw_complex *in, *out;
in = (fftw_complex*) fftw_malloc(sizeof(fftw_complex) * N);
out = (fftw_complex*) fftw_malloc(sizeof(fftw_complex) * N);

in[0][0] = 1;
in[0][1] = 0;

in[1][0] = 2;
in[1][1] = -1;

in[2][0] = 0;
in[2][1] = -1;

in[3][0] = -1;
in[3][1] = 2;



p = fftw_plan_dft_1d(4, in, out, FFTW_FORWARD, FFTW_ESTIMATE);
fftw_execute(p); /* repeat as needed */
fftw_destroy_plan(p);
```

```
Direct Fourier Transformation
        Real part       Imaginary part
X[0]    2.000000        0.000000
X[1]    -2.000000       -2.000000
X[2]    0.000000        -2.000000
X[3]    4.000000        4.000000
```

```c
p = fftw_plan_dft_1d(4, out, in, FFTW_BACKWARD, FFTW_ESTIMATE);
fftw_execute(p); /* repeat as needed */
fftw_destroy_plan(p);
```

```
Inverse Fourier Transformation
        Real part       Imaginary part
x[0]    1.000000        0.000000
x[1]    2.000000        -1.000000
x[2]    0.000000        -1.000000
x[3]    -1.000000       2.000000
```

Equilibrium become

$$C_{ijkl}\bar{u}_k\xi_l\xi_j = -iC_{ijkl}\bar{\epsilon}^0_{kl}\xi_j$$

Using the notations K and X where

$$K_{ik}\left(\xi\right) = C_{ijkl}\xi_l\xi_j$$

$$X_i = -iC_{ijkl}\bar{\epsilon}^0_{kl}\xi_j,$$

We can rewrite

$$K_{11}\bar{u}_1 + K_{12}\bar{u}_2 + K_{13}\bar{u}_3 = X_1$$

$$K_{21}\bar{u}_1 + K_{22}\bar{u}_2 + K_{23}\bar{u}_3 = X_2$$

$$K_{31}\bar{u}_1 + K_{32}\bar{u}_2 + K_{33}\bar{u}_3 = X_3$$

$$C_{1111}u_{1,11}+C_{1122}u_{2,21}+C_{1133}u_{3,31}+2C_{1212}u_{1,22}+2C_{1313}u_{1,33}=C_{1111}\varepsilon^0_{11,1}+C_{1122}\varepsilon^0_{22,1}+C_{1133}\varepsilon^0_{33,1}+2C_{1212}\varepsilon^0_{12,2}+2C_{1313}\varepsilon^0_{13,3}$$

$$2C_{2121}u_{2,11}+C_{2211}u_{1,12}+C_{2222}u_{2,22}+C_{2233}u_{3,32}+2C_{2323}u_{2,33}=2C_{2121}\varepsilon^0_{12,1}+C_{2211}\varepsilon^0_{11,2}+C_{2222}\varepsilon^0_{22,2}+C_{2233}\varepsilon^0_{33,2}+2C_{2323}\varepsilon^0_{23,3}$$

$$2C_{3131}u_{3,11}+2C_{3232}u_{3,22}+C_{3311}u_{1,13}+C_{3322}u_{2,23}+C_{3333}u_{3,33}=2C_{3131}\varepsilon^0_{13,1}+2C_{3232}\varepsilon^0_{23,2}+C_{3311}\varepsilon^0_{11,3}+C_{3322}\varepsilon^0_{22,3}+C_{3333}\varepsilon^0_{33,3}$$

After Fourier transformation

$$C_{1111}\xi_1\xi_1\bar{u}_1\left(\xi\right)+C_{1122}\xi_1\xi_2\bar{u}_2\left(\xi\right)+C_{1133}\xi_1\xi_3\bar{u}_3\left(\xi\right)+2C_{1212}\xi_2\xi_2\bar{u}_1\left(\xi\right)+2C_{1313}\xi_3\xi_3\bar{u}_1\left(\xi\right)=-i(C_{1111}\xi_1\bar{\varepsilon}^0_{11}\left(\xi\right)+C_{1122}\xi_1\bar{\varepsilon}^0_{22}\left(\xi\right)+C_{1133}\xi_1\bar{\varepsilon}^0_{33}\left(\xi\right)+2C_{1212}\xi_2\bar{\varepsilon}^0_{12}\left(\xi\right)+2C_{1313}\zeta_3\bar{\varepsilon}^0_{13}\left(\xi\right))$$

$$2C_{2121}\xi_1\xi_1\bar{u}_2\left(\xi\right)+C_{2211}\xi_1\xi_2\bar{u}_1\left(\xi\right)+C_{2222}\xi_2\xi_2\bar{u}_2\left(\xi\right)+C_{2233}\xi_2\xi_3\bar{u}_3\left(\xi\right)+2C_{2323}\xi_3\xi_3\bar{u}_2\left(\xi\right)=-i(2C_{2121}\xi_1\bar{\varepsilon}^0_{12}\left(\xi\right)+C_{2211}\xi_2\bar{\varepsilon}^0_{11}\left(\xi\right)+C_{2222}\xi_2\bar{\varepsilon}^0_{22}\left(\xi\right)+C_{2233}\xi_2\bar{\varepsilon}^0_{33}\left(\xi\right)+2C_{2323}\xi_3\bar{\varepsilon}^0_{23}\left(\xi\right))$$

$$2C_{3131}\xi_1\xi_1\bar{u}_3\left(\xi\right)+2C_{3232}\xi_2\xi_2\bar{u}_3\left(\xi\right)+C_{3311}\xi_1\xi_3\bar{u}_1\left(\xi\right)+C_{3322}\xi_2\xi_3\bar{u}_2\left(\xi\right)+C_{3333}\xi_3\xi_3\bar{u}_3\left(\xi\right)=-i(2C_{3131}\zeta_1\bar{\varepsilon}^0_{13}\left(\xi\right)+2C_{3232}\zeta_2\bar{\varepsilon}^0_{23}\left(\xi\right)+C_{3311}\zeta_3\bar{\varepsilon}^0_{11}\left(\xi\right)+C_{3322}\zeta_3\bar{\varepsilon}^0_{22}\left(\xi\right)+C_{3333}\zeta_3\bar{\varepsilon}^0_{33}\left(\xi\right))$$

$$K_{ik}(\xi)=C_{ijkl}\xi_l\xi_j$$

$$K_{11}(\xi)=C_{1111}\xi_1\xi_1+C_{1212}\xi_2\xi_2+C_{1313}\xi_3\xi_3 \qquad K_{12}(\xi)=2C_{1122}\xi_1\xi_2 \qquad K_{13}(\xi)=2C_{1133}\xi_1\xi_3$$

$$K_{21}(\xi)=2C_{2211}\xi_1\xi_2 \qquad K_{22}(\xi)=C_{2121}\xi_1\xi_1+C_{2222}\xi_2\xi_2+C_{2323}\xi_3\xi_3 \qquad K_{23}(\xi)=2C_{2233}\xi_2\xi_3$$

$$K_{31}(\xi)=2C_{3311}\xi_1\xi_3 \qquad K_{32}(\xi)=2C_{3322}\xi_2\xi_3 \qquad K_{22}(\xi)=C_{3131}\xi_1\xi_1+C_{3232}\xi_2\xi_2+C_{3333}\xi_3\xi_3$$

$$X_i=-iC_{ijkl}\bar{\varepsilon}^0_{kl}\left(\xi\right)\xi_j$$

$$X_1=-i(C_{1111}\xi_1\bar{\varepsilon}^0_{11}\left(\xi\right)+C_{1122}\xi_1\bar{\varepsilon}^0_{22}\left(\xi\right)+C_{1133}\xi_1\bar{\varepsilon}^0_{33}\left(\xi\right)+2C_{1212}\xi_2\bar{\varepsilon}^0_{12}\left(\xi\right)+2C_{1313}\xi_3\bar{\varepsilon}^0_{13}\left(\xi\right))$$

$$X_2=-i(2C_{2121}\xi_1\bar{\varepsilon}^0_{12}\left(\xi\right)+C_{2211}\xi_2\bar{\varepsilon}^0_{11}\left(\xi\right)+C_{2222}\xi_2\bar{\varepsilon}^0_{22}\left(\xi\right)+C_{2233}\xi_2\bar{\varepsilon}^0_{33}\left(\xi\right)+2C_{2323}\xi_3\bar{\varepsilon}^0_{23}\left(\xi\right))$$

$$X_3=-i(2C_{3131}\xi_1\bar{\varepsilon}^0_{13}\left(\xi\right)+2C_{3232}\xi_2\bar{\varepsilon}^0_{23}\left(\xi\right)+C_{3311}\xi_3\bar{\varepsilon}^0_{11}\left(\xi\right)+C_{3322}\xi_3\bar{\varepsilon}^0_{22}\left(\xi\right)+C_{3333}\xi_3\bar{\varepsilon}^0_{33}\left(\xi\right))$$

# Solve the linear equation using Cholesky decomposition

(from wikipedia)

$$\mathbf{A} = \mathbf{L}\mathbf{L}^T = \begin{pmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{pmatrix} \begin{pmatrix} L_{11} & L_{21} & L_{31} \\ 0 & L_{22} & L_{32} \\ 0 & 0 & L_{33} \end{pmatrix}$$
$$= \begin{pmatrix} L_{11}^2 & & (\text{symmetric}) \\ L_{21}L_{11} & L_{21}^2 + L_{22}^2 & \\ L_{31}L_{11} & L_{31}L_{21} + L_{32}L_{22} & L_{31}^2 + L_{32}^2 + L_{33}^2 \end{pmatrix},$$

$$\mathbf{L} = \begin{pmatrix} \sqrt{A_{11}} & 0 & 0 \\ A_{21}/L_{11} & \sqrt{A_{22} - L_{21}^2} & 0 \\ A_{31}/L_{11} & (A_{32} - L_{31}L_{21})/L_{22} & \sqrt{A_{33} - L_{31}^2 - L_{32}^2} \end{pmatrix}$$

$$Ax = b \;\rightarrow\; Ly = b \;\&\; L^T x = y$$

**Step 1 :** $$Ly = b \;\rightarrow\; \begin{pmatrix} L_{11} & 0 & 0 \\ L_{21} & L_{22} & 0 \\ L_{31} & L_{32} & L_{33} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} L_{11}y_1 \\ L_{21}y_1 + L_{22}y_2 \\ L_{31}y_1 + L_{32}y_2 + L_{33}y_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

$$y_1 = b_1/L_{11}, \quad y_2 = (b_2 - L_{21}y_1)/L_{22}, \quad y_3 = (b_3 - L_{31}y_1 - L_{32}y_2)/L_{33}$$

**Step 2 :** $$L^T x = y \;\rightarrow\; \begin{pmatrix} L_{11} & L_{21} & L_{31} \\ 0 & L_{22} & L_{32} \\ 0 & 0 & L_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} L_{11}x_1 + L_{21}x_2 + L_{31}x_3 \\ L_{22}x_2 + L_{32}x_3 \\ L_{33}x_3 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

$$x_3 = y_3/L_{33}, \quad x_2 = (y_2 - L_{32}x_3)/L_{22}, \quad x_1 = (y_1 - L_{21}x_2 - L_{31}x_3)/L_{11}$$

For 2D $$\begin{bmatrix} c_{22} & c_{23} \\ c_{23} & c_{33} \end{bmatrix} \begin{bmatrix} \bar{\varepsilon}_2 \\ \bar{\varepsilon}_3 \end{bmatrix} = \begin{bmatrix} -c_{12} \\ -c_{13} \end{bmatrix} \bar{\varepsilon}_1$$

For 3D $$\begin{bmatrix} c_{33} & c_{34} & c_{35} \\ c_{34} & c_{44} & c_{45} \\ c_{35} & c_{45} & c_{55} \end{bmatrix} \begin{bmatrix} \bar{\varepsilon}_3 \\ \bar{\varepsilon}_4 \\ \bar{\varepsilon}_5 \end{bmatrix} = \begin{bmatrix} -c_{13} - c_{23} \\ -c_{14} - c_{24} \\ -c_{15} - c_{25} \end{bmatrix} \bar{\varepsilon}_1$$

Step 0 : Create arrays for $\varepsilon_{ij}^{0}$, $\bar{\varepsilon}_{ij}^{0}$ ,$u_i$, $\bar{u}_i$, $\varepsilon_{ij}$

Step 1 : Calculate the eigenstrain

$$\varepsilon_{11}^{0} = Q_{11}P_1^2 + Q_{12}P_2^2 + Q_{13}P_3^2 = Q_{11}P_1^2 + Q_{12}P_2^2 + Q_{12}P_3^2$$

$$\varepsilon_{22}^{0} = Q_{21}P_1^2 + Q_{22}P_2^2 + Q_{23}P_3^2 = Q_{12}P_1^2 + Q_{11}P_2^2 + Q_{12}P_3^2$$

$$\varepsilon_{33}^{0} = Q_{31}P_1^2 + Q_{32}P_2^2 + Q_{33}P_3^2 = Q_{12}P_1^2 + Q_{12}P_2^2 + Q_{11}P_3^2$$

$$\varepsilon_{23}^{0} = Q_{44}P_2P_3$$

$$\varepsilon_{13}^{0} = Q_{44}P_1P_3$$

$$\varepsilon_{12}^{0} = Q_{44}P_1P_2$$

Step 2 : Using direct Fourier transformation to the eigenstrain, finding $\bar{\varepsilon}_{ij}^{0}$

$$\mathscr{F}\left[\varepsilon_{ij}^{0}\right]$$

Step 3 : Calculate the value of K and X

$$K_{ik}(\xi) = C_{ijkl}\xi_l\xi_j$$

$$K_{11}(\xi) = C_{1111}\xi_1\xi_1 + C_{1212}\xi_2\xi_2 + C_{1313}\xi_3\xi_3 \qquad K_{12}(\xi) = 2C_{1122}\xi_1\xi_2 \qquad K_{13}(\xi) = 2C_{1133}\xi_1\xi_3$$

$$K_{21}(\xi) = 2C_{2211}\xi_1\xi_2 \qquad K_{22}(\xi) = C_{2121}\xi_1\xi_1 + C_{2222}\xi_2\xi_2 + C_{2323}\xi_3\xi_3 \qquad K_{23}(\xi) = 2C_{2233}\xi_2\xi_3$$

$$K_{31}(\xi) = 2C_{3311}\xi_1\xi_3 \qquad K_{32}(\xi) = 2C_{3322}\xi_2\xi_3 \qquad K_{33}(\xi) = C_{3131}\xi_1\xi_1 + C_{3232}\xi_2\xi_2 + C_{3333}\xi_3\xi_3$$

$$X_i = -\, iC_{ijkl}\varepsilon_{kl}^{0}\left(\xi\right)\xi_j$$

$$X_1 = -\, i(C_{1111}\xi_1\bar{\varepsilon}_{11}^{0}\left(\xi\right) + C_{1122}\xi_1\bar{\varepsilon}_{22}^{0}\left(\xi\right) + C_{1133}\xi_1\bar{\varepsilon}_{33}^{0}\left(\xi\right) + 2C_{1212}\xi_2\bar{\varepsilon}_{12}^{0}\left(\xi\right) + 2C_{1313}\zeta_3\bar{\varepsilon}_{13}^{0}\left(\xi\right))$$

$$X_2 = -\, i(2C_{2121}\xi_1\bar{\varepsilon}_{12}^{0}\left(\xi\right) + C_{2211}\xi_2\bar{\varepsilon}_{11}^{0}\left(\xi\right) + C_{2222}\xi_2\bar{\varepsilon}_{22}^{0}\left(\xi\right) + C_{2233}\xi_2\bar{\varepsilon}_{33}^{0}\left(\xi\right) + 2C_{2323}\xi_3\bar{\varepsilon}_{23}^{0}\left(\xi\right))$$

$$X_3 = -\, i(2C_{3131}\zeta_1\bar{\varepsilon}_{13}^{0}\left(\xi\right) + 2C_{3232}\zeta_2\bar{\varepsilon}_{23}^{0}\left(\xi\right) + C_{3311}\zeta_3\bar{\varepsilon}_{11}^{0}\left(\xi\right) + C_{3322}\zeta_3\bar{\varepsilon}_{22}^{0}\left(\xi\right) + C_{3333}\zeta_3\bar{\varepsilon}_{33}^{0}\left(\xi\right))$$

Step 4: Solve the linear equation using Cholesky decomposition

Derivative of elastic energy

$$\frac{\partial f_{\mathrm{elas}}}{\partial P_i} = C_{11}\left[(\eta_i - \eta_i^0)\left(-\frac{\partial \eta_i^0}{\partial P_i}\right) + \sum_j \left(\eta_j - \eta_j^0\right)\left(-\frac{\partial \eta_j^0}{\partial P_i}\right)\right] + C_{12}\left[\left(-\frac{\partial \eta_i^0}{\partial P_i}\right)\sum_j \left(\eta_j - \eta_j^0\right) + (\eta_i - \eta_i^0)\sum_j \left(-\frac{\partial \eta_j^0}{\partial P_i}\right) + \sum_{j,k} (\eta_k - \eta_k^0)\left(-\frac{\partial \eta_j^0}{\partial P_i}\right)\right]$$

$$+C_{44}\left[\sum_j \left(\eta_{ij} - \eta_{ij}^0\right)\left(-\frac{\partial \eta_{ij}^0}{\partial P_i}\right)\right]$$

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# Effect of substrate constraint on the stability and evolution of ferroelectric domain structures in thin films

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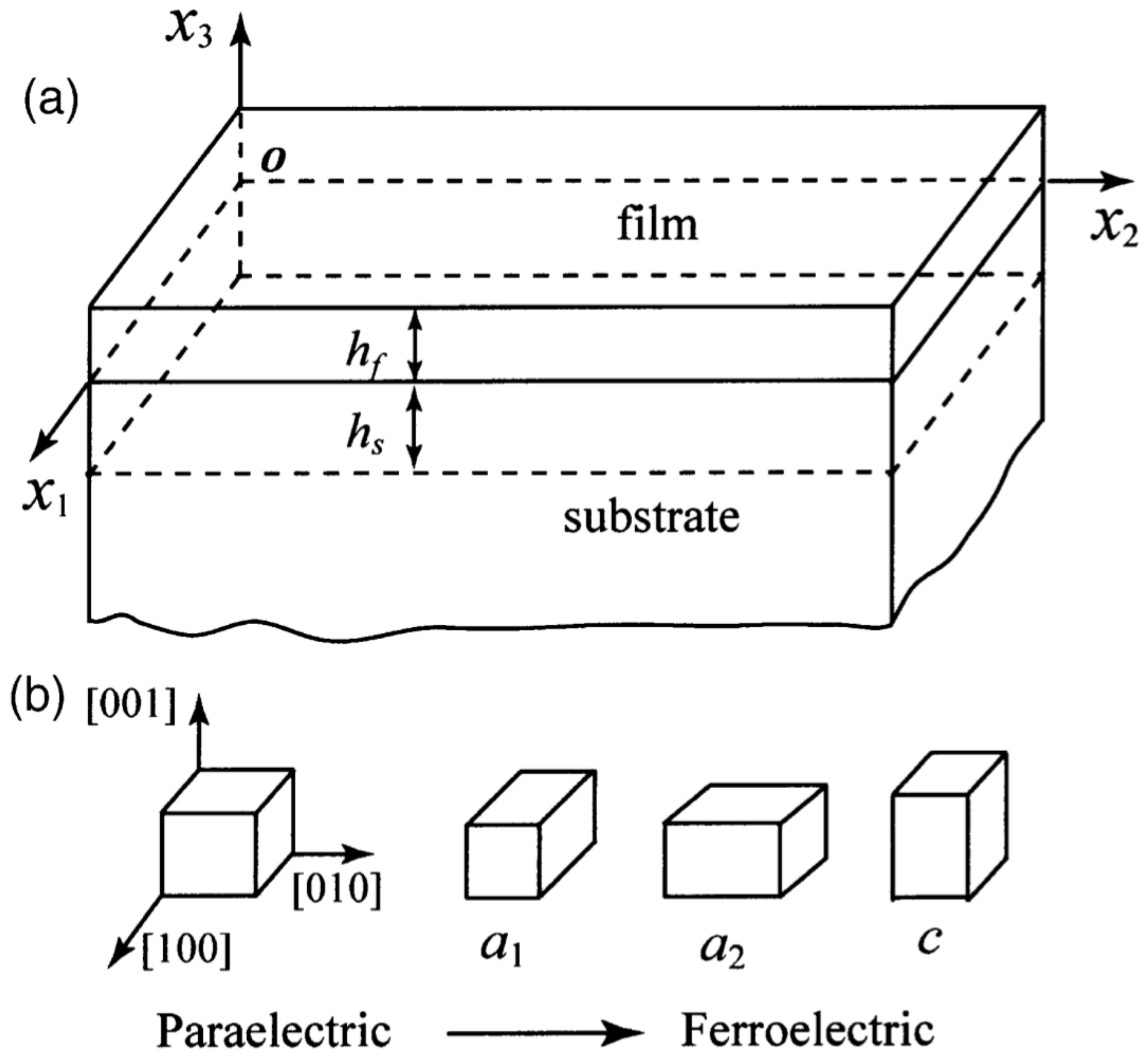


### 3. Elastic field in a constrained film

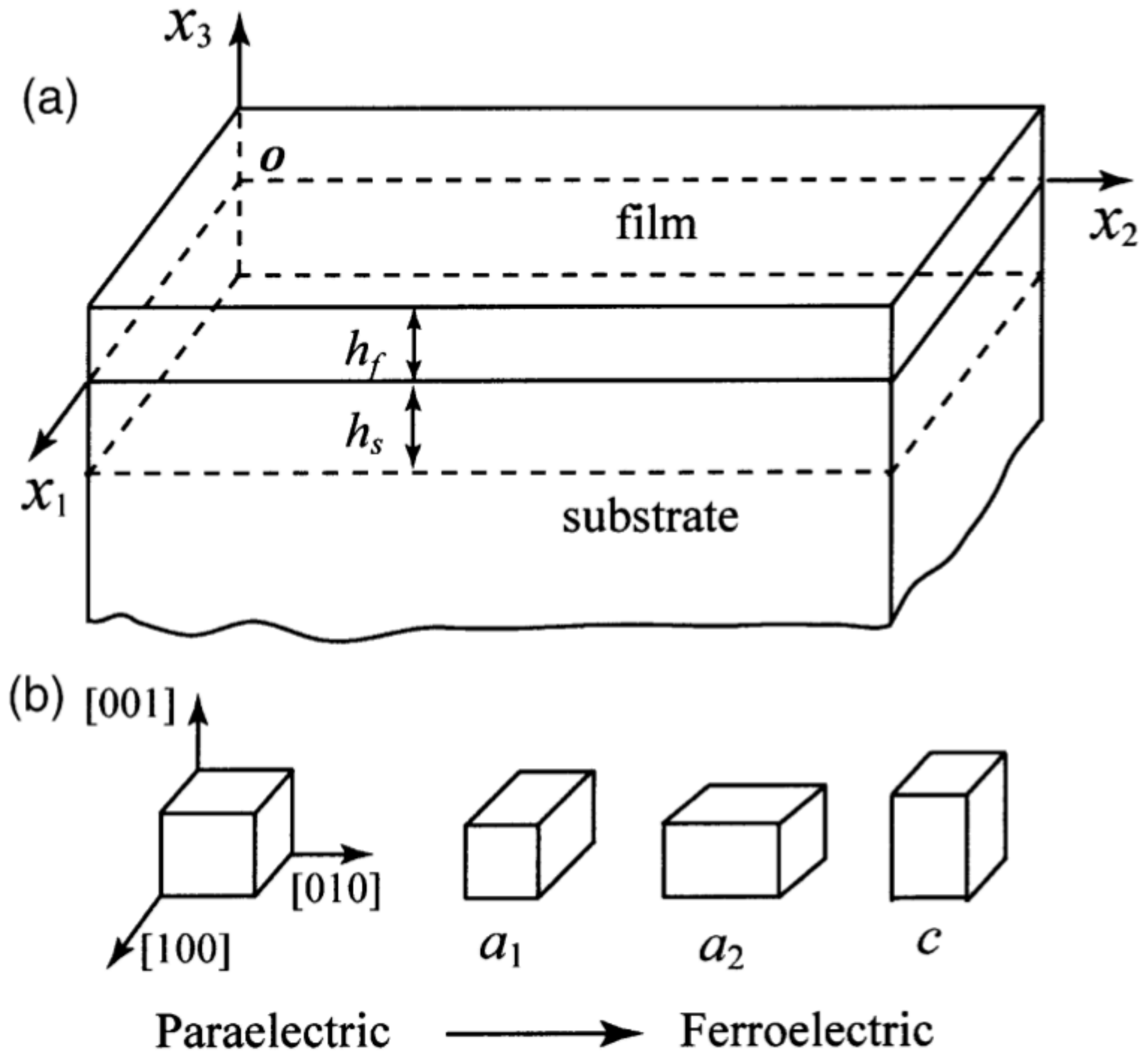



Fig. 2. Schematic illustrations of: (a) a thin film coherently constrained by a substrate, and (b) cubic paraelectric phase and the three ferroelectric tetragonal variants.

We consider a thin film with its top surface stress-free and bottom surface coherently constrained by the substrate.

Stress :

$$\sigma_{ij} = c_{ijkl}e_{kl} = c_{ijkl}(\varepsilon_{kl} - \varepsilon^o_{kl}) \quad \text{( Hooke's law )}$$

The mechanical equilibrium equations

$$\sigma_{ij,j} = 0$$

The stress-free boundary condition

$$\sigma_{i3}|_{x_3 = h_f} = 0$$

Total strain : $\varepsilon_{ij}(\mathbf{x}) = \bar{\varepsilon}_{ij} + \eta_{ij}(\mathbf{x})$

Stress : $\sigma_{ij}(\mathbf{x}) = \bar{\sigma}_{ij} + s_{ij}(\mathbf{x})$

Homogeneous part:

$$\bar{\sigma}_{ij}(\mathbf{x}) = c_{ijkl}\bar{\varepsilon}_{kl},$$

Heterogeneous part:

$$s_{ij}(\mathbf{x}) = c_{ijkl}[\eta_{kl}(\mathbf{x}) - \varepsilon^o_{kl}(\mathbf{x})]$$

$$\iiint_V \eta_{\alpha\beta}(\mathbf{x}) d^3x = 0$$

### Determine the homogeneous strains

$\bar{\varepsilon}_{11} = \bar{\varepsilon}_{22} = (a_s - a_f)/a_s, \bar{\varepsilon}_{12} = 0$ (misfit strains by the substrate)

The macroscopic shape deformation of the film along $x_3$

$$\sigma_{i3} = c_{i3kl}\bar{\varepsilon}_{kl} = 0$$

$$\sigma_{33} = c_{33kl}\bar{\varepsilon}_{kl} = c_{12}(\bar{\varepsilon}_{11} + \bar{\varepsilon}_{22}) + c_{11}\bar{\varepsilon}_{33} = 0 \rightarrow \bar{\varepsilon}_{33} = -\frac{2c_{12}}{c_{11}}\bar{\varepsilon}_{11}$$

$$\sigma_{13} = c_{13kl}\bar{\varepsilon}_{kl} = c_{44}\bar{\varepsilon}_{13} = 0 \rightarrow \bar{\varepsilon}_{13} = \bar{\varepsilon}_{23} = 0$$

### Determine the heterogeneous strains

Heterogeneous strain : $\eta_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ $\quad$ $u_i(\mathbf{x})$ : displacements

$$s_{ij}(\mathbf{x}) = c_{ijkl}[\eta_{kl}(\mathbf{x}) - \varepsilon^o_{kl}(\mathbf{x})] \xrightarrow[\sigma_{ij,j} = 0]{(i\text{ : force },\, j\text{ : surface})} \boxed{c_{ijkl}u_{k,lj} = c_{ijkl}\varepsilon^o_{ki,j}} \qquad (20)$$

The boundary conditions : $c_{i3kl}(u_{k,l} - \varepsilon^o_{kl})|_{x_3 = h_f} = 0. \qquad u_i|_{x_3 = -h_s} = 0$

**Step 1 (superscript A) : to solve Eq. (20) in a 3D space with eigenstrain distribution $\varepsilon^0_{ij}$ within $0 < x_3 < h_f$**

$$u_i^A(\mathbf{x}) = \iiint \hat{u}_i^A(\zeta) e^{I\mathbf{x}\cdot\zeta} d^3\zeta, \qquad \hat{\varepsilon}^o_{ij}(\zeta) = \frac{1}{(2\pi)^3}\iiint \varepsilon^o_{ij}(\mathbf{x}) e^{-I\mathbf{x}\cdot\zeta} d^3x, \longrightarrow \hat{u}_i^A = -Ig_{ij}c_{jmkl}\hat{\varepsilon}^o_{kl}\zeta_m \qquad (20)$$

**Step 2 (superscript B) : to find elastic solution in an infinite plate of thickness $h_f + h_s$, satisfying the equation of equilibrium with our body-force.**

$$\boxed{c_{ijkl}u^B_{k,lj} = 0,}$$ with boundary conditions : $$c_{i3kl}u^B_{k,l}|_{x_3=h_f} = -c_{i3kl}(u^A_{k,l}-\varepsilon^o_{kl})|_{x_3=h_f},\quad u^B_i|_{x_3=-h_s} = -u^A_i|_{x_3=-h_s}.$$

$$\hat{u}^B_i(\zeta_1,\zeta_2,x_3) = \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} u^B_i(x_1,x_2,x_3)e^{-I(\zeta_1x_1+\zeta_2x_2)}dx_1\,dx_2$$

$$c_{i\alpha k\beta}(I\zeta_\alpha)(I\zeta_\beta)\hat{u}^B_k + (c_{i\alpha k3} + c_{i3k\alpha})(I\zeta_\alpha)\hat{u}^B_{k,3} + c_{i3k3}\hat{u}^B_{k,33} = 0, \qquad (28)$$

$$k=1:-\left[c_{11}\zeta_1^2+c_{44}\zeta_2^2+(c_{44}+c_{12})\zeta_1\zeta_2\right]\hat{u}^B_1 + i(c_{44}+c_{12})\zeta_1\hat{u}^B_{1,3}+c_{44}\hat{u}^B_{1,33}=0$$

**For 2D :** $-c_{11}\zeta_1^2\hat{u}^B_1 + i(c_{44}+c_{12})\zeta_1\hat{u}^B_{1,2}+c_{44}\hat{u}^B_{1,22}=0$

$$\hat{\mathbf{u}}^B(\zeta_1,\zeta_2,x_3) = \mathbf{a}e^{Ip\zeta x_3} \qquad \zeta = \sqrt{\zeta_1^2+\zeta_2^2},$$

$$\left[c_{i\alpha k\beta}\zeta_\alpha\zeta_\beta + p(c_{i\alpha k3}+c_{i3k\alpha})\zeta_\alpha\zeta + c_{i3k3}p^2\zeta^2\right]a_k = 0$$

$$\left[c_{11}\zeta_1^2+c_{44}\zeta_2^2+(c_{44}+c_{12})\zeta_1\zeta_2+p(c_{44}+c_{12})\zeta_1\zeta+p^2c_{44}\zeta^2\right]a_1=0$$

**For 2D :** $\left[c_{11}\zeta_1^2+p(c_{44}+c_{12})\zeta_1\zeta+p^2c_{44}\zeta^2\right]a_1=0$

$\rightarrow \left[c_{11}+p(c_{44}+c_{12})+p^2c_{44}\right]a_1=0 \quad (\zeta=\zeta_1)$

$\left[c_{44}+p(c_{44}+c_{12})+p^2c_{11}\right]a_2=0$

$$n_1 = \zeta_1/\zeta,\quad n_2 = \zeta_2/\zeta$$

$$\left[c_{i\alpha k\beta}n_\alpha n_\beta + p(c_{i\alpha k3}+c_{i3k\alpha})n_\alpha + c_{i3k3}p^2\right]a_k = 0$$

$$W_{ik} = c_{ijkl}n_jn_l,\quad R_{ik} = c_{ijkl}n_jm_l,\quad U_{ik} = c_{ijkl}m_jm_l$$

$$\mathbf{m} = (0,0,1)^T,\quad \mathbf{n} = (n_1,n_2,0)^T$$

$$\{W + p(R+R^T) + p^2U\}\mathbf{a} = \mathbf{0}, \longrightarrow N\boldsymbol{\xi} = p\boldsymbol{\xi}, N = \begin{pmatrix} N_1 & N_2 \\ N_3 & N_1^T \end{pmatrix}, \boldsymbol{\xi} = \begin{pmatrix}\mathbf{a}\\ \mathbf{b}\end{pmatrix}$$

$$W_{ik} = c_{ijkl}n_jn_l,\quad R_{ik} = c_{ijkl}n_jm_l,\quad U_{ik} = c_{ijkl}m_jm_l \qquad \{W + p(R + R^T) + p^2U\}\mathbf{a} = \mathbf{0}, \qquad (30)$$

$$\mathbf{m} = (0,0,1)^T,\quad \mathbf{n} = (n_1,n_2,0)^T$$

$$W_{ik} = C_{ijkl}n_jn_l = \begin{bmatrix} C_{1111}n_1n_1 + C_{1212}n_2n_2 & C_{1122}n_1n_2 + C_{1221}n_2n_1 & 0 \\ C_{2112}n_1n_2 + C_{2211}n_2n_1 & C_{2222}n_2n_2 + C_{2121}n_1n_1 & 0 \\ 0 & 0 & C_{3131}n_1n_1 + C_{3232}n_2n_2 \end{bmatrix}$$

$$R_{ik} = C_{ijkl}n_jm_l = \begin{bmatrix} 0 & 0 & C_{1133}n_1 \\ 0 & 0 & C_{2233}n_2 \\ C_{3113}n_1 & C_{3223}n_2 & 0 \end{bmatrix}$$

$$R_{ik}^T = \begin{bmatrix} 0 & 0 & C_{1331}n_1 \\ 0 & 0 & C_{2332}n_2 \\ C_{3311}n_1 & C_{3322}n_2 & 0 \end{bmatrix}$$

$$U_{ik} = C_{ijkl}m_jm_l = \begin{bmatrix} C_{1313} & 0 & 0 \\ 0 & C_{2323} & 0 \\ 0 & 0 & C_{3333} \end{bmatrix}$$

| | |
|---|---|
| $C_{i\alpha k\beta}$ | $C_{1111}, C_{2222}, C_{1122}, C_{2211}, C_{1212}, C_{2112}, C_{1221}, C_{2121}, C_{3232}, C_{3131}$ |
| $C_{i\alpha k3}$ | $C_{2233}, C_{1133}, C_{3223}, C_{3113}$ |
| $C_{i3k\alpha}$ | $C_{3322}, C_{3311}, C_{2332}, C_{1331}$ |
| $C_{i3k3}$ | $C_{1313}, C_{2323}, C_{3333}$ |
| **Voigt notation** | |
| $C_{11}$ | $C_{1111} = C_{2222} = C_{3333}$ |
| $C_{12}$ | $C_{2233}=C_{3322}$ |
| | $C_{1133}=C_{3311}$ |
| | $C_{1122}=C_{2211}$ |
| $C_{44}$ | $C_{2323}=C_{3223}=C_{2332}=C_{3232}$ |
| | $C_{1313}=C_{3113}=C_{1331}=C_{3131}$ |
| | $C_{1212}=C_{2112}=C_{1221}=C_{2121}$ |

$$\begin{bmatrix} C_{1111}n_1^2 + C_{1212}n_2^2 + p^2C_{1313} & C_{1122}n_1n_2 + C_{1221}n_1n_2 & p(C_{1133} + C_{3113})n_1 \\ C_{2112}n_1n_2 + C_{2211}n_1n_2 & C_{2222}n_2^2 + C_{2121}n_1^2 + p^2C_{2323} & p(C_{2233} + C_{3223})n_2 \\ p(C_{3113} + C_{1133})n_1 & p(C_{3223} + C_{2233})n_2 & p^2C_{3333} \end{bmatrix} a = 0 \qquad (30)$$

$$N_1 = -U^{-1}R^T$$

$$U^{-1} = \begin{bmatrix} \frac{1}{C_{1313}} & 0 & 0 \\ 0 & \frac{1}{C_{2323}} & 0 \\ 0 & 0 & \frac{1}{C_{3333}} \end{bmatrix} \quad R_{ik}^T = \begin{bmatrix} 0 & 0 & C_{3113}n_1 \\ 0 & 0 & C_{3223}n_2 \\ C_{1133}n_1 & C_{2233}n_2 & 0 \end{bmatrix}$$

$$N_1 = \begin{bmatrix} 0 & 0 & -n_1 \\ 0 & 0 & -n_2 \\ -\frac{C_{1133}n_1}{C_{3333}} & -\frac{C_{2233}n_2}{C_{3333}} & 0 \end{bmatrix}$$

$$R_{ik} = C_{ijkl}n_j m_l = \begin{bmatrix} 0 & 0 & C_{1133}n_1 \\ 0 & 0 & C_{2233}n_2 \\ C_{3113}n_1 & C_{3223}n_2 & 0 \end{bmatrix}$$

$$N_2 = U^{-1} \qquad N_2 = \begin{bmatrix} \frac{1}{C_{1313}} & 0 & 0 \\ 0 & \frac{1}{C_{2323}} & 0 \\ 0 & 0 & \frac{1}{C_{3333}} \end{bmatrix}$$

$$N_3 = RU^{-1}R^T - W$$

$$RU^{-1} = \begin{bmatrix} 0 & 0 & \frac{c_{1133}n_1}{C_{3333}} \\ 0 & 0 & \frac{c_{2233}n_2}{C_{3333}} \\ n_1 & n_2 & 0 \end{bmatrix} \quad RU^{-1}R^T = \begin{bmatrix} \frac{C_{1133}^2 n_1^2}{C_{3333}} & \frac{C_{1133}C_{2233}n_1n_2}{C_{3333}} & 0 \\ \frac{C_{1133}C_{2233}n_1n_2}{C_{3333}} & \frac{C_{2233}^2 n_2^2}{C_{3333}} & 0 \\ 0 & 0 & C_{3113}n_1^2 + C_{3223}n_2^2 \end{bmatrix}$$

$$N_3 = \begin{bmatrix} \frac{C_{1133}^2 n_1^2 - C_{1111}C_{3333}n_1^2 - C_{1212}C_{3333}n_2^2}{C_{3333}} & \frac{(C_{1133}C_{2233} - C_{1122}C_{3333} - C_{1221}C_{3333})n_1n_2}{C_{3333}} & 0 \\ \frac{(C_{1133}C_{2233} - C_{2112}C_{3333} - C_{2211}C_{3333})n_1n_2}{C_{3333}} & \frac{C_{2233}^2 n_2^2 - C_{2222}C_{3333}n_2^2 - C_{2121}C_{3333}n_1^2}{C_{3333}} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\hat{s}^b = I\zeta b e^{Ip\zeta x_3} = \sum_{t=1}^{6} q_t I\zeta b e^{Ip\zeta x_3} = \sum_{t=1,2,4,5} q_t I\zeta b e^{Ip\zeta x_3} + q_3' \left[ I\zeta b_3' e^{Ip_3\zeta x_3} - \zeta^2 x_3 b_2 e^{Ip_3\zeta x_3} \right] + q_6' \left[ I\zeta b_6' e^{Ip_6\zeta x_3} - \zeta^2 x_3 b_5 e^{Ip_6\zeta x_3} \right]$$

$$p_1 = p_2 = p_3 = \overset{-I}{\cancel{I}}, p_4 = p_5 = p_6 = \qquad (35)$$

$$I \; -\cancel{I},$$

$$\xi_1 = \left( -\frac{In_2}{\mu n_1}, \frac{I}{\mu}, 0, -\frac{n_2}{n_1}, 1, 0 \right)^T, \qquad \xi_4 = \bar{\xi}_1,$$

$$\xi_2 = \left( -\frac{In_1}{4\mu v}, -\frac{In_2}{4\mu v}, -\frac{1}{4\mu v}, -\frac{n_1}{2v}, -\frac{n_2}{2v}, \frac{I}{2v} \right)^T, \qquad \xi_5 = \bar{\xi}_2,$$

$$\xi_3' = \left( \frac{1-2v}{2\mu v n_1}, 0, \frac{I}{4\mu v}, -\frac{I(1-2v)}{2v n_1}, 0, 1 \right)^T, \qquad \xi_6' = \bar{\xi}_3'.$$

$$\hat{s}_1^b = [-I\zeta \frac{n_2}{n_1} q_1 - I\zeta \frac{n_1}{2v} q_2 + (\zeta \frac{1-2v}{2v n_1} + \zeta^2 x_3 \frac{n_1}{2v}) q_3'] e^{\zeta x_3} + [-I\zeta \frac{n_2}{n_1} q_4 - I\zeta \frac{n_1}{2v} q_5 + (-\zeta \frac{1-2v}{2v n_1} + \zeta^2 x_3 \frac{n_1}{2v}) q_6'] e^{-\zeta x_3}$$

$$\hat{s}_2^b = [I\zeta q_1 + I\zeta \frac{-n_2}{2v} q_2 + \zeta^2 x_3 \frac{n_2}{2v} q_3'] e^{\zeta x_3} + [I\zeta q_4 - I\zeta \frac{n_2}{2v} q_5 + \zeta^2 x_3 \frac{n_2}{2v} q_6'] e^{-\zeta x_3}$$

$$\hat{s}_3^b = [-\zeta \frac{1}{2v} q_2 + (I\zeta - I\zeta^2 x_3 \frac{1}{2v}) q_3'] e^{\zeta x_3} + [\zeta \frac{1}{2v} q_5 + (I\zeta + I\zeta^2 x_3 \frac{1}{2v}) q_6'] e^{-\zeta x_3}$$

$$\hat{u}_1{}^B(\zeta_1, \zeta_2, x_3) = \left[\left(\frac{1-2\nu}{2\mu\nu n_1} + \frac{n_1\zeta x_3}{4\mu\nu}\right) q_3' - i\left(\frac{n_2}{\mu n_1} q_1 + \frac{n_1}{4\mu\nu} q_2\right)\right] e^{\zeta x_3} + \left[\left(\frac{1-2\nu}{2\mu\nu n_1} - \frac{n_1\zeta x_3}{4\mu\nu}\right) q_6' + i\left(\frac{n_2}{\mu n_1} q_4 + \frac{n_1}{4\mu\nu} q_5\right)\right] e^{-\zeta x_3}$$

$$\hat{u}_2{}^B(\zeta_1, \zeta_2, x_3) = \left[\frac{n_2\zeta x_3}{4\mu\nu} q_3' + i\left(\frac{1}{\mu} q_1 - \frac{n_2}{4\mu\nu} q_2\right)\right] e^{\zeta x_3} + \left[-\frac{n_2\zeta x_3}{4\mu\nu} q_6' - i\left(\frac{1}{\mu} q_4 - \frac{n_2}{4\mu\nu} q_5\right)\right] e^{-\zeta x_3}$$

$$\hat{u}_3{}^B(\zeta_1, \zeta_2, x_3) = \left[-\frac{1}{4\mu\nu} q_2 + i\frac{1-\zeta x_3}{4\mu\nu} q_3'\right] e^{\zeta x_3} + \left[-\frac{1}{4\mu\nu} q_5 - i\frac{1+\zeta x_3}{4\mu\nu} q_6'\right] e^{-\zeta x_3}$$

# Electrostatic energy density

For an electrically inhomogeneous system the long-range electric dipole–dipole interaction energy density is given by

$$f_{elec} = -\frac{1}{2}\sum_i \mathbf{E}_i \cdot \mathbf{P}_i$$

where $E_i$ denotes the inhomogeneous electric field due to dipole–dipole interactions.

## CHARGE-CHARGE (C-C) INTERACTION

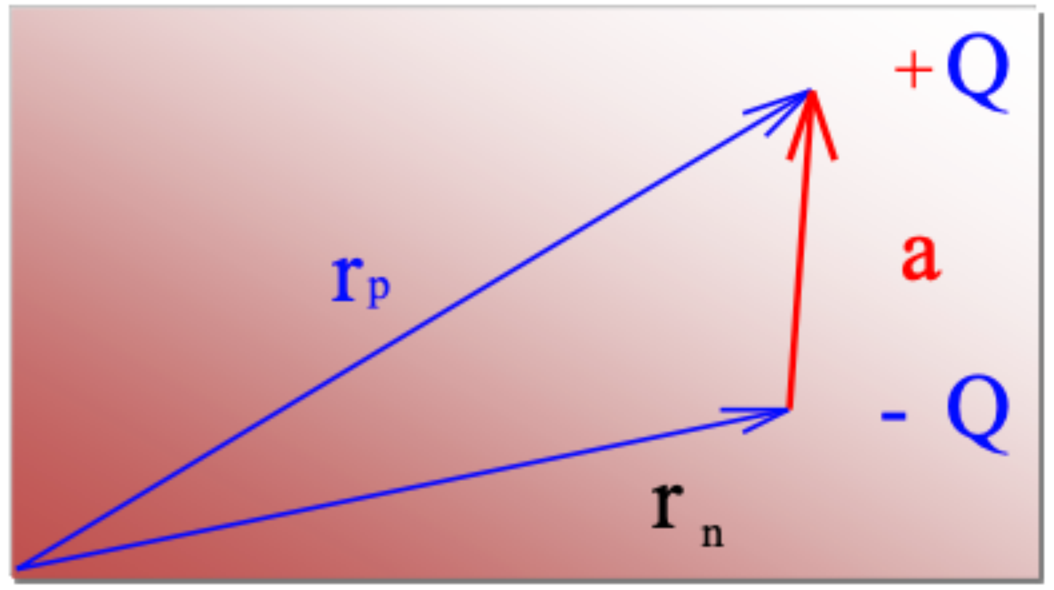
The coulomb potential $\phi_C$ from the point charge $Q_i$ at $\mathbf{r_i}$ is given by

$$\phi_C\left(|\mathbf{r}-\mathbf{r_i}|\right) = \frac{Q_i}{4\pi\varepsilon_0}\frac{1}{|\mathbf{r}-\mathbf{r_i}|}$$

If we put the other point charge $Q_j$ at at $\mathbf{r_j}$ the electrostatic energy Vcc is

$$V_{cc} = Q_j\phi_C\left(|\mathbf{r_j}-\mathbf{r_i}|\right) = \frac{Q_iQ_j}{4\pi\varepsilon_0}\frac{1}{|\mathbf{r_j}-\mathbf{r_i}|}$$

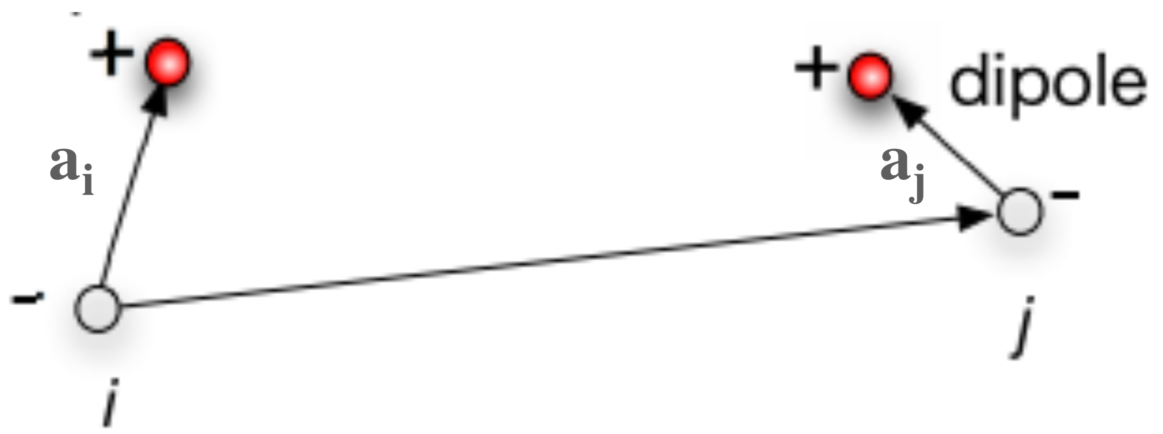
# DIPOLE-DIPOLE (C-C) INTERACTION




Electric dipole moment of the system is electric moment of a system of charges with zero net charge

$$\mu = (\mathbf{r}_\mathbf{p} - \mathbf{r}_\mathbf{n})Q = \mathbf{a}Q$$

The difference $\mathbf{r}_\mathbf{p} - \mathbf{r}_\mathbf{n}$ is equal to the vector distance between the centers of gravity, represented by a vector $\mathbf{a}$, pointing from the negative to the positive center




$$+\frac{1}{\left(1-2\mathbf{r_{ji}}\cdot\mathbf{a_i}/r_{ji}^2+\mathbf{r_{ji}}\cdot\mathbf{a_j}/r_{ji}^2+\mathbf{a_i^2}/r_{ji}^2+\mathbf{a_j^2}/r_{ji}^2-2\mathbf{a_i^2}\cdot\mathbf{a_j^2}/r_{ji}^2\right)^{\frac{1}{2}}}$$

$$-1+\frac{1}{2}\frac{-2\mathbf{r_{ji}}\cdot\mathbf{a_i}}{r_{ji}^2}+\frac{1}{2}\frac{\mathbf{a_i^2}}{r_{ji}^2}-\frac{3}{8}\left(-2\mathbf{r_{ji}}\cdot\mathbf{a_i}/r_{ji}^2+\mathbf{a_i^2}/r_{ji}^2\right)^2$$

Electrostatic energy Vdd of dipole-dipole (D-D) interaction can be obtain as

$$V_{dd}=\frac{(-Q_i)\left(-Q_j\right)}{4\pi\varepsilon_0}\frac{1}{|\mathbf{r}_j-\mathbf{r}_i|}+\frac{(-Q_i)\,Q_j}{4\pi\varepsilon_0}\frac{1}{|\mathbf{r}_j+\mathbf{a}_j-\mathbf{r}_i|}+\frac{Q_i\left(-Q_j\right)}{4\pi\varepsilon_0}\frac{1}{|\mathbf{r}_j-\mathbf{r}_i-\mathbf{a}_i|}+\frac{Q_iQ_j}{4\pi\varepsilon_0}\frac{1}{|\mathbf{r}_j+\mathbf{a}_j-\mathbf{r}_i-\mathbf{a}_i|}$$

$$=\frac{Q_iQ_j}{4\pi\varepsilon_0}\left(\frac{1}{r_{ji}}-\frac{1}{\sqrt{r_{ji}^2+2\mathbf{r}_{ji}\cdot\mathbf{a}_j+\mathbf{a}_j^2}}-\frac{1}{\sqrt{r_{ji}^2-2\mathbf{r}_{ji}\cdot\mathbf{a}_i+\mathbf{a}_i^2}}+\frac{1}{\sqrt{r_{ji}^2-2\mathbf{r_{ji}}\cdot\mathbf{a}_i+2\mathbf{r}_{ji}\cdot\mathbf{a}_j+\mathbf{a}_i^2+\mathbf{a}_j^2-2\mathbf{a}_i\cdot\mathbf{a}_j}}\right)$$

$$=\frac{Q_iQ_j}{4\pi\varepsilon_0 r_{ji}}\left[1-\frac{1}{\left(1+2\mathbf{r}_{ji}\cdot\mathbf{a}_j/r_{ji}^2+\mathbf{a}_j^2/r_{ji}^2\right)^{1/2}}-\frac{1}{\left(1-2\mathbf{r}_{ji}\cdot\mathbf{a}_i/r_{ji}^2+\mathbf{a}_i^2/r_{ji}^2\right)^{1/2}}+\frac{1}{\left(1-2\mathbf{r}_{ji}\cdot\mathbf{a}_i/r_{ji}^2+2\mathbf{r_{ji}}\cdot\mathbf{a}_j/r_{ji}^2+\mathbf{a}_i^2/r_{ji}^2+\mathbf{a}_j^2/r_{ji}^2-2\mathbf{a}_i\cdot\mathbf{a}_j/r_{ji}^2\right)^{1/2}}\right]$$

Binomial approximation $(1+x)^{-1/2}\simeq 1-x/2+3x^2/8\ldots$

$$V_{dd}=\frac{Q_iQ_j}{4\pi\varepsilon_0 r_{ji}}\left[1-1+\frac{1}{2}\frac{2\mathbf{r}_{ji}\cdot\mathbf{a}_j}{r_{ji}^2}+\frac{1}{2}\frac{\mathbf{a}_j^2}{r_{ji}^2}-\frac{3}{8}\left(2\mathbf{r}_{ji}\cdot\mathbf{a}_j/r_{ji}^2+\mathbf{a}_j^2/r_{ji}^2\right)^2-1+\frac{1}{2}\frac{-2\mathbf{r}_{ji}\cdot\mathbf{a}_i}{r_{ji}^2}+\frac{1}{2}\frac{\mathbf{a}_i^2}{r_{ji}^2}-\frac{3}{8}\left(-2\mathbf{r}_{ji}\cdot\mathbf{a}_i/r_{ji}^2+\mathbf{a}_i^2/r_{ji}^2\right)^2\right.$$

$$\left.+1+\frac{1}{2}\frac{2\mathbf{r}_{ji}\cdot\mathbf{a}_i}{r_{ji}^2}-\frac{1}{2}\frac{2\mathbf{r}_{ji}\cdot\mathbf{a}_j}{r_{ji}^2}-\frac{1}{2}\frac{\mathbf{a}_i^2}{r_{ji}^2}-\frac{1}{2}\frac{\mathbf{a}_j^2}{r_{ji}^2}+\underbrace{\frac{1}{2}\frac{2\mathbf{a}_i\cdot\mathbf{a}_j}{r_{ji}^2}}_{\text{Survive}}+\frac{3}{8}\left(\underbrace{\frac{-2\mathbf{r}_{ji}\cdot\mathbf{a}_i}{r_{ji}^2}+\frac{2\mathbf{r}_{ji}\cdot\mathbf{a}_j}{r_{ji}^2}}_{\text{Cross term survive}}+\frac{\mathbf{a}_i^2}{r_{ji}^2}+\frac{\mathbf{a}_j^2}{r_{ji}^2}-\frac{2\mathbf{a}_i\cdot\mathbf{a}_j}{r_{ji}^2}\right)^2\right]$$

we assume $r_{ij}>>a_i$

$$V_{dd} = \frac{Q_i Q_j}{4\pi\varepsilon_0 r_{ji}} \left[ \frac{\mathbf{a}_i \cdot \mathbf{a}_j}{r_{ji}^2} - 3\frac{\left(\mathbf{r}_{ji} \cdot \mathbf{a}_i\right)\left(\mathbf{r}_{ji} \cdot \mathbf{a}_j\right)}{r_{ji}^4} \right]$$

Substitute $\mu = \mathbf{a}Q$

$$V_{dd} = \frac{1}{4\pi\varepsilon_0} \left[ \frac{\mu_i \cdot \mu_j}{r_{ij}^3} - 3\frac{\left(\mu_i \cdot \mathbf{r}_{ij}\right)\left(\mathbf{r}_{ij} \cdot \mu_j\right)}{r_{ij}^5} \right]$$

Electrostatic energy for n dipoles

$$V_{dd} = \frac{1}{2} \sum_{i,j} \frac{1}{4\pi\varepsilon_0} \left[ \frac{\mu_i \cdot \mu_j}{r_{ij}^3} - 3\frac{\left(\mu_i \cdot \mathbf{r}_{ij}\right)\left(\mathbf{r}_{ij} \cdot \mu_j\right)}{r_{ij}^5} \right]$$

Electrostatic energy density, $f_{\text{elec}}$ with $\mathbf{P}_i \equiv \frac{\mu_i}{V}$

$$f_{\text{elec}} = \frac{V_{dd}}{V} = \frac{V}{2} \sum_{i,j} \frac{1}{4\pi\varepsilon_0} \left[ \frac{\mathbf{P_i} \cdot \mathbf{P_j}}{r_{ij}^3} - 3\frac{\left(\mathbf{P_i} \cdot \mathbf{r_{ij}}\right)\left(\mathbf{r_{ij}} \cdot \mathbf{P_j}\right)}{r_{ij}^5} \right] = -\frac{1}{2} \sum_i \mathbf{E}_i \cdot \mathbf{P}_i$$

$$\mathbf{E}_i = -\sum_j \frac{V}{4\pi\varepsilon_0} \left[ \frac{\mathbf{P_j}}{r_{ij}^3} - 3\frac{\mathbf{r_{ij}}\left(\mathbf{r_{ij}} \cdot \mathbf{P_j}\right)}{r_{ij}^5} \right]$$

It can be obtained by solving the electrostatic equilibrium (Gauss' law) equation given by $\nabla \cdot \overrightarrow{D} = 0$ where $\overrightarrow{D}$ is the electrical displacement represented by

$$\nabla \cdot \overrightarrow{D} = \nabla \cdot \left(\varepsilon_0 \kappa \overrightarrow{E} + \overrightarrow{P}\right) = \rho_f$$

where $\rho_f$ is the density of free electrons. The electric field $\overrightarrow{E}$ is related to the electric potential through $-\nabla\phi = \overrightarrow{E}$. Hence, by assuming $\kappa_{ij} = 0$ for $i \neq j$

For $\rho_f = 0$

$$\nabla \cdot \left(\varepsilon_0 \kappa \overrightarrow{E} + \overrightarrow{P}\right) = 0$$

$$-\nabla \cdot \left(\kappa \overrightarrow{E}\right) = \frac{1}{\varepsilon_0}\overrightarrow{P}$$

$$-\nabla \cdot \left(\kappa_{11}E_1 + \kappa_{22}E_2 + \kappa_{33}E_3\right) = \frac{1}{\varepsilon_0}\overrightarrow{P}$$

$$\kappa_{11}\phi_{,11} + \kappa_{22}\phi_{,22} + \kappa_{33}\phi_{,33} = \frac{1}{\varepsilon_0}\left(P_{1,1} + P_{2,2} + P_{3,3}\right)$$

By transforming into Fourier space, we obtain

$$-\kappa_{11}\xi_1^2\bar{\phi}(\xi) - \kappa_{22}\xi_2^2\bar{\phi}(\xi) - \kappa_{33}\xi_3^2\bar{\phi}(\xi) = \frac{1}{\varepsilon_0}\left(i\xi_1\bar{P}_1(\xi) + i\xi_2\bar{P}_2(\xi) + i\xi_3\bar{P}_3(\xi)\right)$$

$$\bar{\phi}\left(\xi\right) = -\frac{i}{\varepsilon_0}\frac{\xi_1\bar{P}_1\left(\xi\right) + \xi_2\bar{P}_2\left(\xi\right) + \xi_3\bar{P}_3\left(\xi\right)}{\kappa_{11}\xi_1^2 + \kappa_{22}\xi_2^2 + \kappa_{33}\xi_3^2}$$

# TDGL Equation

For a proper ferroelectric phase transition, the polarization vector **P**=($P_1$, $P_2$, $P_3$) is the primary order parameter, and its spatial distribution in the ferroelectric state describes a domain structure.

The temporal evolution of the polarization field, and thus the domain structure evolution, is described by the Time Dependent Ginzburg–Landau (TDGL) equations

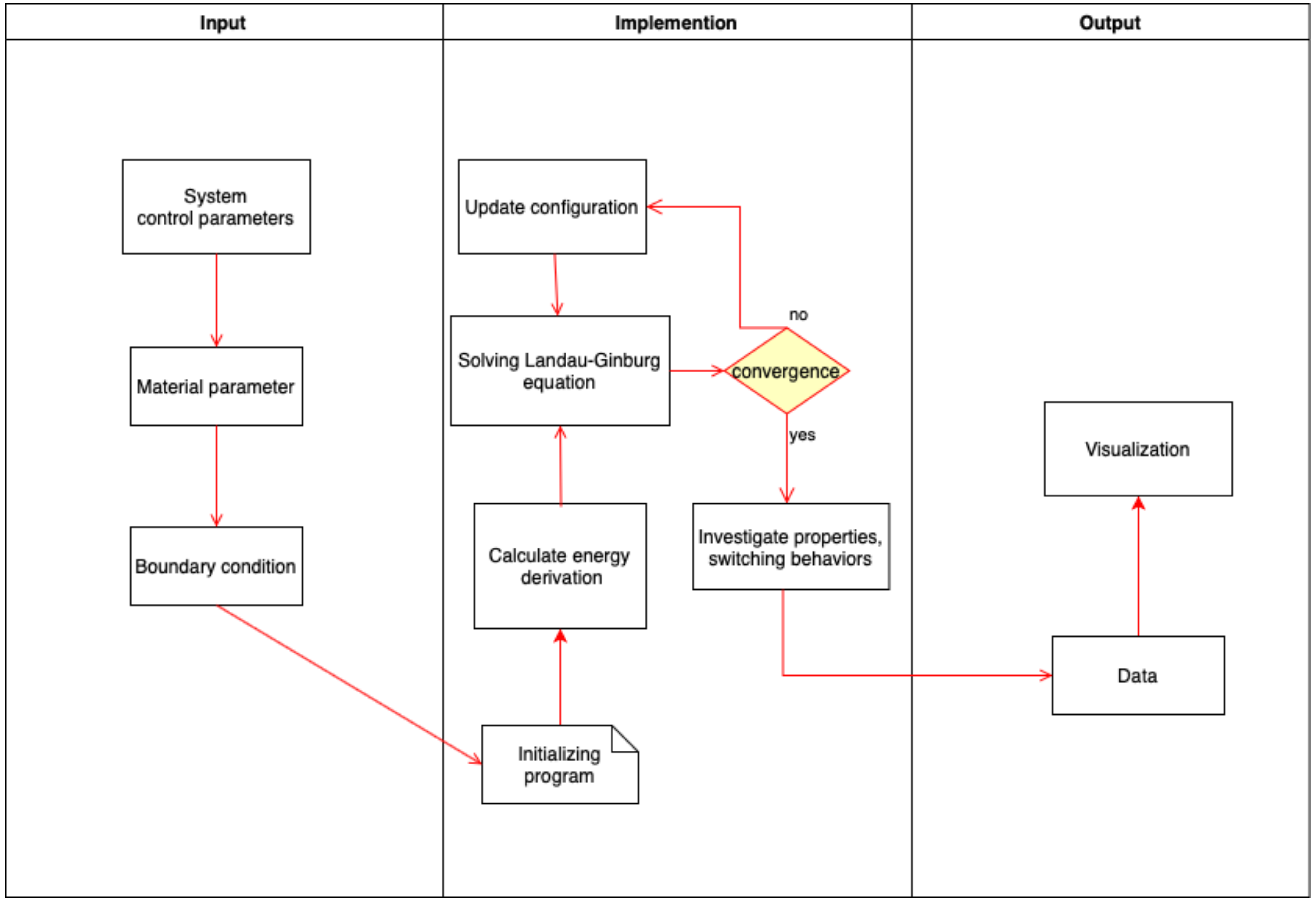
$$\frac{\partial P_i(\mathbf{x},t)}{\partial t} = -L\frac{\delta F}{\delta P_i(\mathbf{x},t)}, \quad (i = 1,2,3)$$

The total free energy of the system includes the bulk free energy, the domain wall energy, the elastic energy,

# Phase-field Program

The Phase-field program is implemented by C language with the support from Intel MKL Library

We use Python scripts for analyzing data and visualization



# Phase-field Program

| | $BaTiO_3$ | | | $PbTiO_3$ | | |
|---|---|---|---|---|---|---|
| | unit | | reduced | unit | | reduced |
| $\alpha_1$ | -2.772E+07 | $JmC^{-2}$ | -1.0000E+00 | -1.725E+08 | $JmC^{-2}$ | -1.0000E+00 |
| $\alpha_{11}$ | 1.701E+08 | $Jm^5C^{-4}$ | 4.1482E-01 | -7.3E+07 | $Jm^5C^{-4}$ | -2.4251E-01 |
| $\alpha_{12}$ | -3.441E+08 | $Jm^5C^{-2}$ | -8.3915E-01 | 7.5E+08 | $Jm^5C^{-2}$ | 2.4915E+00 |
| $\alpha_{111}$ | 8.004E+09 | $Jm^9C^{-2}$ | 1.3195E+00 | 2.6E+08 | $Jm^9C^{-2}$ | 4.9496E-01 |
| $\alpha_{112}$ | 4.47E+09 | $Jm^9C^{-2}$ | 7.3690E-01 | 6.1E+08 | $Jm^9C^{-2}$ | 1.1612E+00 |
| $\alpha_{123}$ | 4.91E+09 | $Jm^9C^{-2}$ | 8.0943E-01 | -3.7E+09 | $Jm^9C^{-2}$ | -7.0436E+00 |
| $G_{11}$ | 5.1E-10 | $Jm^3C^{-2}$ | 1E+00 | 1.73E-10 | $Jm^3C^{-2}$ | 1E+00 |
| $G_{14}$ | 0E+00 | $Jm^3C^{-2}$ | 0E+00 | 0E+00 | $Jm^3C^{-2}$ | 0E+00 |
| $G_{44}$ | 2E-11 | $Jm^3C^{-2}$ | 3.9216E-02 | 1.73E-10 | $Jm^3C^{-2}$ | 1.0000E+00 |
| $c_{11}$ | 2.75E+11 | $Jm^{-3}$ | 1.4675E+05 | 1.746E+11 | $Jm^{-3}$ | 1.7663E+03 |
| $c_{12}$ | 1.79E+11 | $Jm^{-3}$ | 9.5524E+04 | 7.937E+10 | $Jm^{-3}$ | 8.0293E+02 |
| $c_{44}$ | 4.43E+10 | $Jm^{-3}$ | 2.3641E+04 | 1.111E+11 | $Jm^{-3}$ | 1.1239E+03 |
| $Q_{11}$ | 1.104E-01 | $m^4C^{-2}$ | 7.4630E-03 | 8.9E-02 | $m^4C^{-2}$ | 5.1001E-02 |
| $Q_{12}$ | -4.52E-02 | $m^4C^{-2}$ | -3.0555E-03 | -2.6E-02 | $m^4C^{-2}$ | -1.4899E-02 |
| $Q_{44}$ | 2.89E-02 | $m^4C^{-2}$ | 1.9536E-03 | 3.375E-02 | $m^4C^{-2}$ | 1.9340E-02 |
| $P_0$ | 2.6E-01 | $Cm^{-2}$ | 1.0000E+00 | 7.57E-01 | $Cm^{-2}$ | 1.0000E+00 |

$$\alpha_1^* = \alpha_1/|\alpha_1|$$
$$\alpha_{11}^* = \alpha_{11}P_0^2/|\alpha_1|$$
$$\alpha_{12}^* = \alpha_{12}P_0^2/|\alpha_1|$$
$$\alpha_{111}^* = \alpha_{111}P_0^4/|\alpha_1|$$
$$\alpha_{112}^* = \alpha_{112}P_0^4/|\alpha_1|$$
$$\alpha_{123}^* = \alpha_{123}P_0^4/|\alpha_1|$$
$$G_{11}^* = G_{11}/G_{11}$$
$$G_{14}^* = G_{14}/G_{11}$$
$$G_{44}^* = G_{44}/G_{11}$$
$$c_{11}^* = c_{11}/(|\alpha_1|P_0^2)$$
$$c_{12}^* = c_{12}/(|\alpha_1|P_0^2)$$
$$c_{44}^* = c_{44}/(|\alpha_1|P_0^2)$$
$$Q_{11}^* = Q_{11}P_0^2$$
$$Q_{12}^* = Q_{12}P_0^2$$
$$Q_{44}^* = Q_{44}P_0^2$$
$$\mathbf{P}^* = \mathbf{P}/P_0$$

# Phase-field Program

control.in

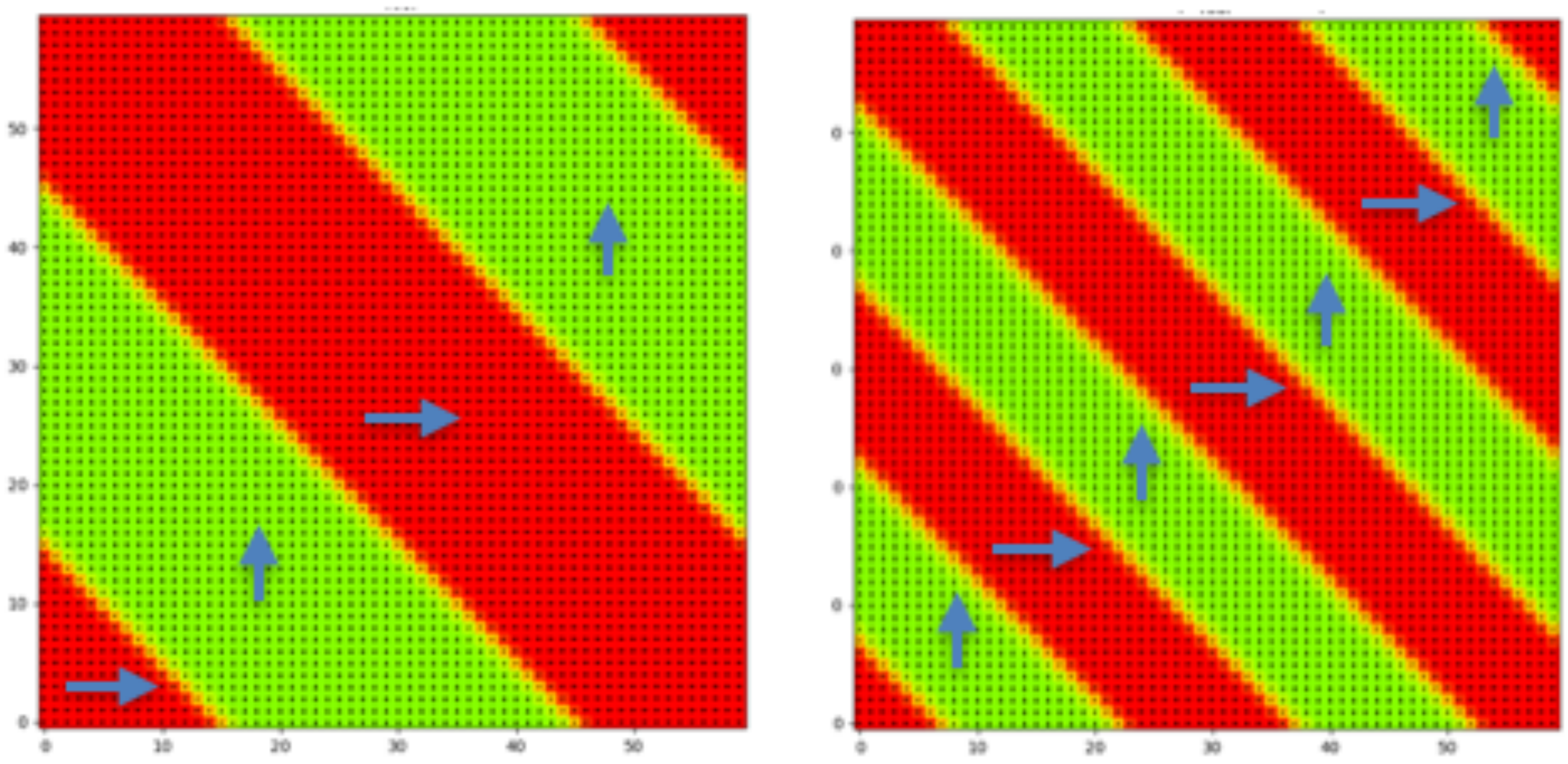
```
nmat = 1      #
nx = 128      # (default:1) the number of UCs along x
ny = 128       # (default:1) the number of UCs along y
nz = 36        #
bd_condition = 2 # 0: non_periodic 1:periodic 2: periodic along x non-periodic along y
electric_bc = 2 #
dim = 3       # (default:1) 2 will be fine for any
dt =  0.01     # (default:1) time interval
gridspace = 1 # (default:1) distance between grid points
xgridspace = 1 # (default:1) distance between grid points
ygridspace = 1 # (default:1) distance between grid points
zgridspace = 1 # (default:1) distance between grid points
landau = 1        # (default:1) Landau free energy (1:on, 0:off)
gradient = 1      # (default:1) Gradient free energy
elastic = 1       # (default:1) Elastic free energy
electric = 1   # (default:1) Dipole diple interaction free energy
ex_electric = 1 #
l = 5.0        # (default:1.0) kinetic coefficient of Ginzburg-Landau equation
iter_max = 2000 #
iter_out = 1900 #
start = 1 #
potbz = -0.0 #
random_ex_electric = 0 #
```

# Phase-field Program

param.in

```
name = BTO       # T: 30 C
a1 = -1.000       #
a11 = -0.404      #
a12 = 1.538      #
a111 = 0.169     #
a112 = -0.254     #
a123 = -0.326     #
a1111 = 0.340     #
a1112 = 0.223     #
a1122 = 0.144     #
a1123 = 0.120     #
g11 = 1.000      #
g44 = 1.000      #
g14 = 0.000      #
c11 = 75117      #
c12 = 40681      #
c44 = 51484      #
Q11 = 0.0068      #
Q12 = -0.0023      #
Q44 = 0.0020      #
permitivity = 0.1  #
aalpha = -0.25 #
abeta = -0.304086723984696 #
misfit_strain = 0.000 #
END-OF-BTO  #
```

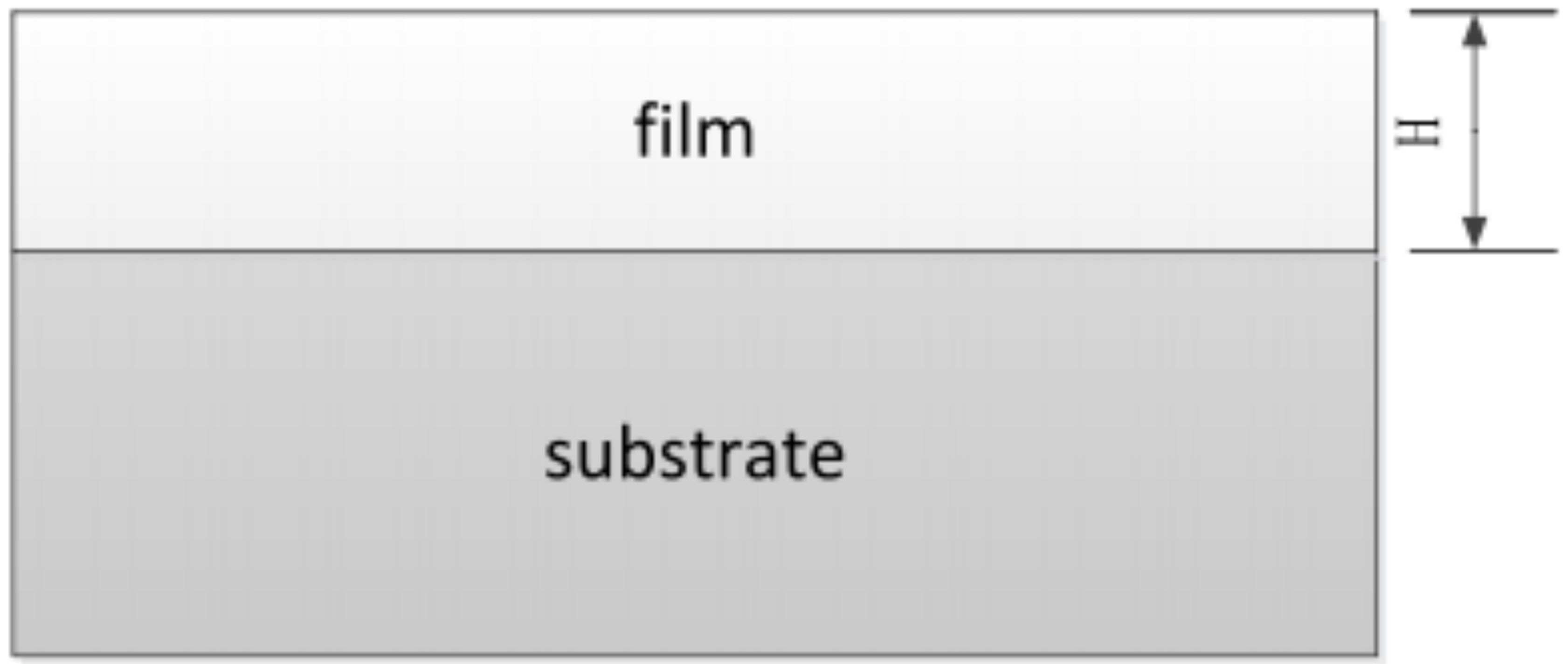
# 2D Simulation



4 and 8 domain pattern of PTO at 25°C : 2D simulation

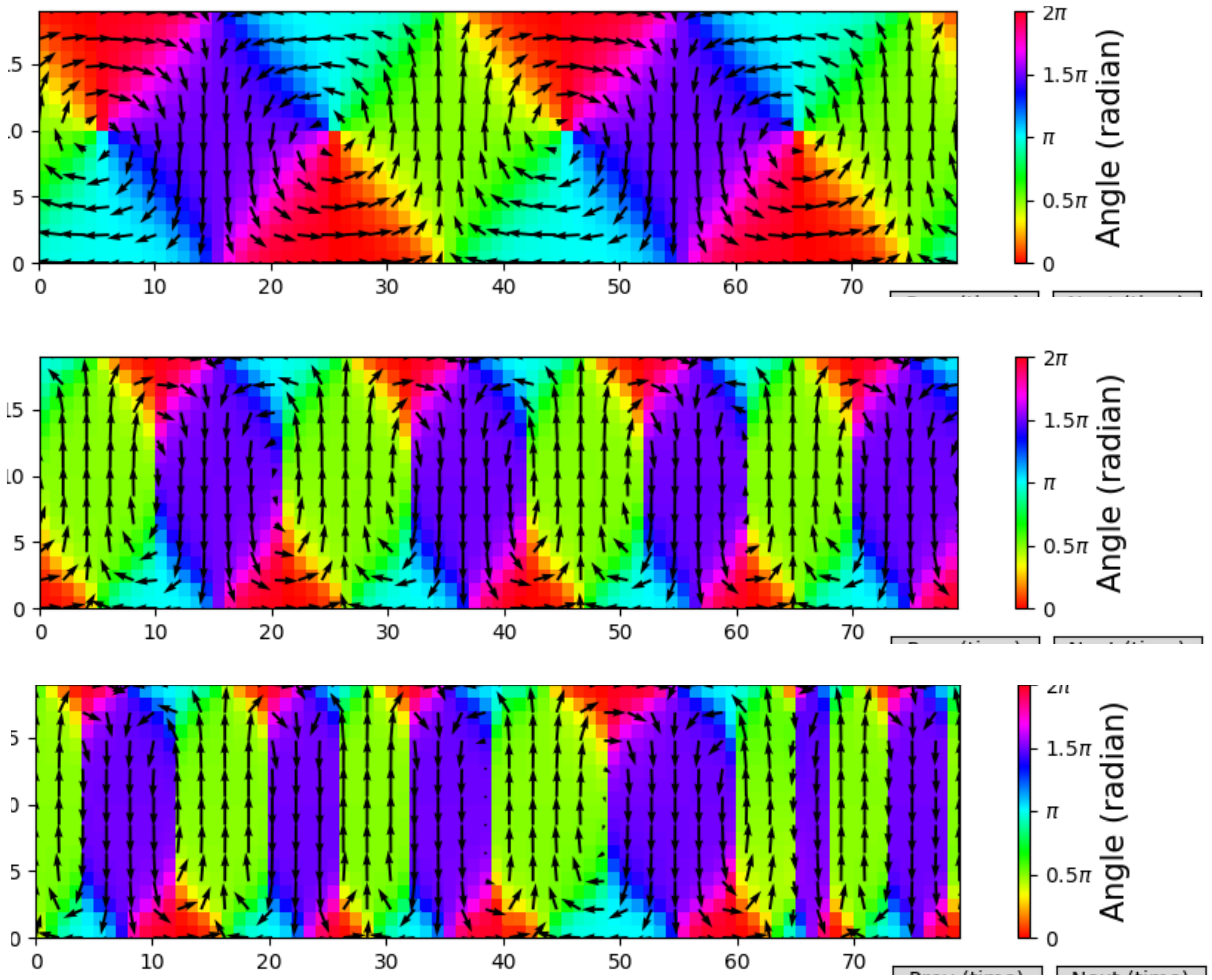
# 2D PTO ferroelectric thin film

Periodic condition along x direction
Non-periodic condition along y direction
Mechanical boundary conditions on epitaxial ferroelectric thin films
Open circuit or Short circuit electrical boundary condition



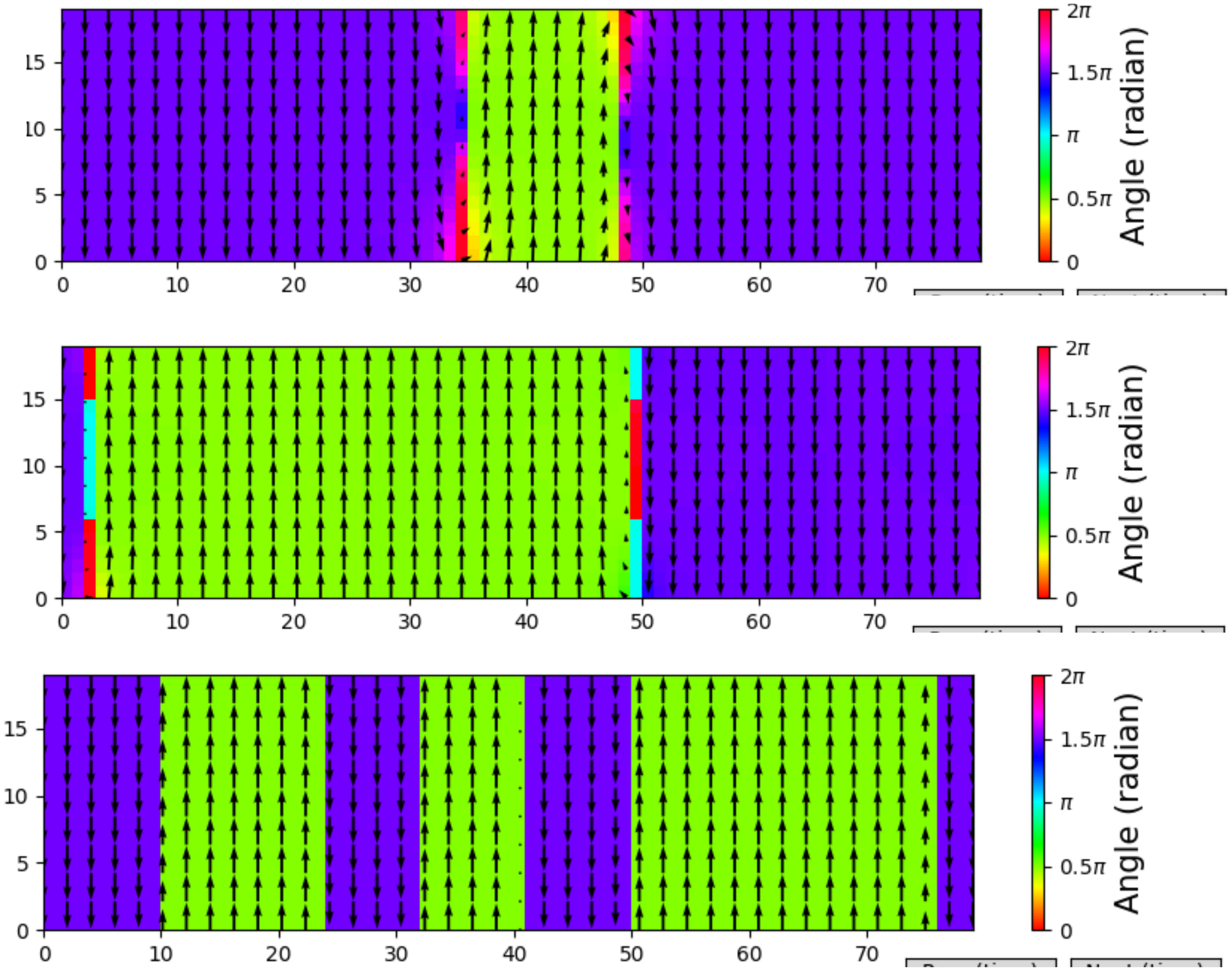

```
PTO            # Material
20             # Number of thickness layers

PTO            #
a1 = -1.0      # Free energy coefficients
a11 = 1.34     # Renormalized Landau coefficients
a22 = 0.176    # - include elastic and electrostriction terms
a12 = 1.527    #
a111 = 0.49    #
a112 = 1.2     #
a123 = -7.0    #
g11 = 1.0      #
g44 = 1.0      #
permitivity = 0.07       #
END-OF-PTO               #

nx = 80        # The number of UCs along x
ny = 20        # The number of UCs along y
nz = 1         # The number of UCs along z
bd_condition = 2 #  2: periodic along x non-periodic along y
dim = 2        # Dimension
gridspace = 1  # Distance between grid points:
```

# 2D ferroelectric thin film



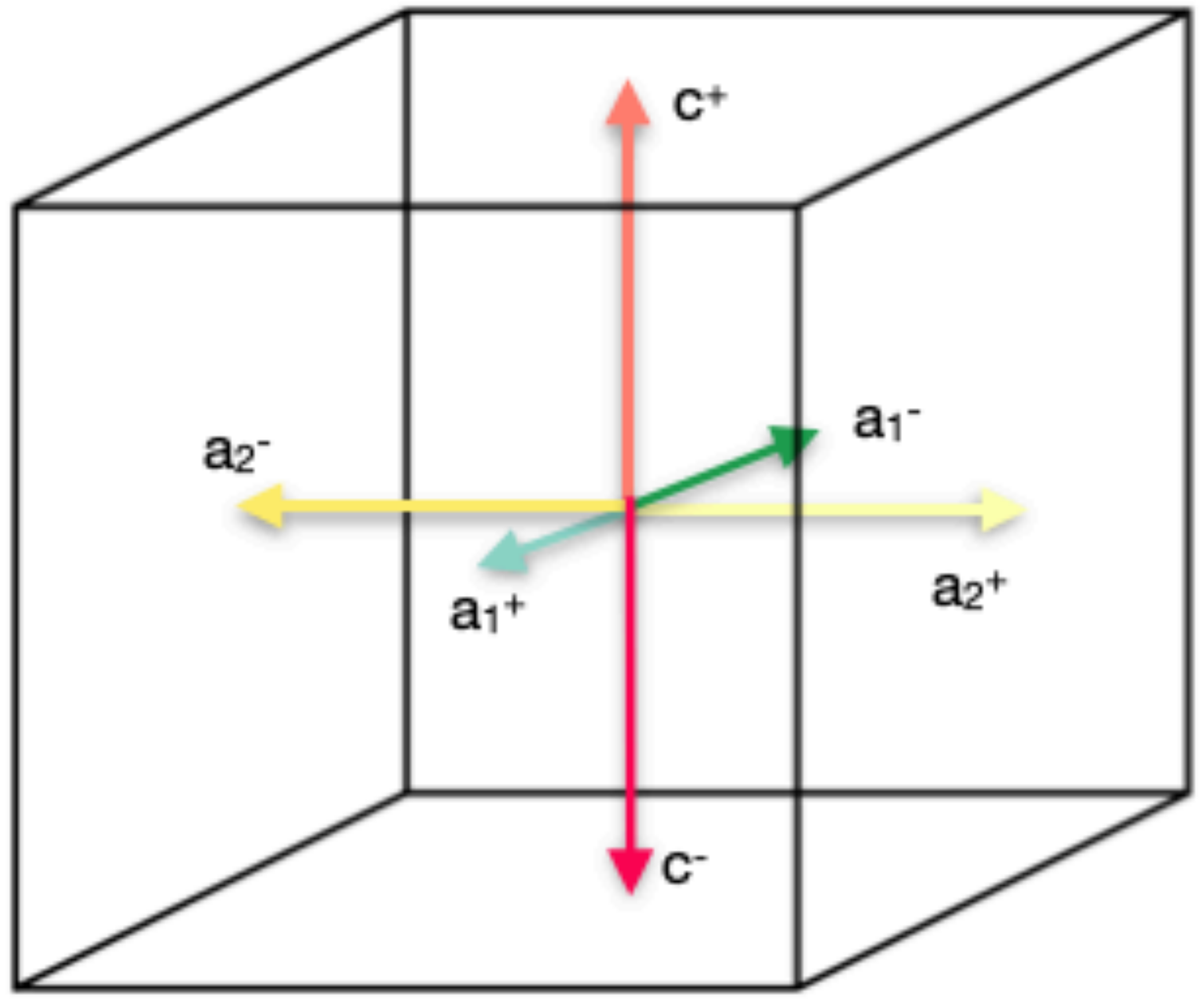

**Domain structures of different thickness of film under OC electrical boundary condition: 10nm, 15nm, 20nm**

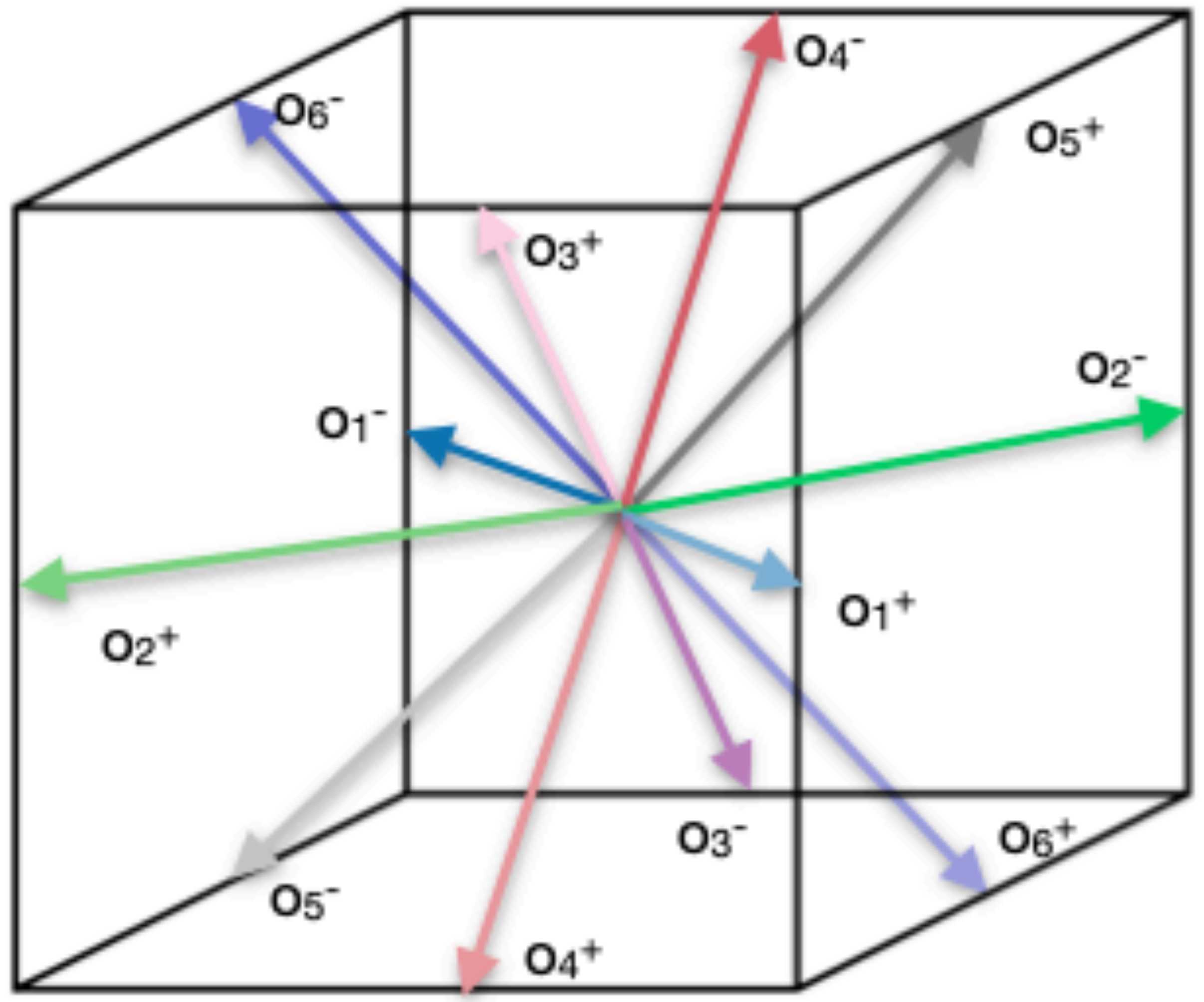
# 2D ferroelectric thin film

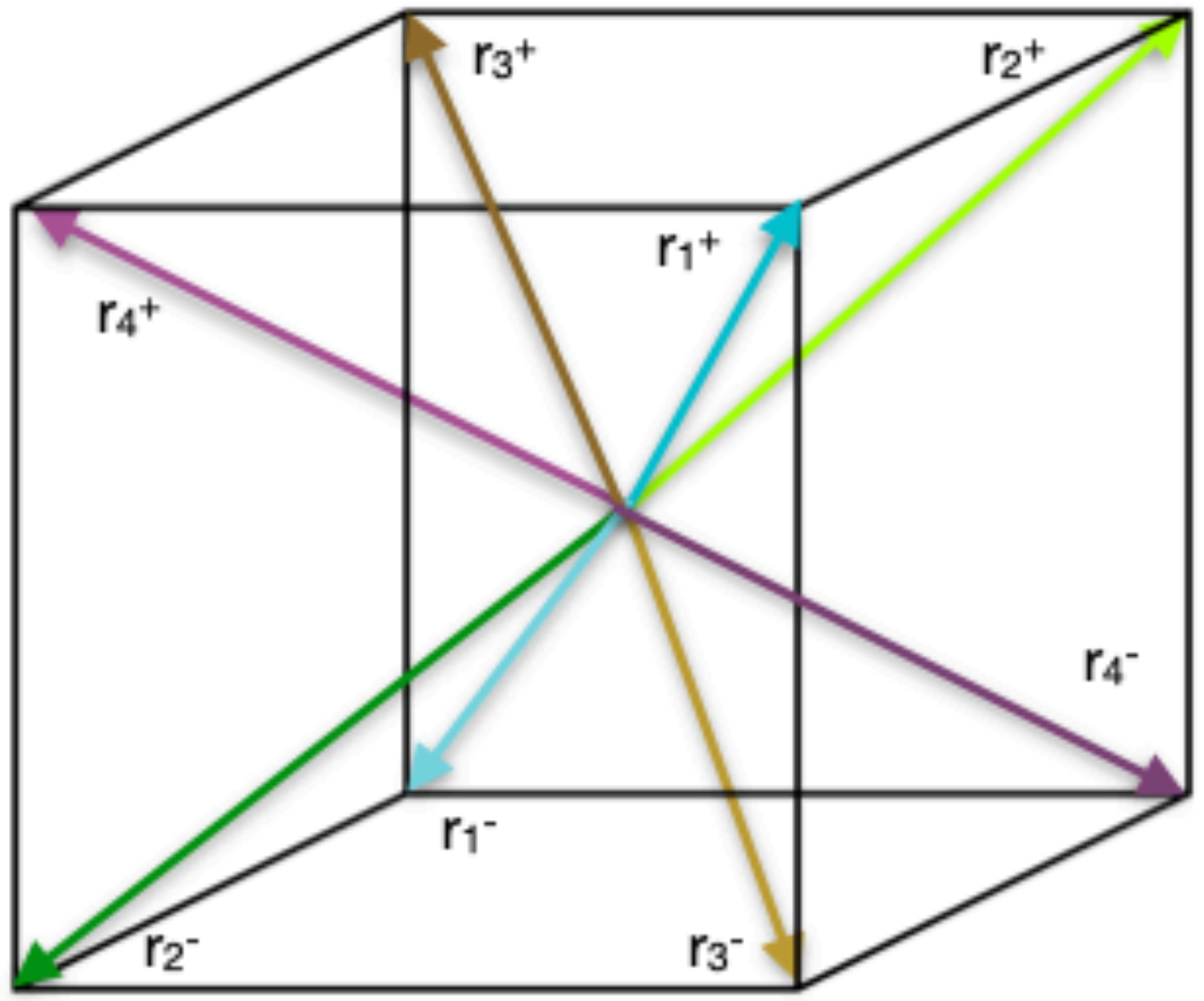



**Domain structures of different thickness of film under SC electrical boundary condition: 10nm, 15nm, 20nm**

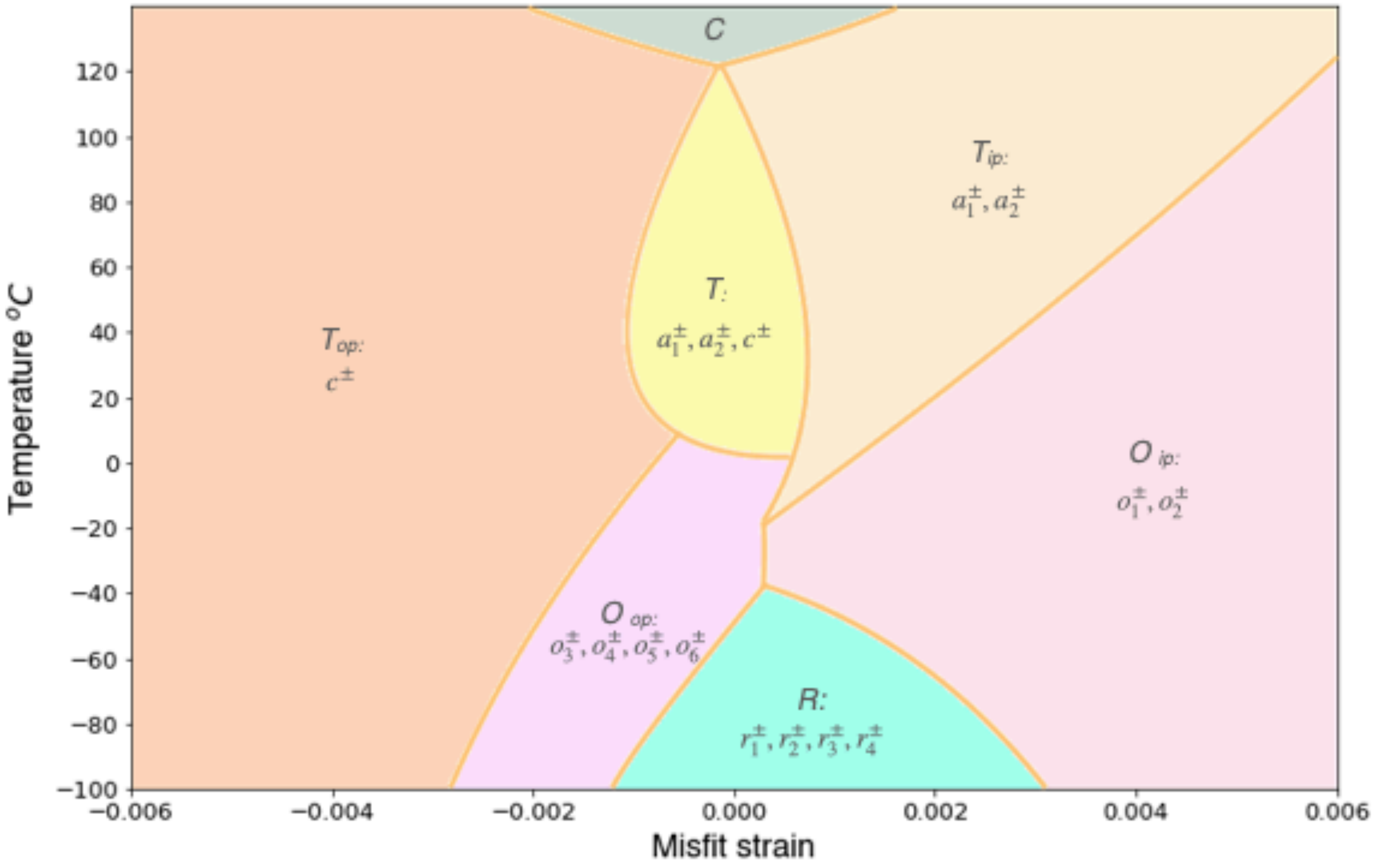
# 3D- Polarization color code

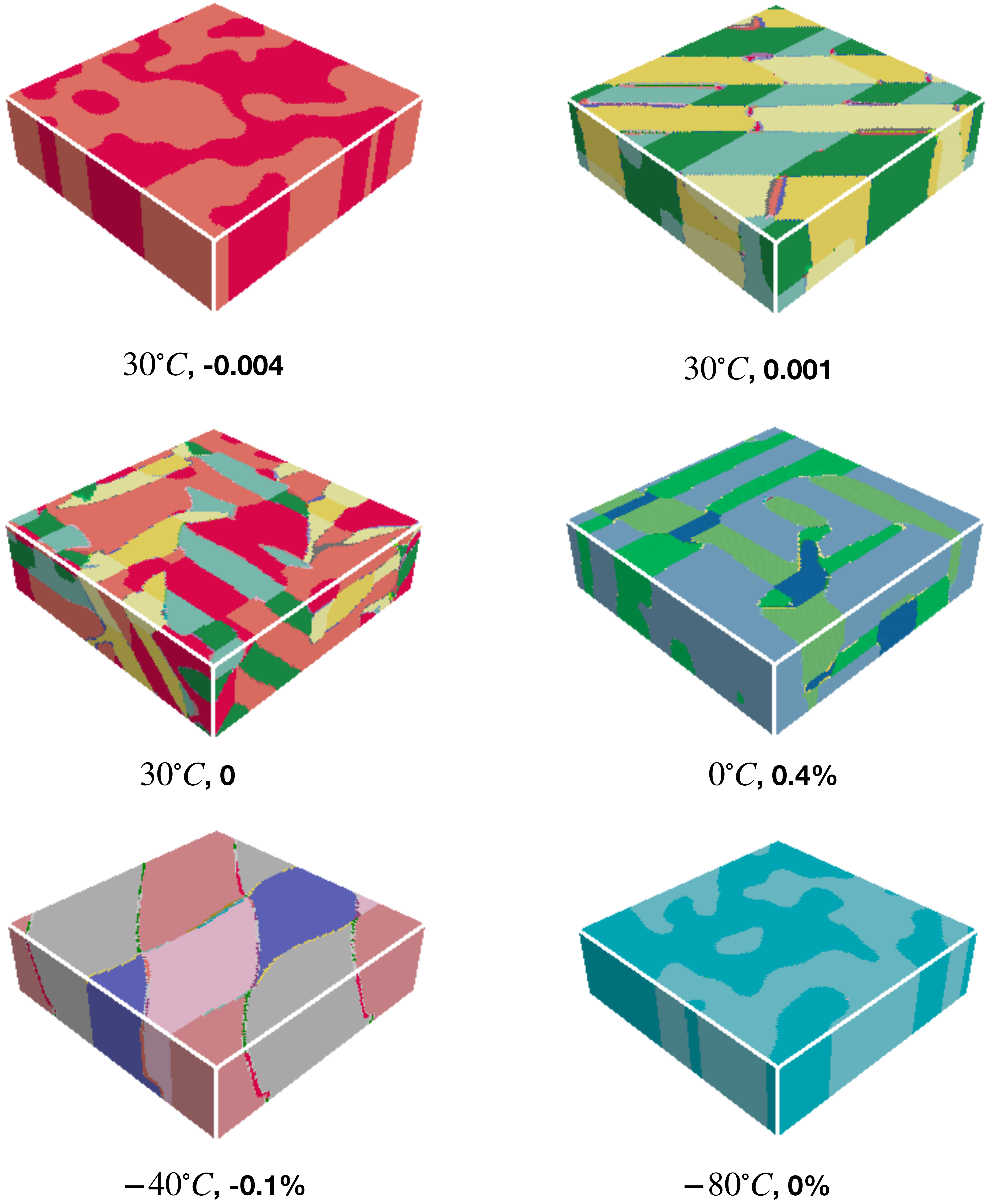


# Phase stability and domain structure



# Wiki - Documentation

https://gitlab.com/yhshin/phase-field/-/wikis/home