Komatsuzaki Seminar
10:00~, March 10th, 2026.

Toward scientific discovery with AI
Part III

Yoh-ichi Mototake
Hitotsubashi university

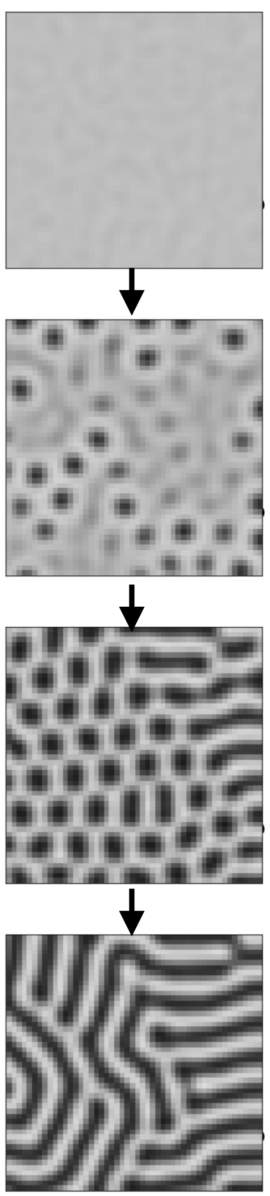
My approaches for Interpretable AI in physics

Our approach to interpretable AI

Part I | Part II

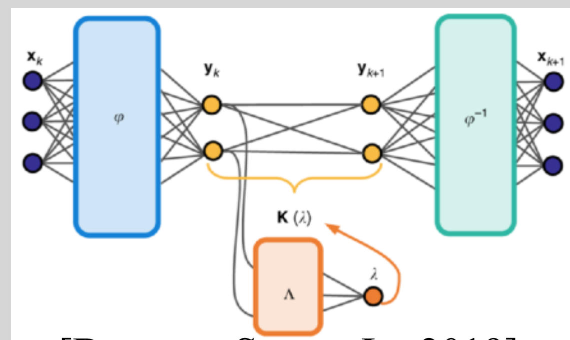
Complex phenomenon

dynamics



Bayesian inference

Deep neural network-type approach



[Brunton, Steven L.. 2019]

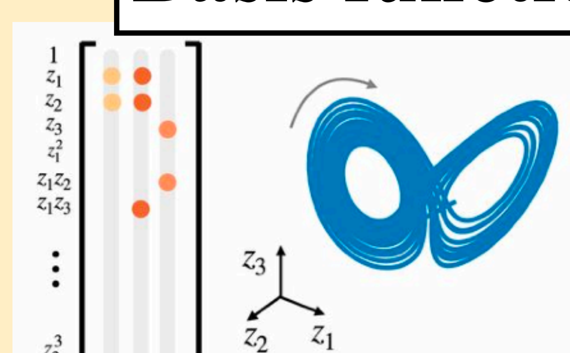
Cons: low interpretability

extract **Interpretable** physical information from DNN

Interpretable and high expressive model

Part III

Basis function type approach



[Steven L. Brunton et al., PNAS, 2016]

Cons: Poor expressive power

Construction of a reduced model based on **topological data analysis**

Expressive Power

Interpretability

Topological data analysis of pattern dynamics in material science

[Y. Mototake, M. Mizumaki, K. Kudo, K. Fukumizu, Physica D, 470(A), 2024]

The Institute of Statistical Mathematics
Yoh-ichi Mototake

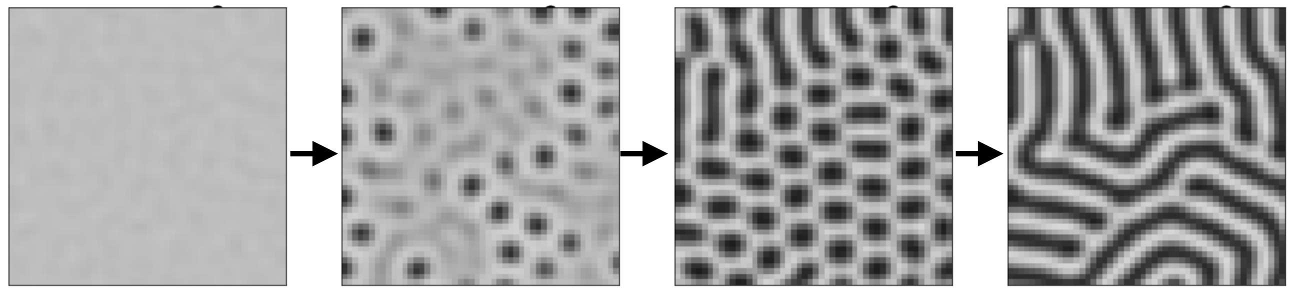
PRESTO
SAKIGAKE

1. Background

Pattern dynamics in material science

Magnetic materials

Time evolution of magnetic domain structure

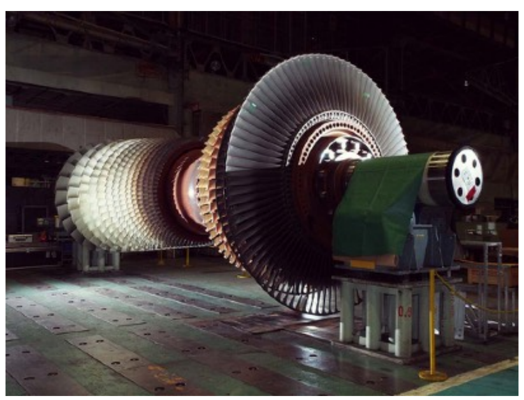


Magnetic properties

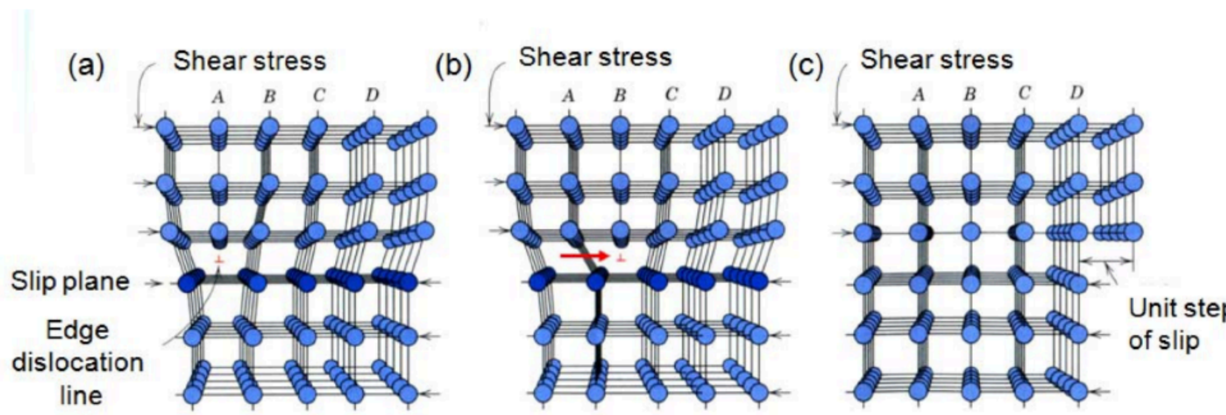
Coercivity (energy storage)
Mechanism of coercivity

Loss of coercivity

Structural materials



Destruction process



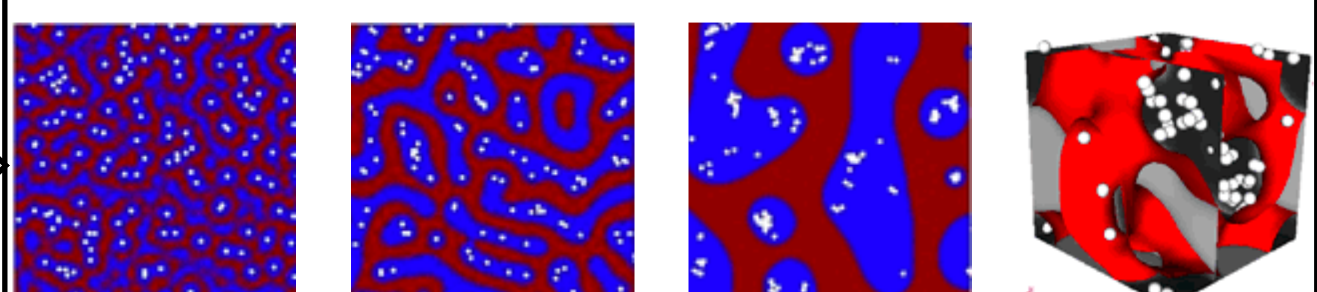
Predicting destruction

Creep prediction in environments with varying temperature and stress

Refinement of time control for quenching and tempering

Polymer Materials

Crystallization process



Prediction of dynamic formation and destruction processes

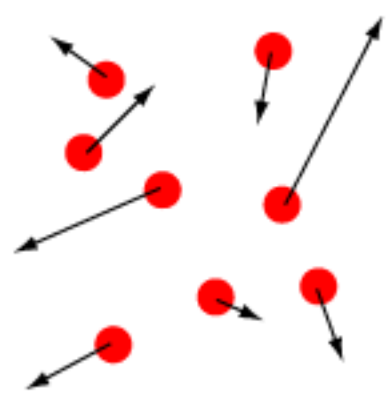
Optimization of the time factor in the material formation process

Optimization of mechanical properties by clarifying the fracture process

Feature of pattern dynamics

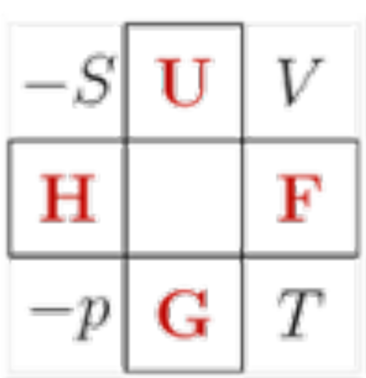
Random ⟷ **Ordered**

Random structure

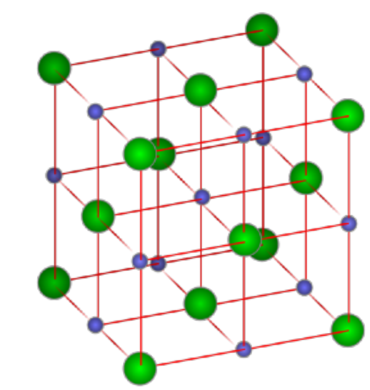


Molecular motion of gas

Statistics



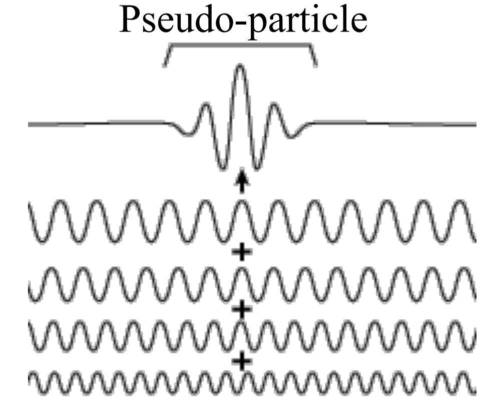
Periodic structure



NaCl crystal (Wikipedia)

Fourier basis

Pseudo-particle



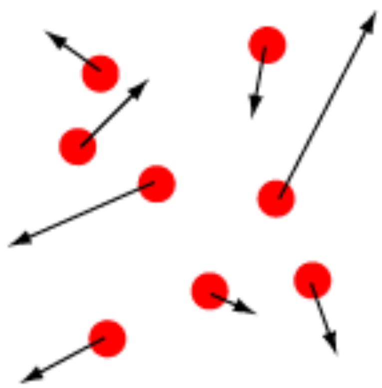
http://k-hiura.cocolog-nifty.com/

[Ippei Obayashi, 数理解析研究所講究録「位相的データ解析の現在」]

Feature of pattern dynamics

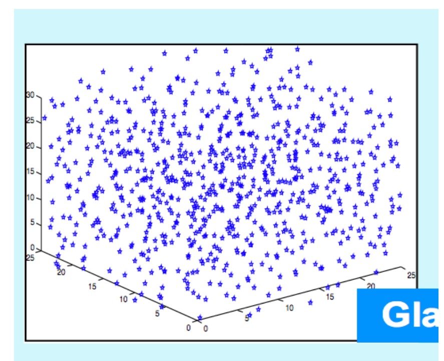
Random ⟵⟶ **Ordered**

Random structure



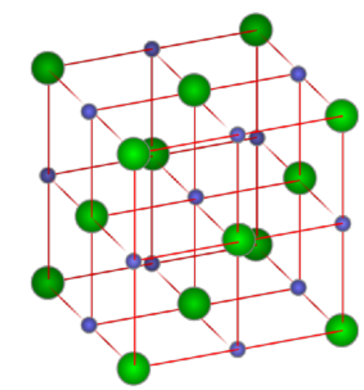
Molecular motion of gas

Non-periodic ordered structure



平岡先生スライド:「パーシステントホモロジーとその応用」
http://www.math.chuo-u.ac.jp/ENCwMATH/EwM70_Hiraoka.pdf

Periodic structure



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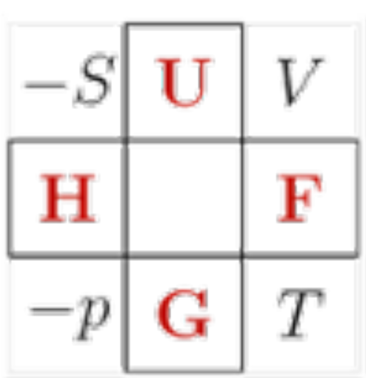
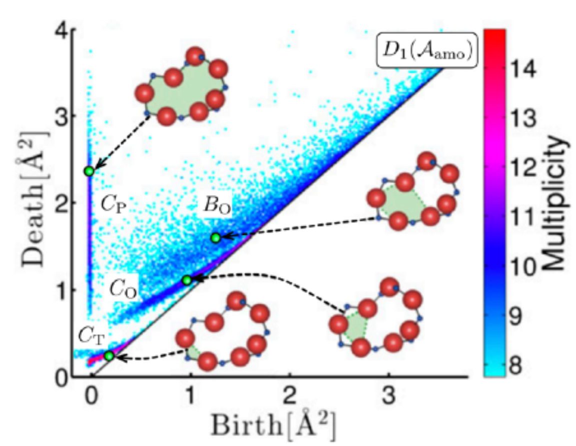
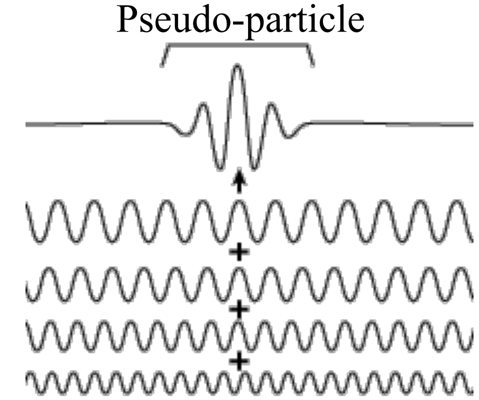


Topological feature



[Yasuaki Hiraoka et al., PNAS, 2016]

Fourier basis



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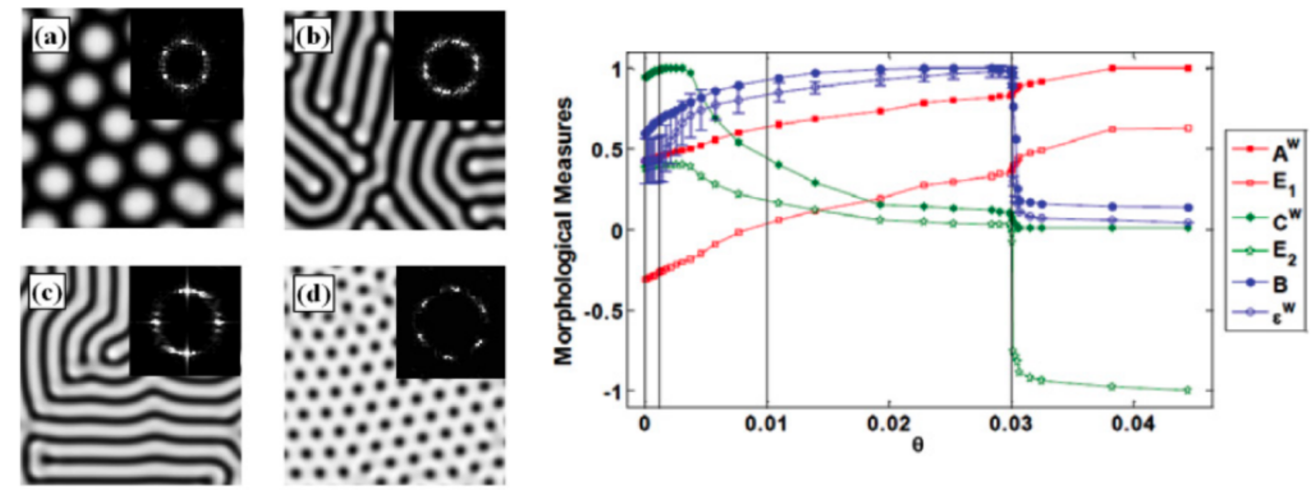
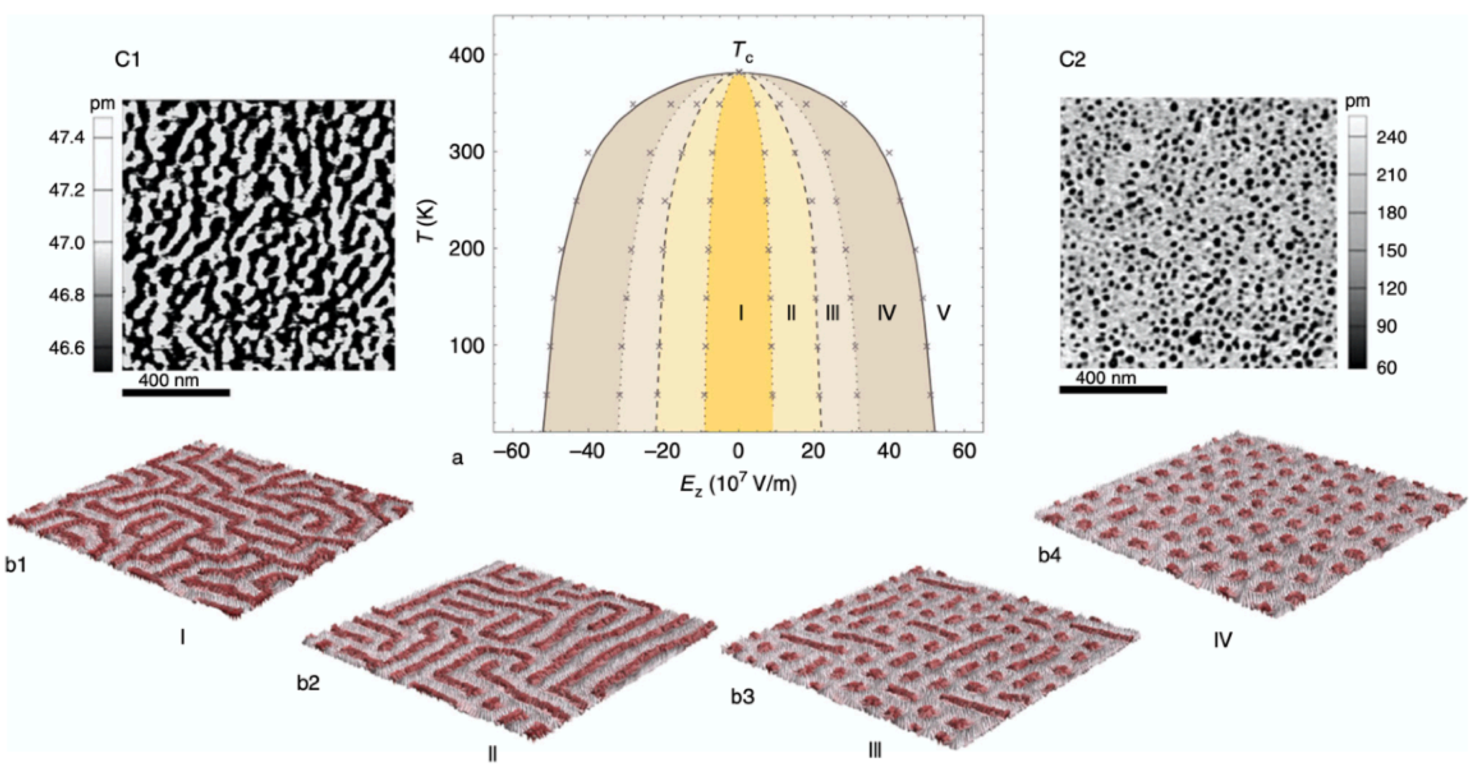
[Ippei Obayashi, 数理解析研究所講究録「位相的データ解析の現在」]

Analysis of domain patterns using topological features

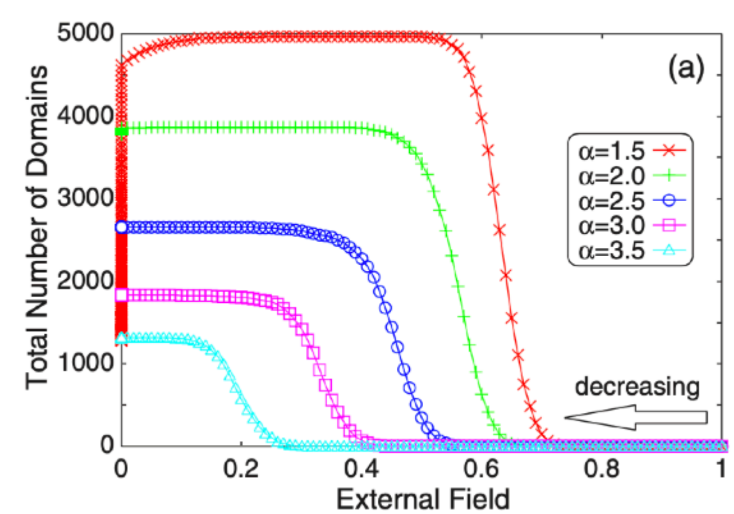
http://park18.wakwak.com/



[Jacobo Guiu-Souto et al., PRE, 12]



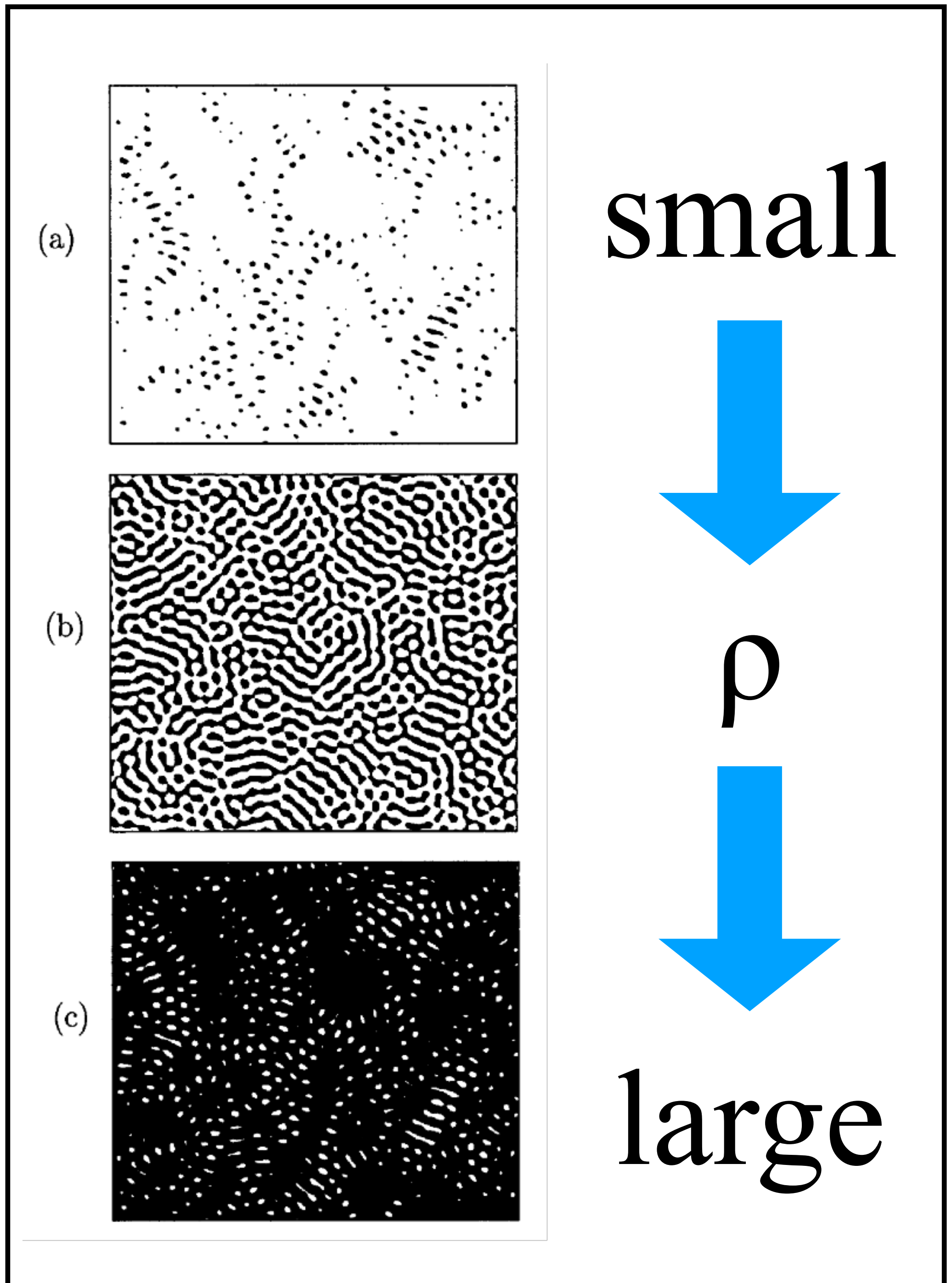
[Y. Nahas et al., *Nature*, 2020]

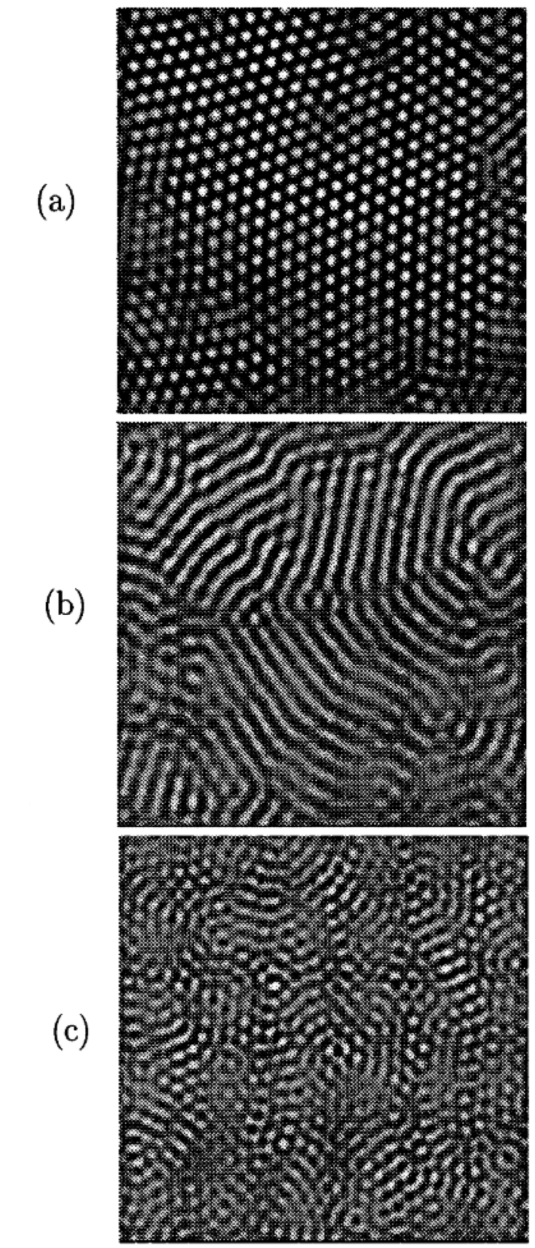


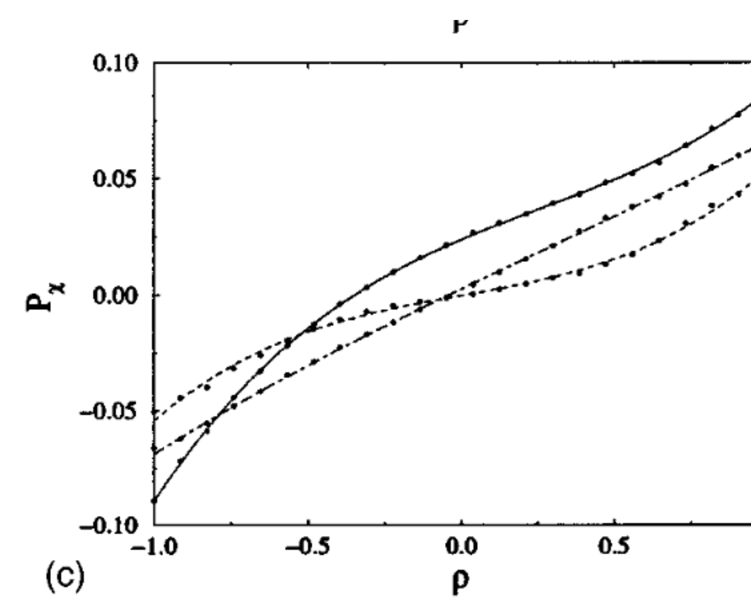
[Kazue Kudo et al., PRB, 07]

Analysis of domain patterns using topological features

- Level set information is important [K. R. Mecke 96]

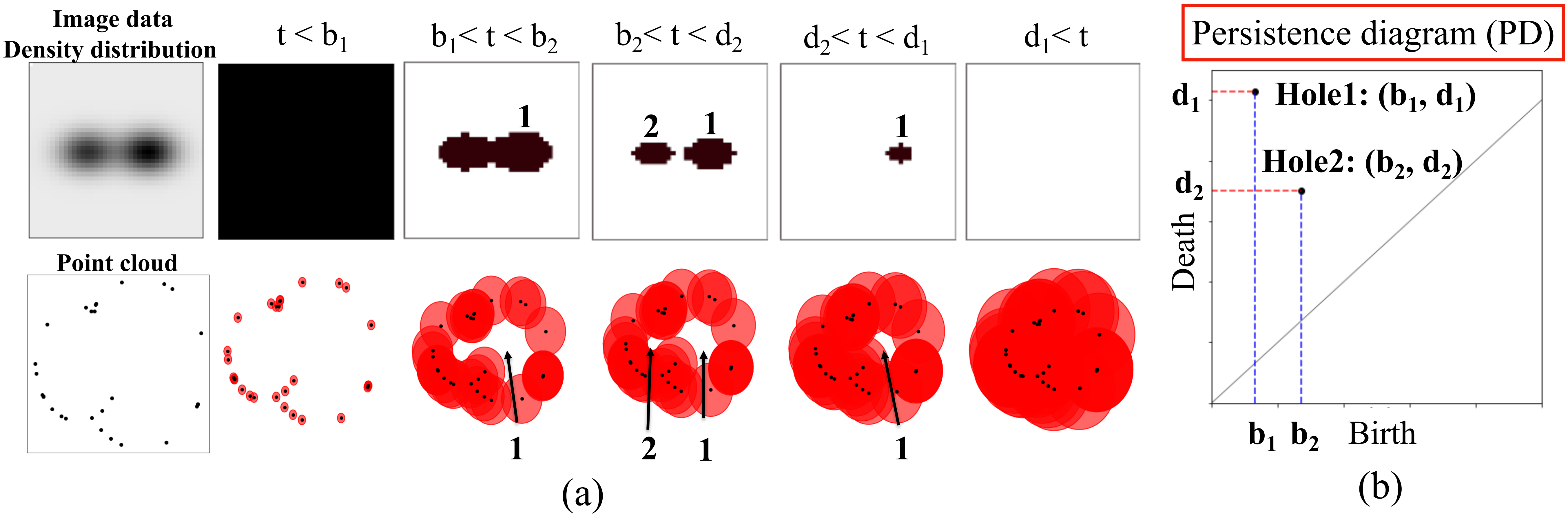




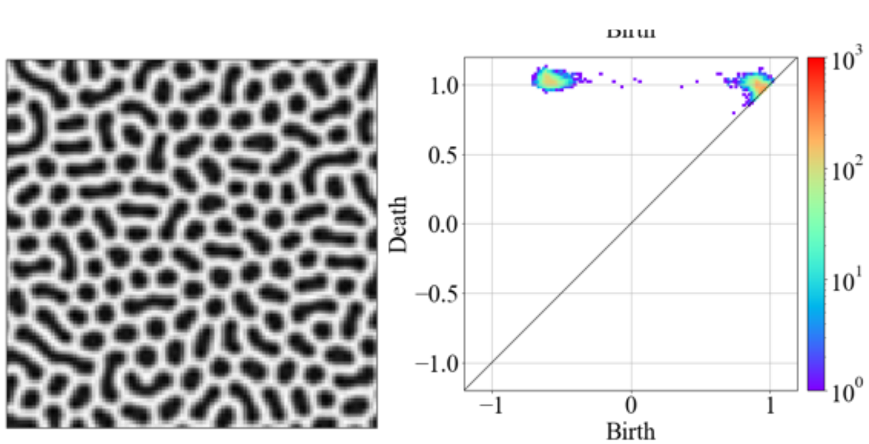


→Low interpretability

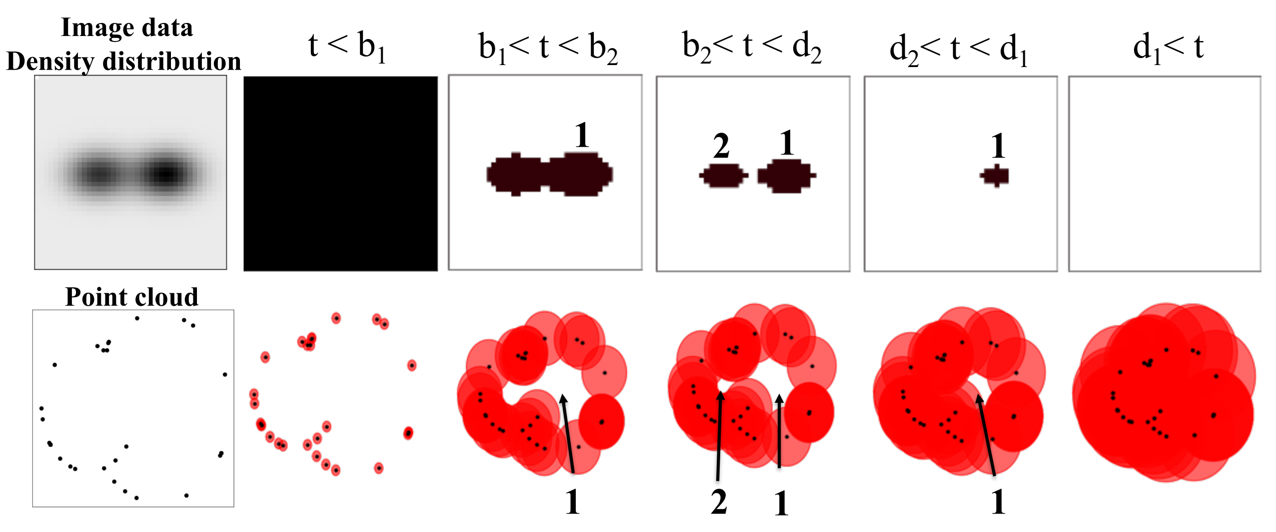
Persistent homology group

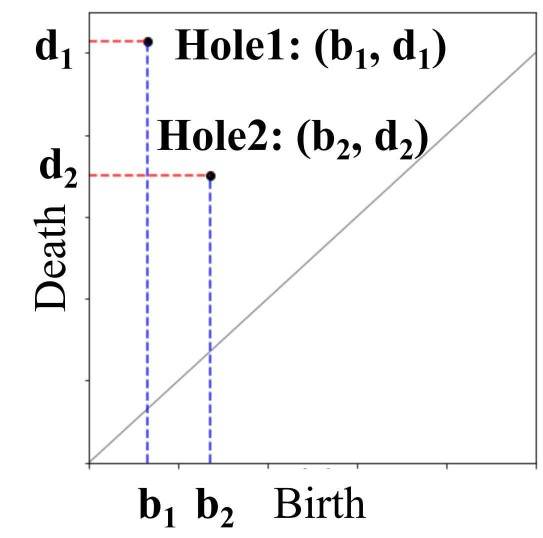


Y. Mototake, M. Mizumaki, K. Kudo, and K. Fukumizu, "Topological Data Analysis of Domain Pattern Formation in Materials," Journal of Smart Processing, 10(3), 2021.



Persistent homology group

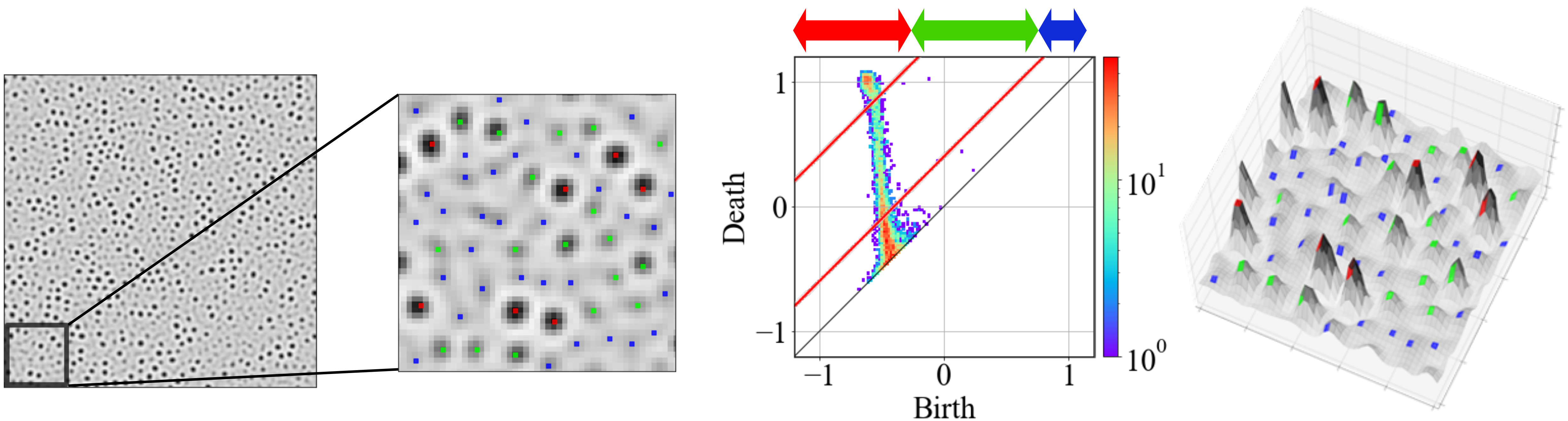




1. Contains information on changes in topological features with one parameter
→Varying topological information depending on patameters such as threshold and scale
2. Contains the topological features of each isolated domain
→Retain topological information of each hole structure
3. Inverse analysis is possible
→Correspondence between features and geometric structures in the original space is clear.
4. The stability theorem holds
→Features behave stably with respect to small changes in geometry in the original space

Persistent homology group

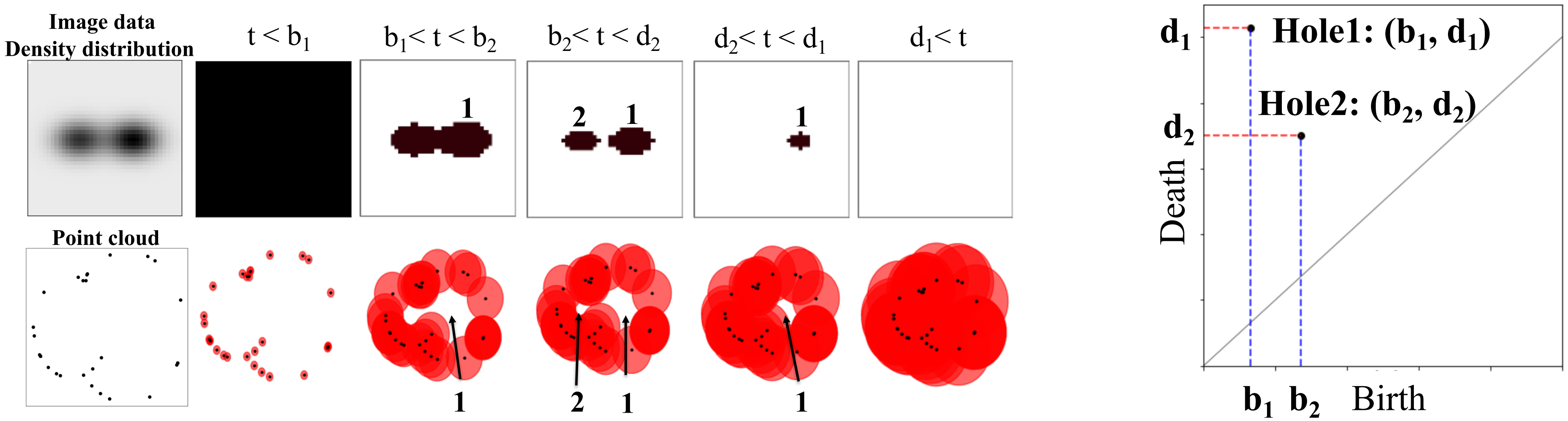
Inverse analysis



(a1) (a2) (a3)

Red: strong intensity peaks around 0.8 (= **Domain structure**)
Green: intermediate intensity peaks (= **Intermediate structure**)
Blue: weak intensity peak around 0.1 (= **Inter-domain structure**)

Persistent homology group



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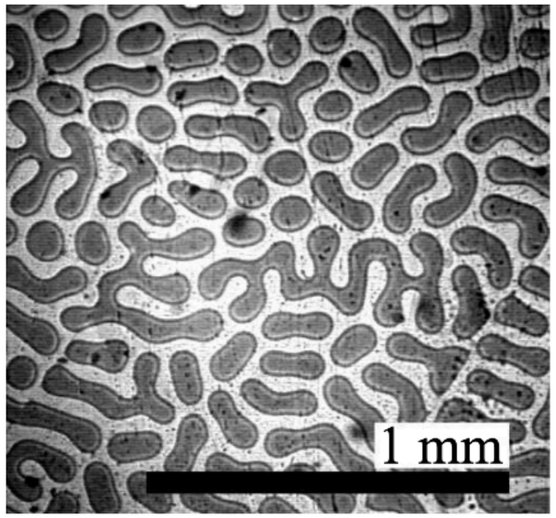
Topological data analysis of pattern dynamics in material science

Magnetic domain pattern

Y. Mototake, M. Mizumaki, K. Kudo, and K. Fukumizu, "Topological Data Analysis of Domain Pattern Formation in Materials," Journal of Smart Processing, 10(3), 2021.

[Y. Mototake, M. Mizumaki, K. Kudo, K. Fukumizu, (in prep)]



Sea island structure

Labyrinth structure

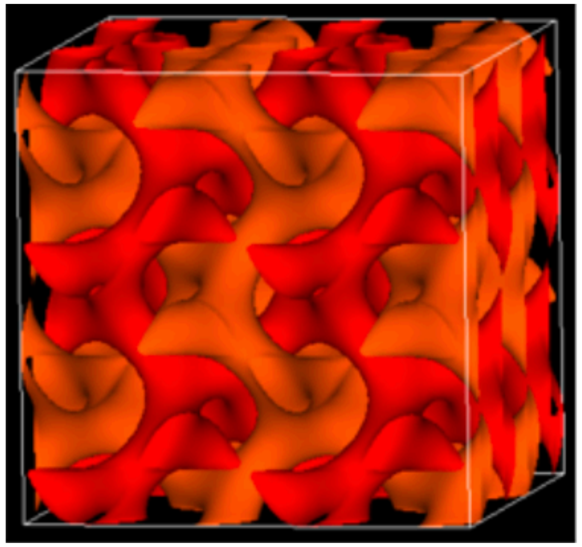
[Kazue Kudo, Michinobu Mino and Katsuhiro Nakamura 07]

Polymer pattern

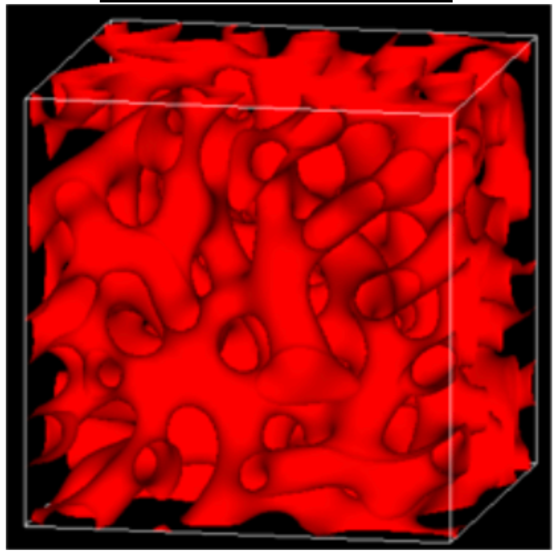
[Y. Mototake, S. Yamanaka, T. Aoyagi, T. Ohnishi, K. Fukumizu, NOLTA2020 , 517 - 520, 2020]

[Y. Mototake, S. Yamanaka, T. Aoyagi, T. Ohnishi, K. Fukumizu, J. Comp. Chem., Japan, 2021 (in press)]

Stable



Meta-stable



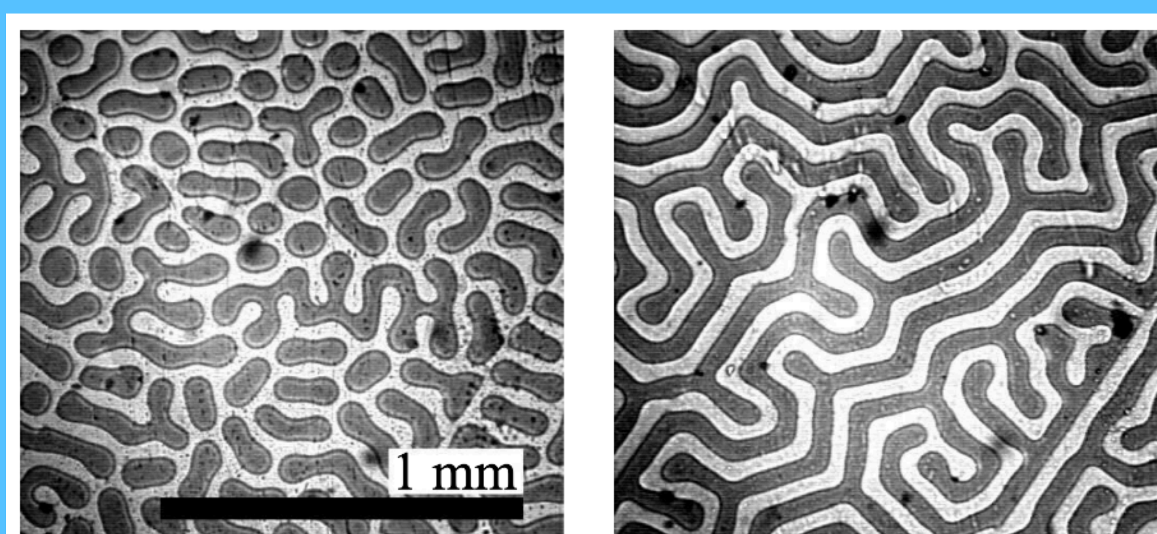
Double Gyroid Structure

Topological data analysis of pattern dynamics in material science

Magnetic domain pattern

Y. Mototake, M. Mizumaki, K. Kudo, and K. Fukumizu,
“Topological Data Analysis of
Domain Pattern Formation in Materials,” Journal of Smart
Processing, 10(3), 2021.

[Y. Mototake, M. Mizumaki, K. Kudo, K. Fukumizu, (in prep)]



Sea island structure   Labyrinth structure

[Kazue Kudo, Michinobu Mino and Katsuhiro Nakamura 07]

Polymer pattern

[Y. Mototake, S. Yamanaka, T. Aoyagi, T. Ohnishi, K. Fukumizu,
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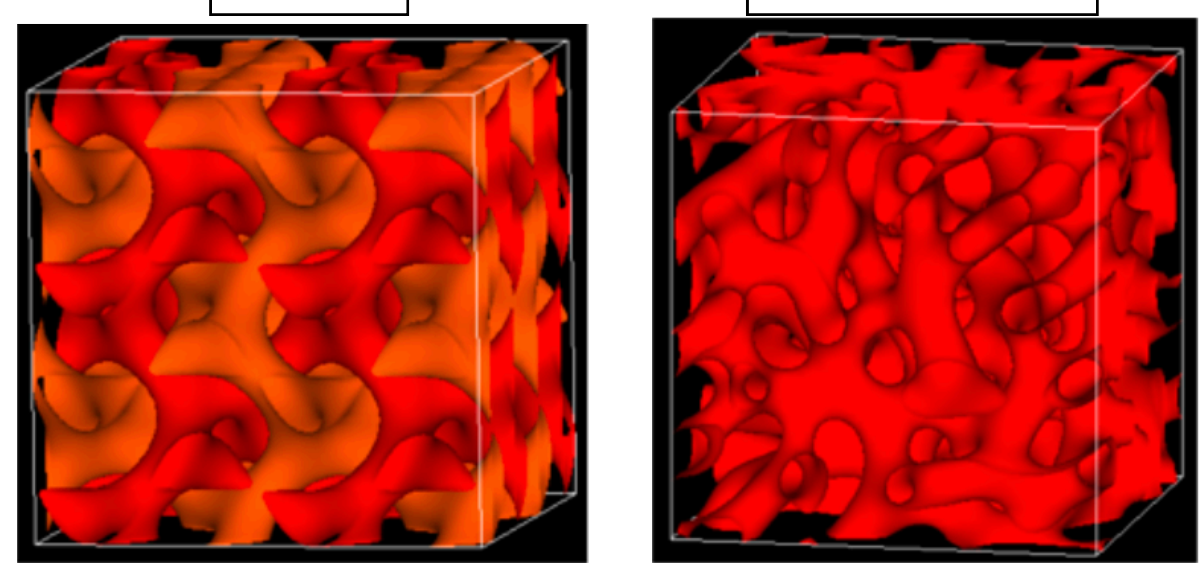
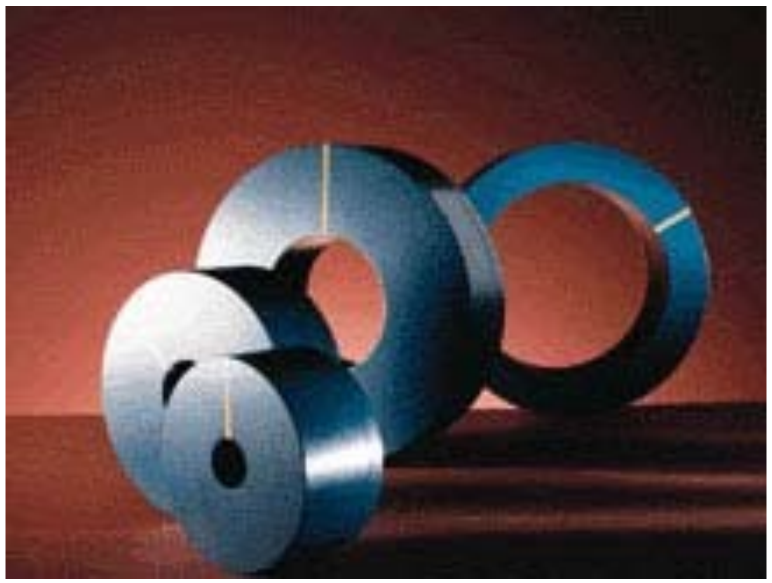
J. Comp. Chem., Japan, 2021 (in press)]

Stable   **Meta-stable**



Double Gyroid Structure

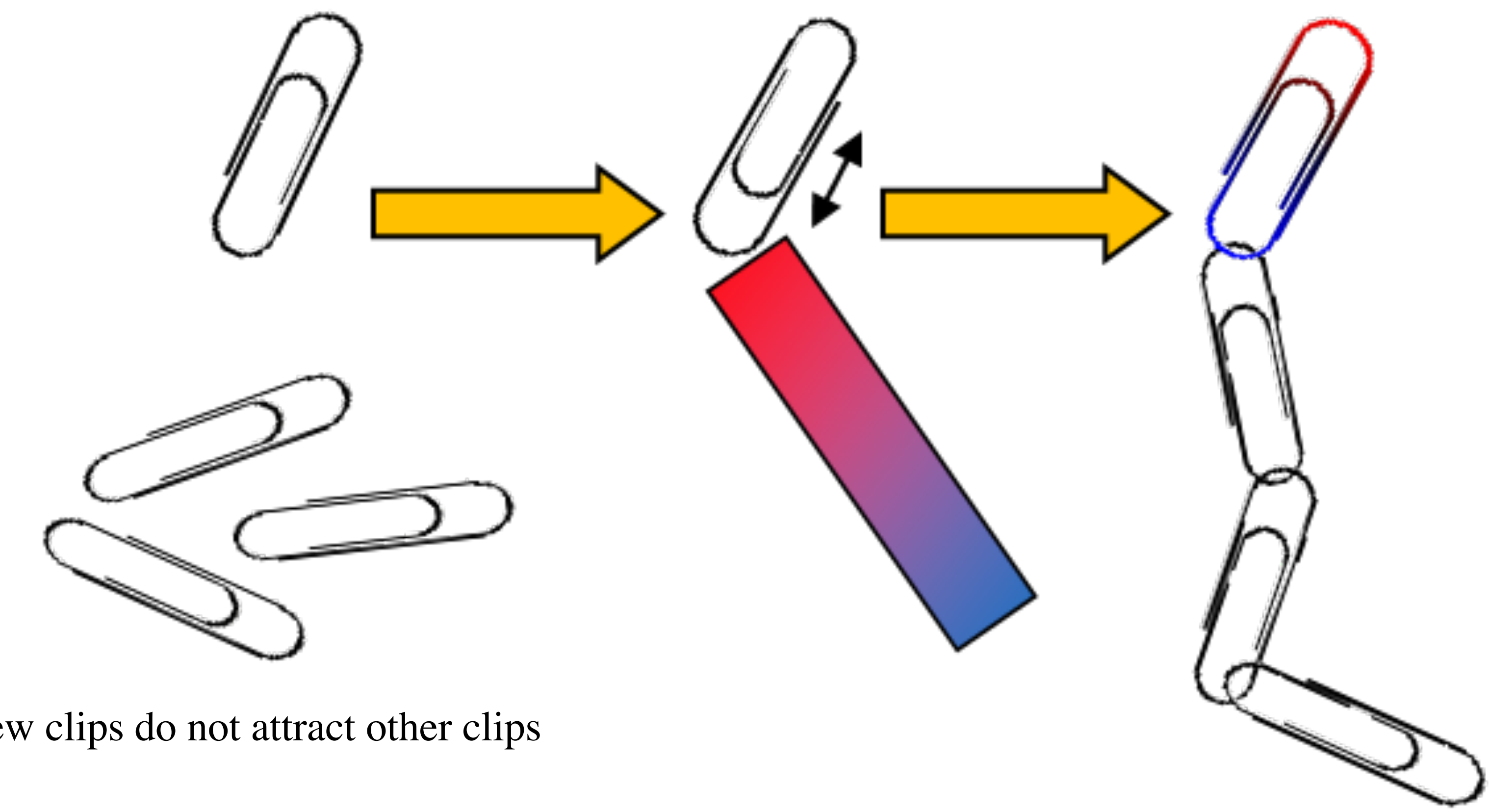
Domain pattern of ferromagnetic materials



[Katsuaki Sato, 「ようこそ、まぐねの国に」より]

Domain pattern of ferromagnetic materials

When you rub an iron clip with a magnet, it becomes magnetized.



(a) New clips do not attract other clips

(b) Clip rubbed with a magnet attract other clips

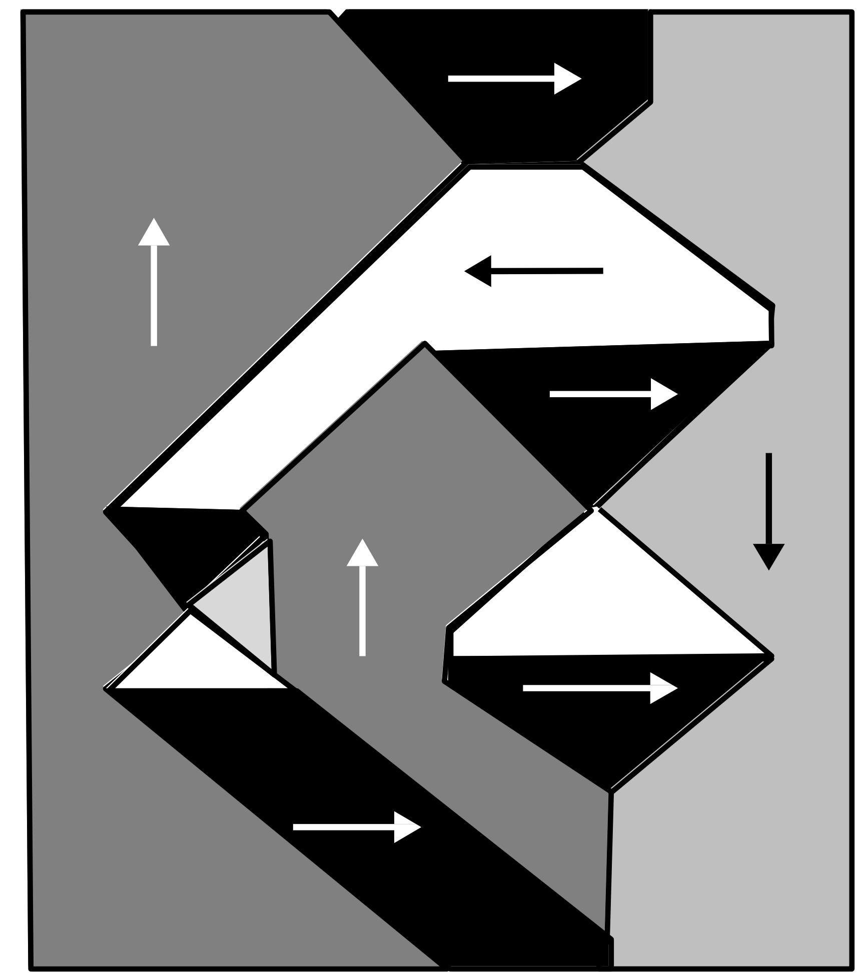
[Katsuaki Sato, 「ようこそ、まぐねの国に」より]

Domain pattern of ferromagnetic materials

1. If we zoom in on the iron clip with a polarized light microscope, we can see that it is divided into many regions with different directions of the magnetic moment as shown schematically in the right figure.
   In this case, the magnetic moment vector sum is zero and the entire magnetization is canceled.

2. When you rub a clip with a magnet, the magnetic domain of the clip aligns with the direction of the magnetic field becomes large and cannot be completely regained, whereas the magnetic field is removed, so the clip becomes magnet.

3. A region where the magnetic moment has the same direction is called a "**magnetic domain**".



Schematic diagram of the magnetic domain structure of a magnetic material before magnetization

[Katsuaki Sato, 「ようこそ、まぐねの国に」より]

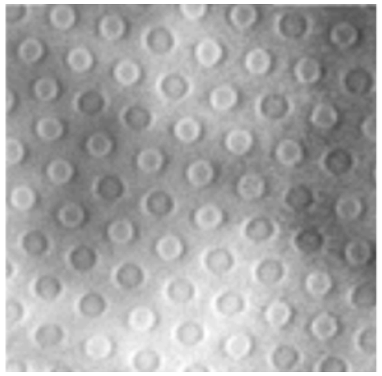
Domain pattern of ferromagnetic materials

Magnetic domain pattern: pattern structure generated by the antagonism of short- and long-range correlations

Stripe

Labyrinth

Hexagonal bubbles



[Iglesias, Jose Roberto, et al., *PRB,* 65.6, 2002]

[Xiuzhen Yu et al., PNAS, 109 (23), 2012]

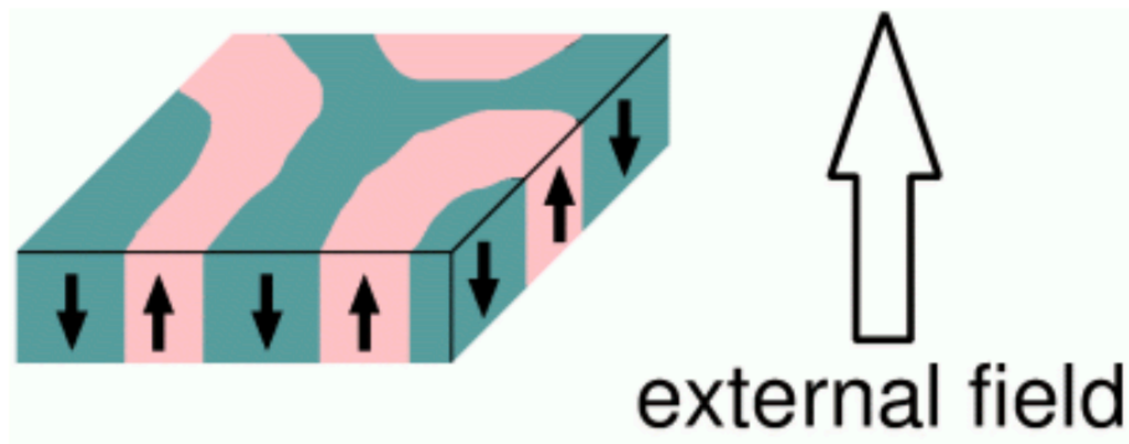
➡Domain patterns have a strong relationship with the functions required for magnetic materials

➡It has long been understood that domain structure is an important component of magnetic properties.
But it is **unclear** how domain structure correlates with physical property, such as coercivity.

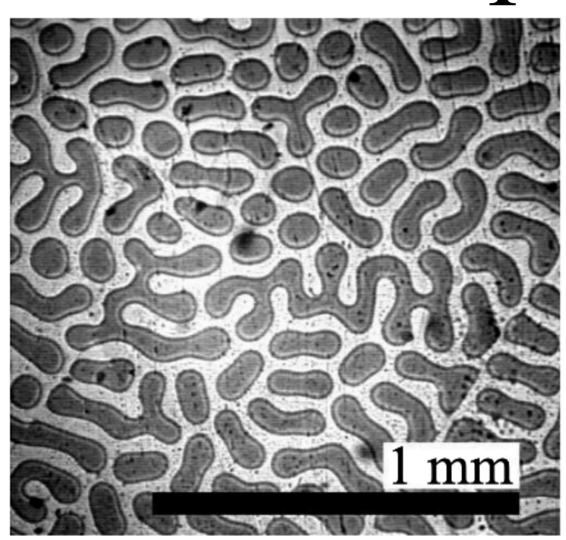
[Kurima Kobayashi, 「磁石の内部磁場分布とMFM及びMOKEによる 表面磁区構造の相関性の検討」より]

Domain pattern formation process

文部科学省委託事業
『次世代自動車エキスパート養成教育プログラム開発事業』
『EV車のモーター技術』より



Fast sweep | Slow sweep



Sea island structure

Labyrinth structure

[Kazue Kudo, Michinobu Mino and Katsuhiro Nakamura 07]

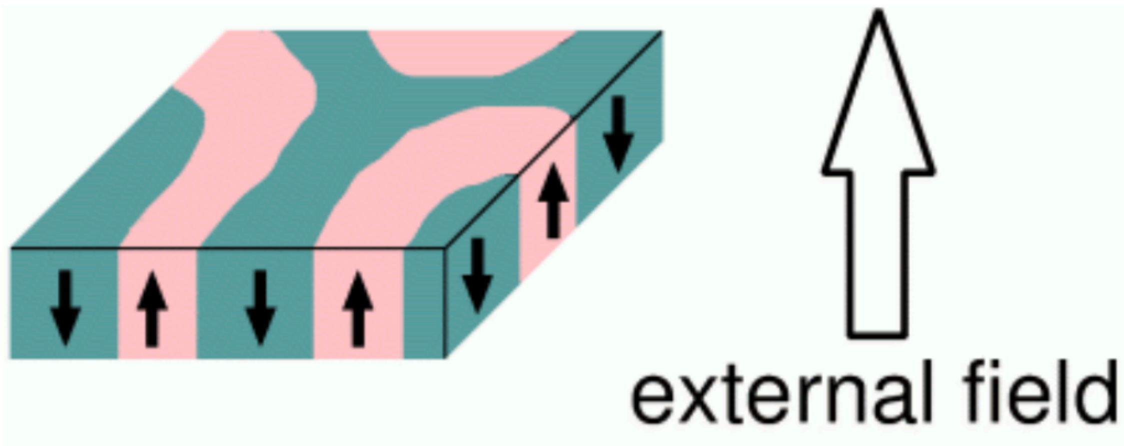
➡Rapidly changing the external magnetic field, a **sea island** structure appears

Time Dependent Gintzburg Landau (TDGL) Equation

$$\phi(\mathbf{r}) \sim \{-1, 1\}$$

➡A time-evolution model of the mean magnetization field $\phi(r)$ of spin populations in a small region

$$\phi(\mathbf{r}) : \mathbf{R}^2 \to \mathbf{R},\ \mathbf{r} = (x, y)$$



Anisotropy energy | **Ferromagnetic interaction** | **Dipolar interaction** | **External field**

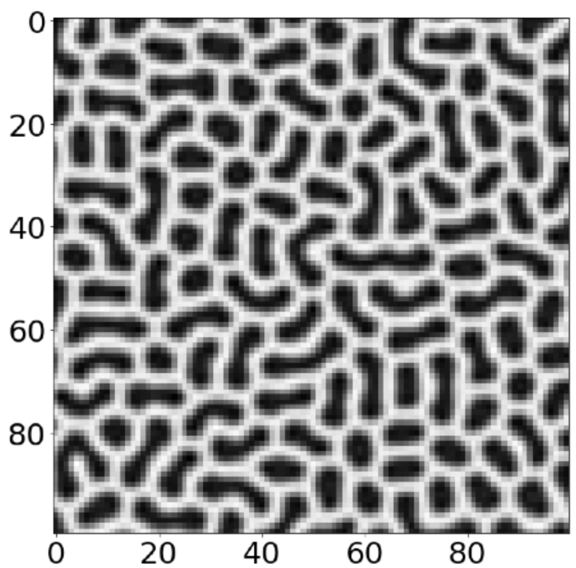
$$\frac{\partial \phi(\mathbf{r})}{\partial t} = -\frac{\delta\left[\alpha \int d\mathbf{r} \lambda(\mathbf{r}) \left(-\frac{\phi(\mathbf{r})^2}{2} + \frac{\phi(\mathbf{r})^4}{4}\right) + \beta \int d\mathbf{r} \frac{|\nabla \phi(\mathbf{r})|}{2} + \gamma \int d\mathbf{r} d\mathbf{r}' \phi(\mathbf{r}) \phi(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') + -h(t) \int d\mathbf{r} \phi(\mathbf{r})\right]}{\delta \phi(\mathbf{r})}$$

$$\lambda(\mathbf{r}) = 1 + \frac{\mu(\mathbf{r})}{4}, \quad G(\mathbf{r}, \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|^3}, \quad h(t) = h_0 - vt \ \ (h(t) > 0).$$

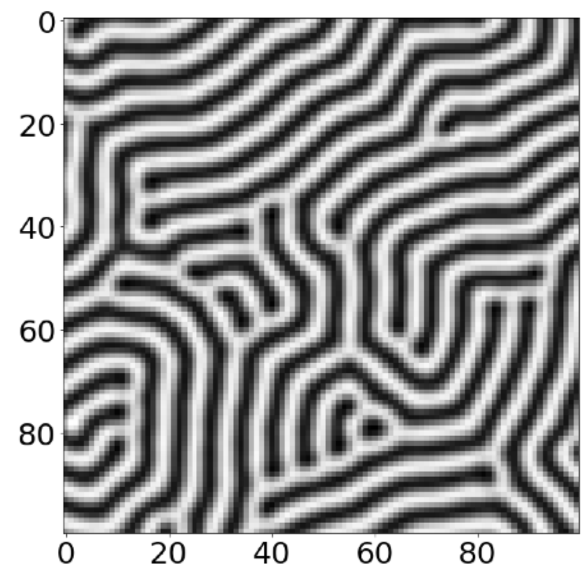
[Kazue Kudo, Michinobu Mino and Katsuhiro Nakamura 07]

2. Model of domain pattern formation

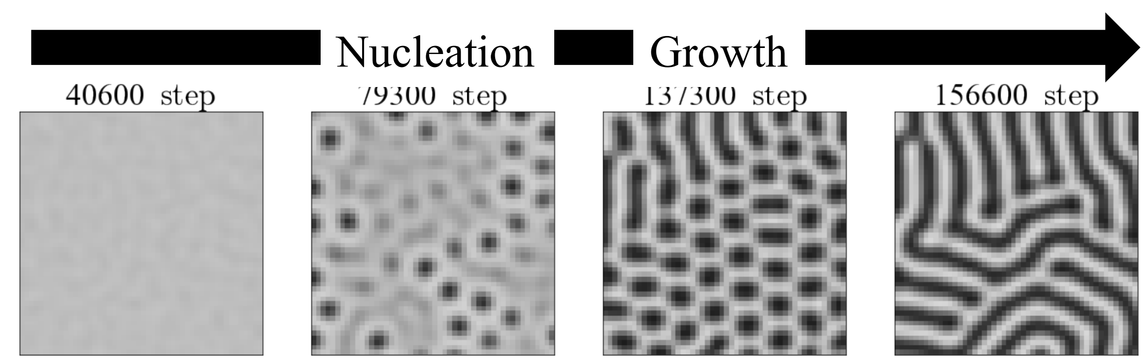
TDGL equation

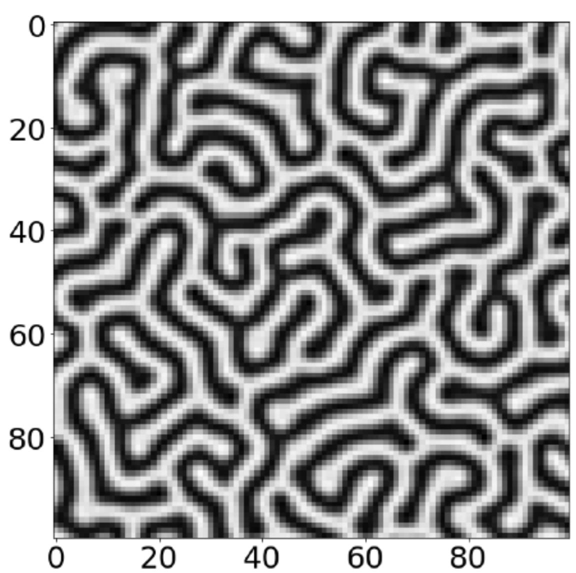


Sea island structure

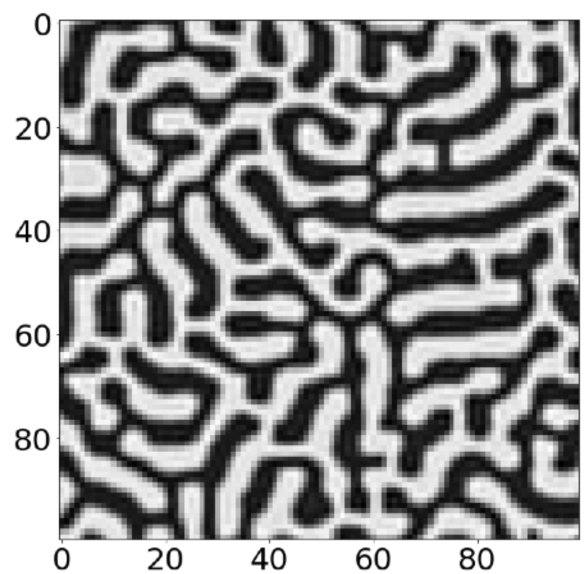


Labyrinth structure

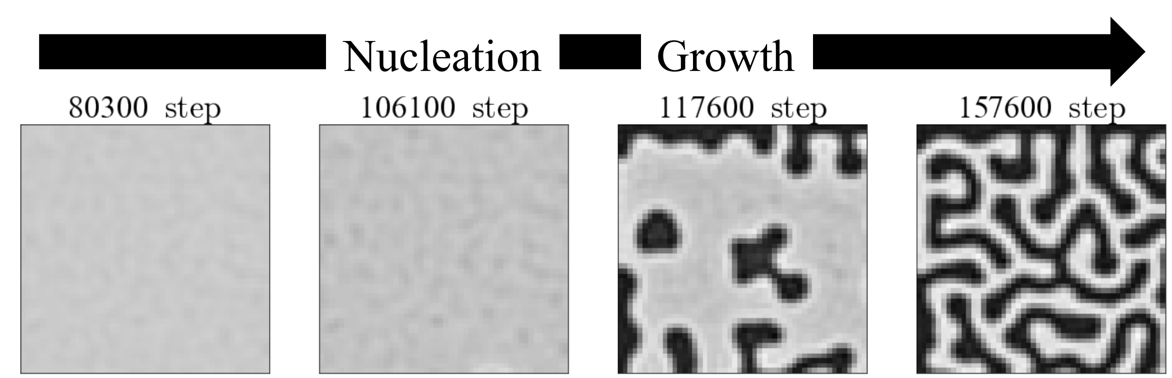




Labyrinth structure

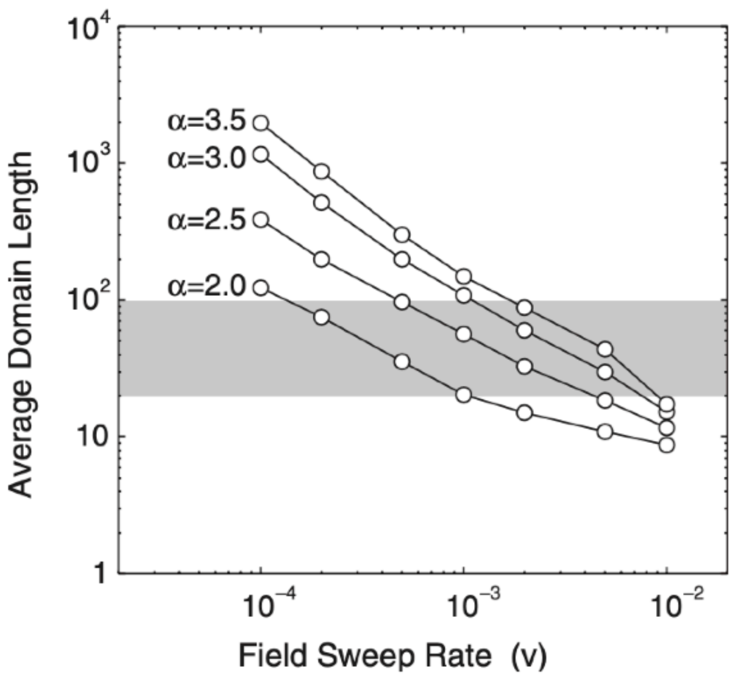


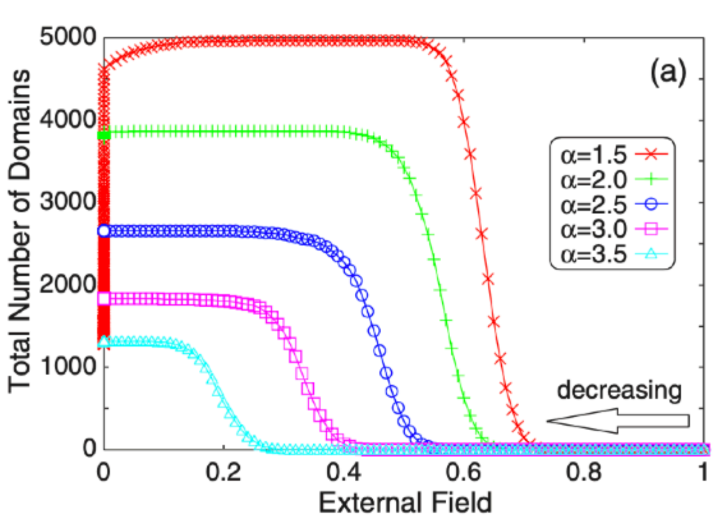
Labyrinth structure



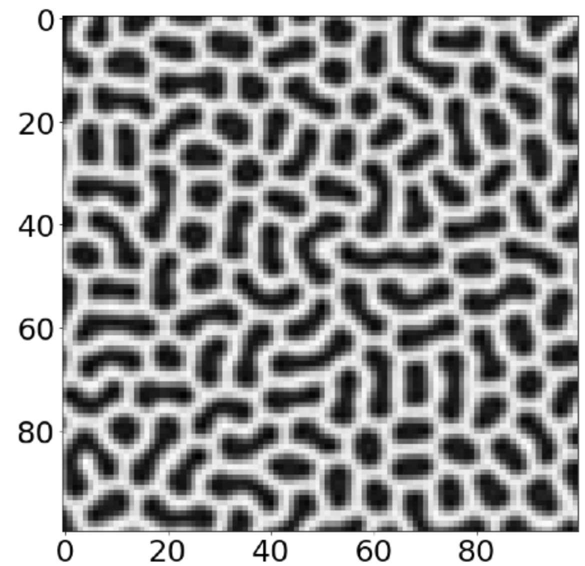
Domain pattern formation process

Results of TDGL:

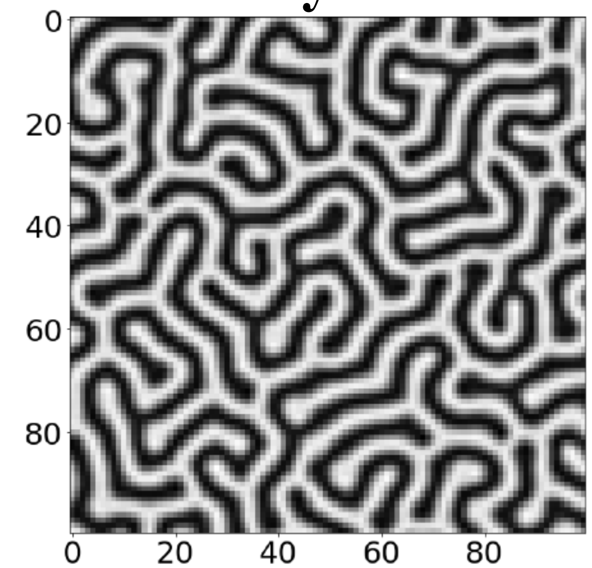




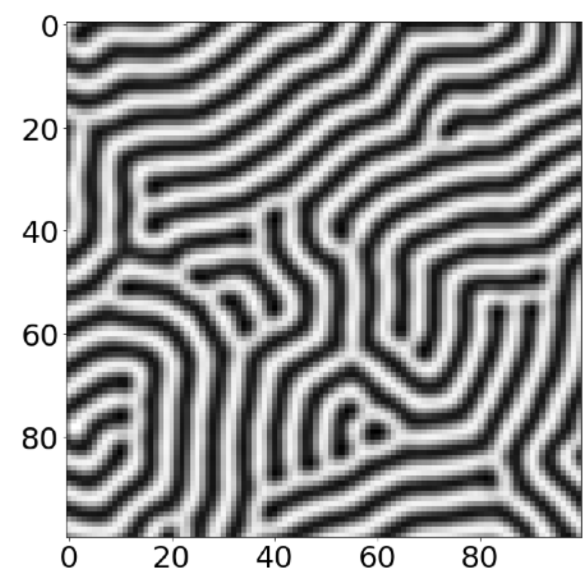
Sea island



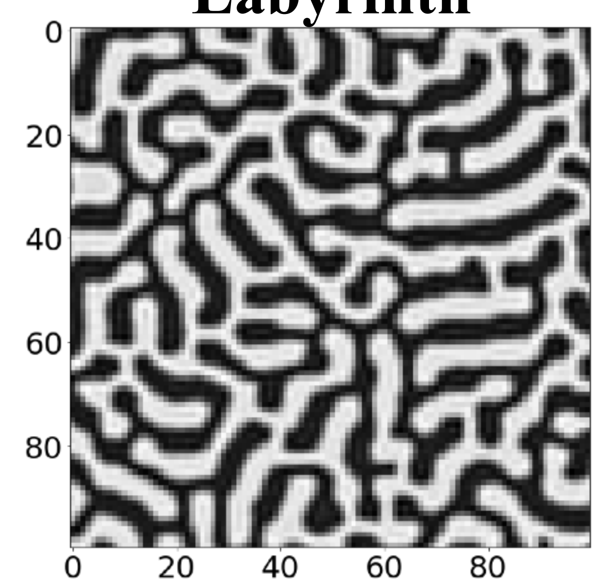
Labyrinth



Labyrinth



Labyrinth



[Kazue Kudo, Michinobu Mino and Katsuhiro Nakamura 07]

➡Isn't it necessary to analyze $\phi(r)$ as a continuous value?

Purpose of the study

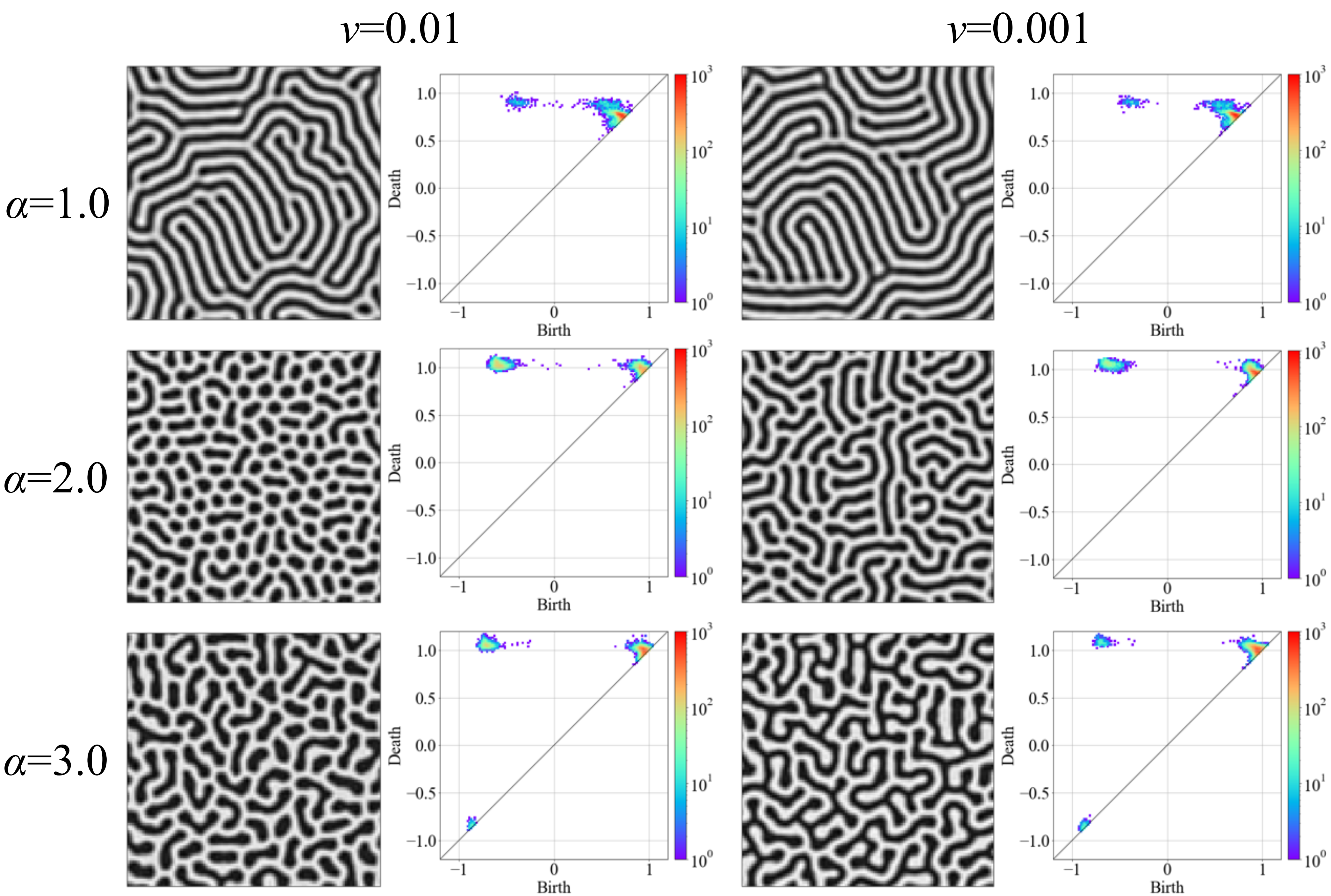
- From the topological feature of $\phi(r)$ where it is treated as a continuous value,

1. Can we do inverse estimation of model parameters?
2. Is there an unknown domain pattern class?
3. Can we obtain insight into the mechanism of the magnetic domain-pattern formation process?

3. Results

Result 1: Inverse estimation of model parameter

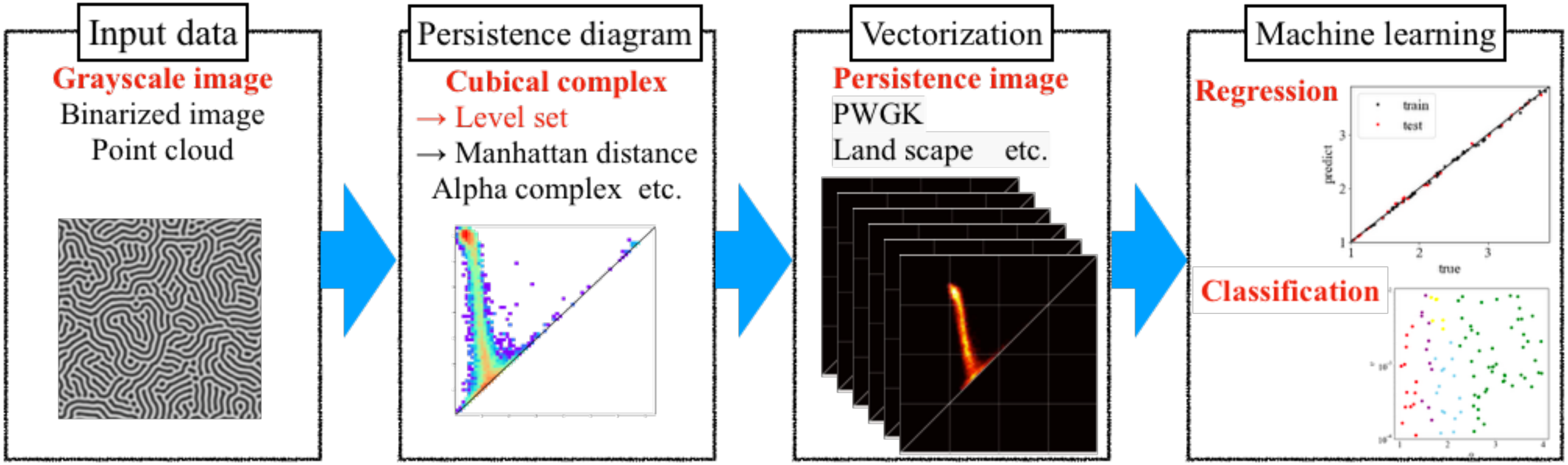
Result 1: Inverse estimation of model parameter



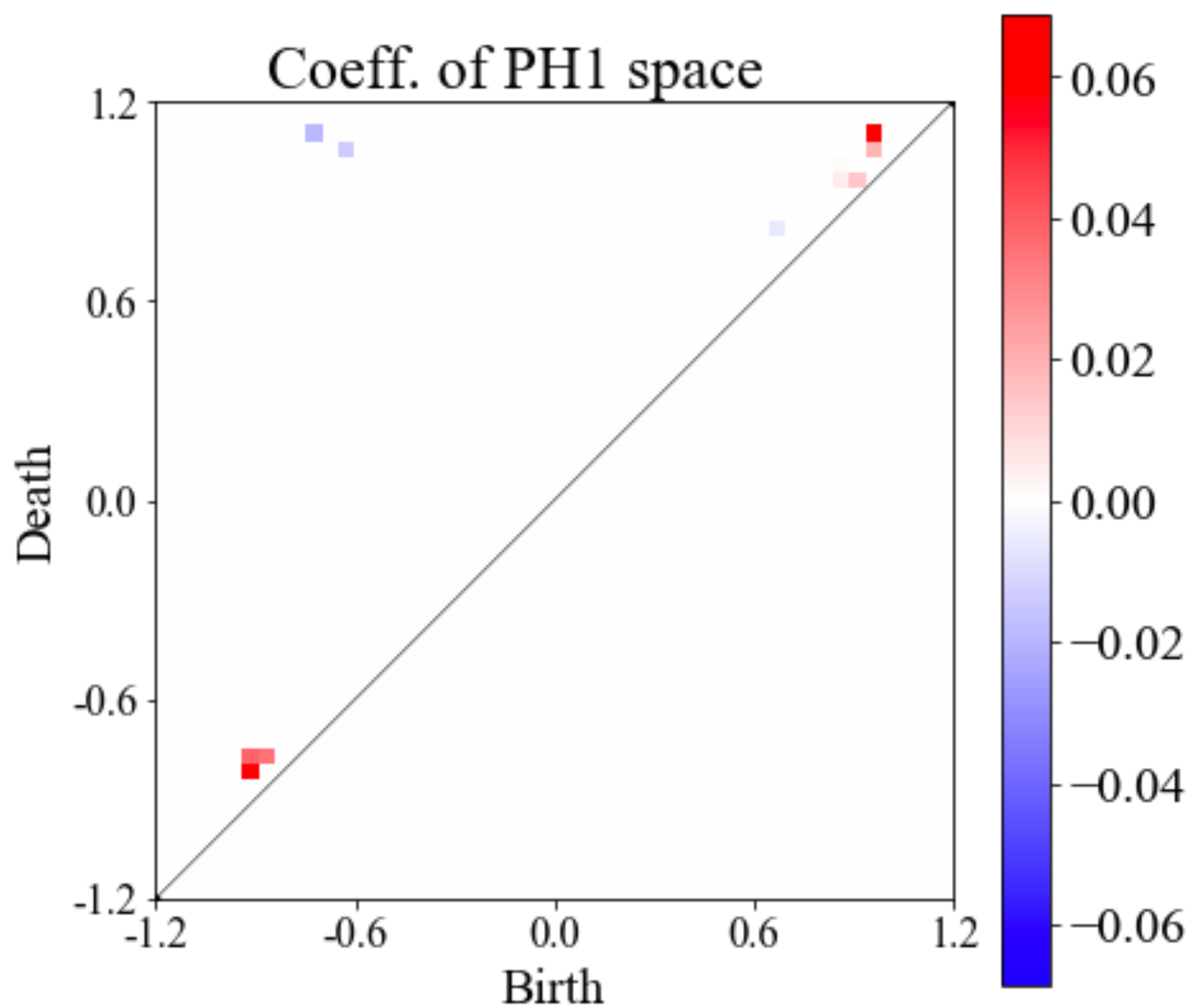
➡The PD is likely to be related to changes in patterns due to differences in α and v.

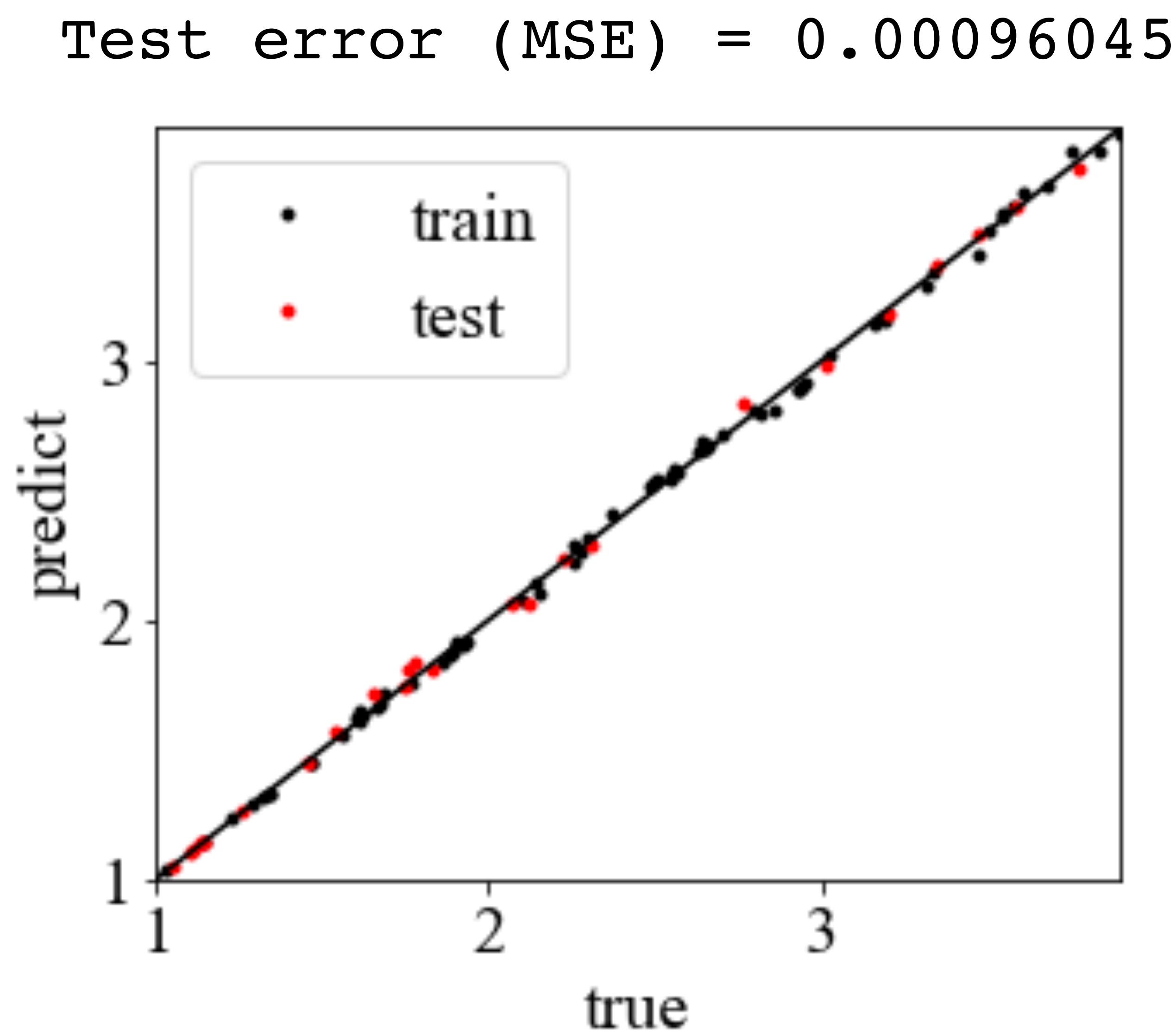
Result 1: Inverse estimation of model parameter

Analysis procedure of PD



Result 1: Inverse estimation of model parameter

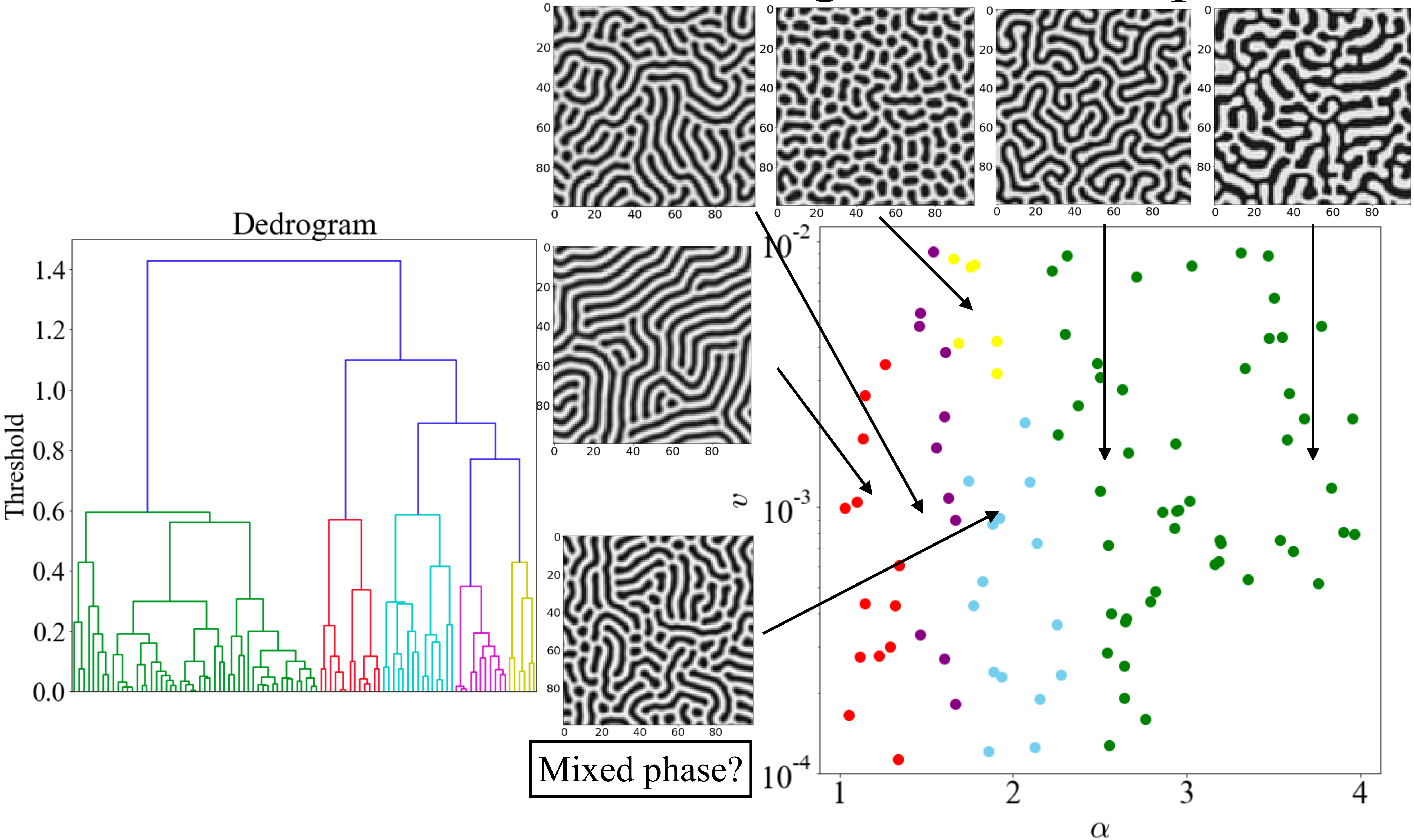




➡LASSO enabled regression with a very high predictive accuracy of α.
➡The three regions on the PD diagram contained the information needed for the regression.

Result 2: Classification of magnetic domain patterns

Result 2: Classification of magnetic domain patterns

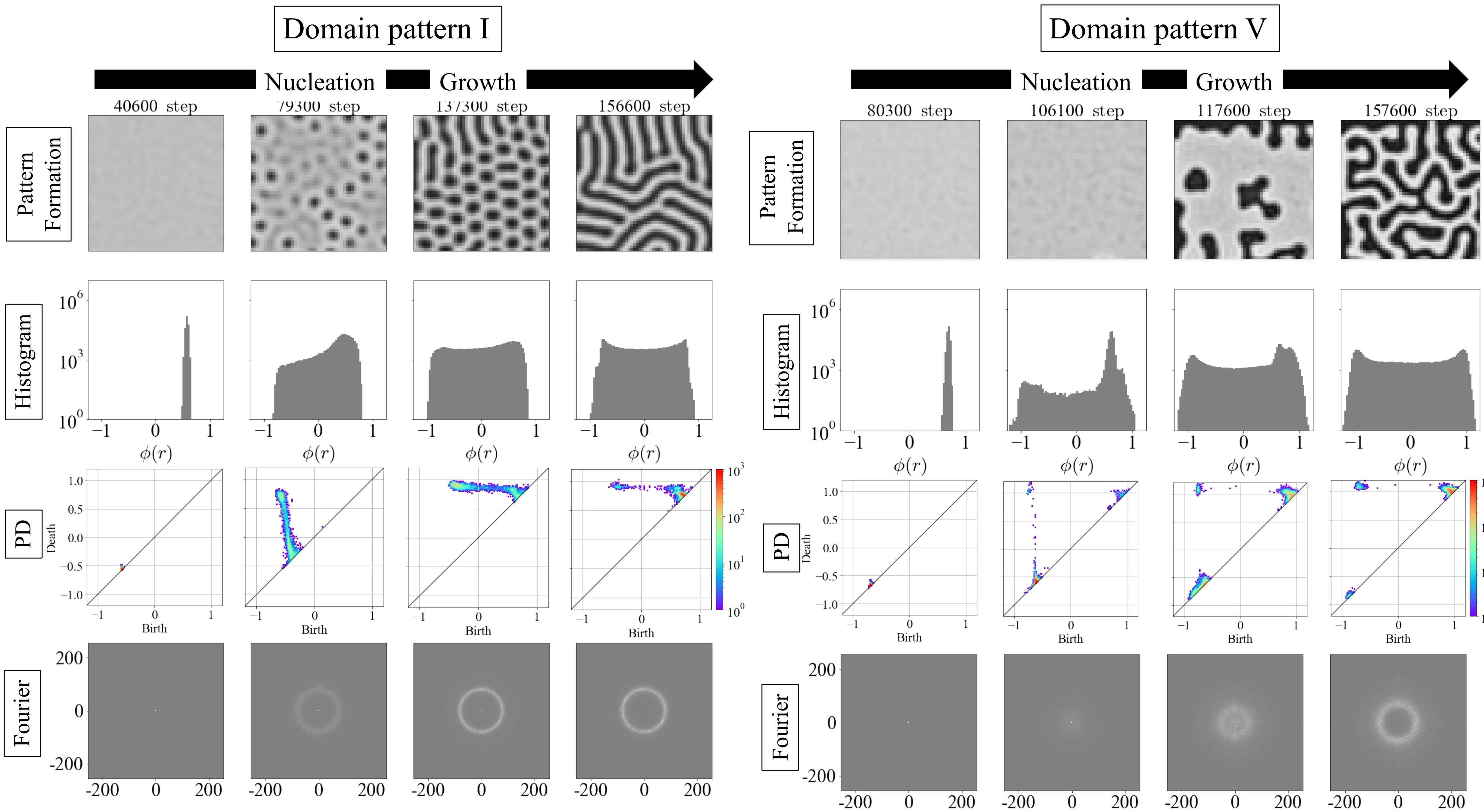


➡As the anisotropy α grows stronger, the pattern change to labyrinth → island (or mixed) →labyrinth.

Result 3: Analysis of the pattern formation process

Result 3: Analysis of the pattern formation process

Time evolution of PD about the domain formation process

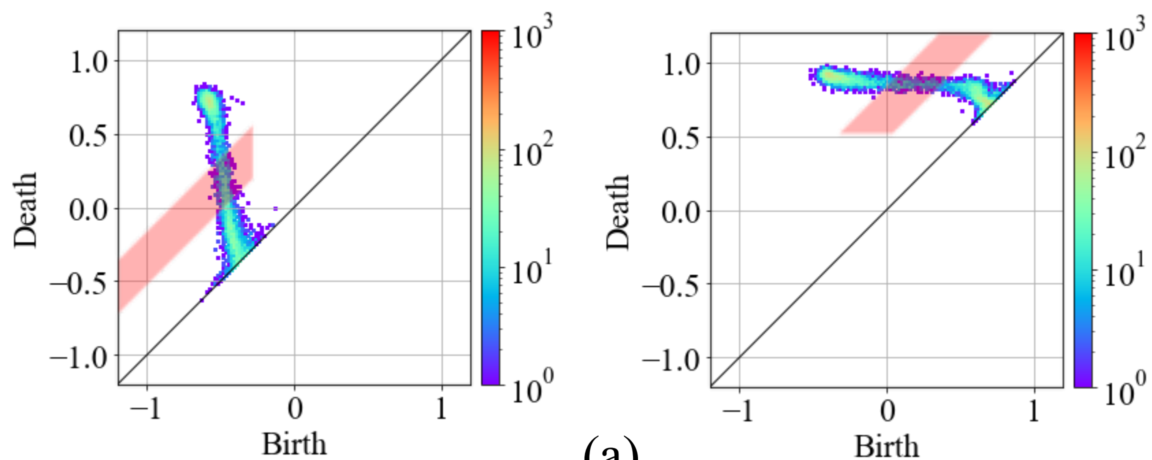


(a) (b)

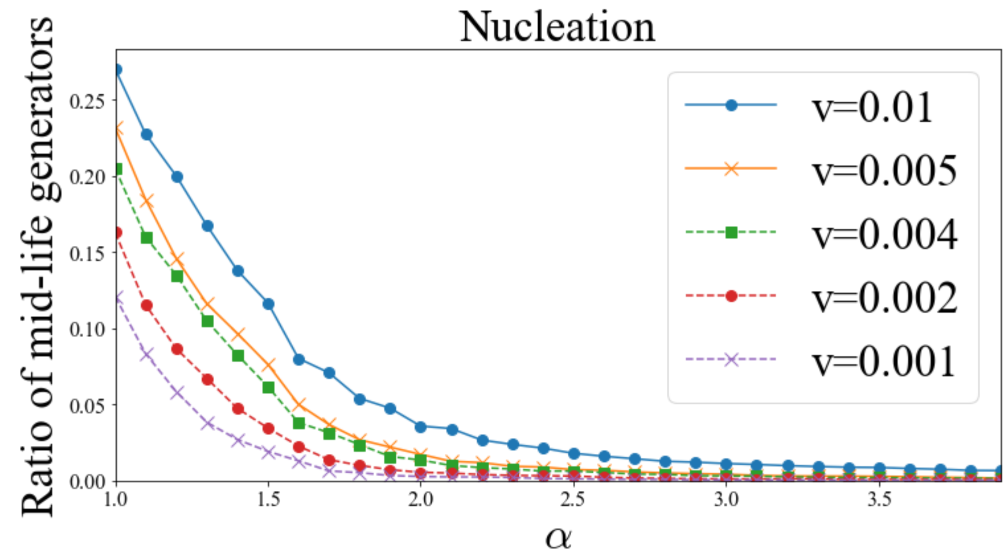
➡The process of domain formation in $\alpha = 1.0$ appears to take an intermediate state around the nucleation and its growth time.

Result 3: Analysis of the pattern formation process

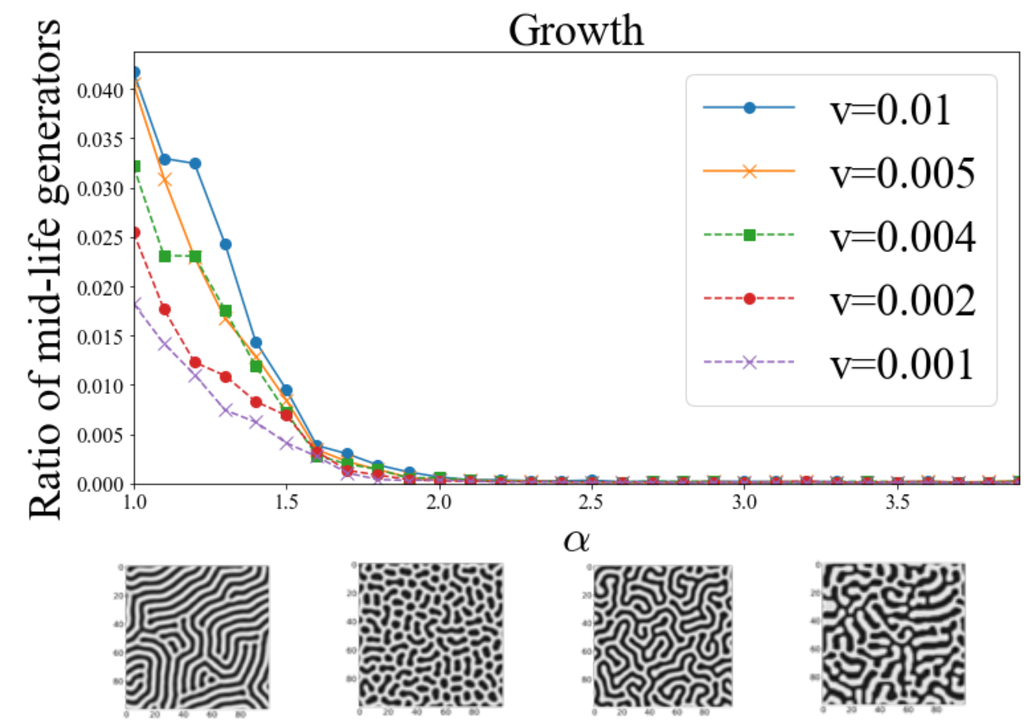
Evaluating the existence of the intermediate state by the ratio of the number of the generator in the **intermediate state** to the total number of generator



(a)



(b)



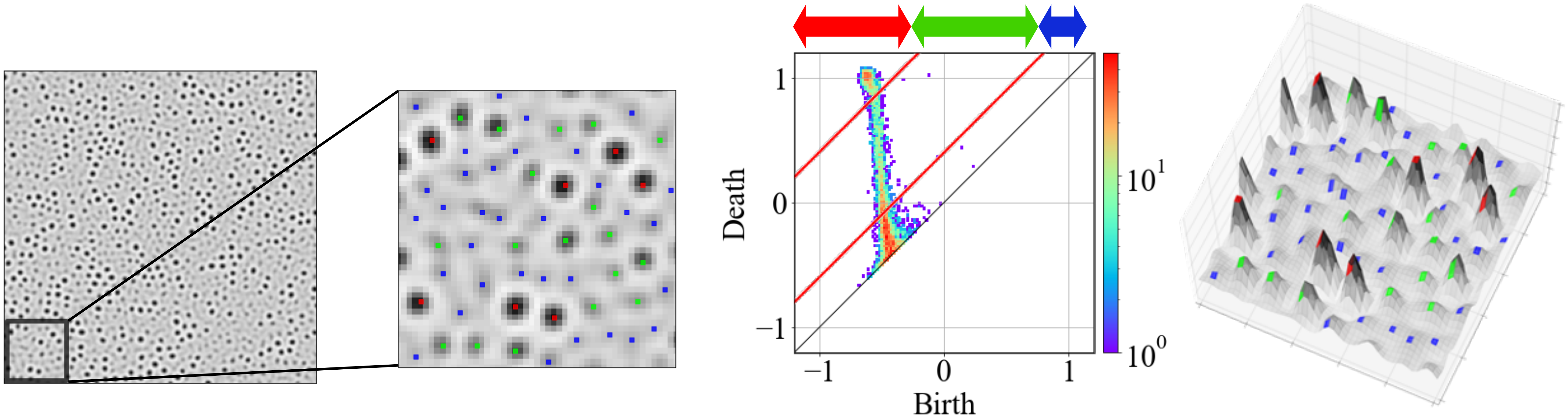
(c)

➡Around $\alpha = 2.0$, where the island structure is observed, the property of nucleation changes significantly.
And it is independent of the changing rate v of the external magnetic field.

3. Discussion

Inverse analysis

Death position of the hole

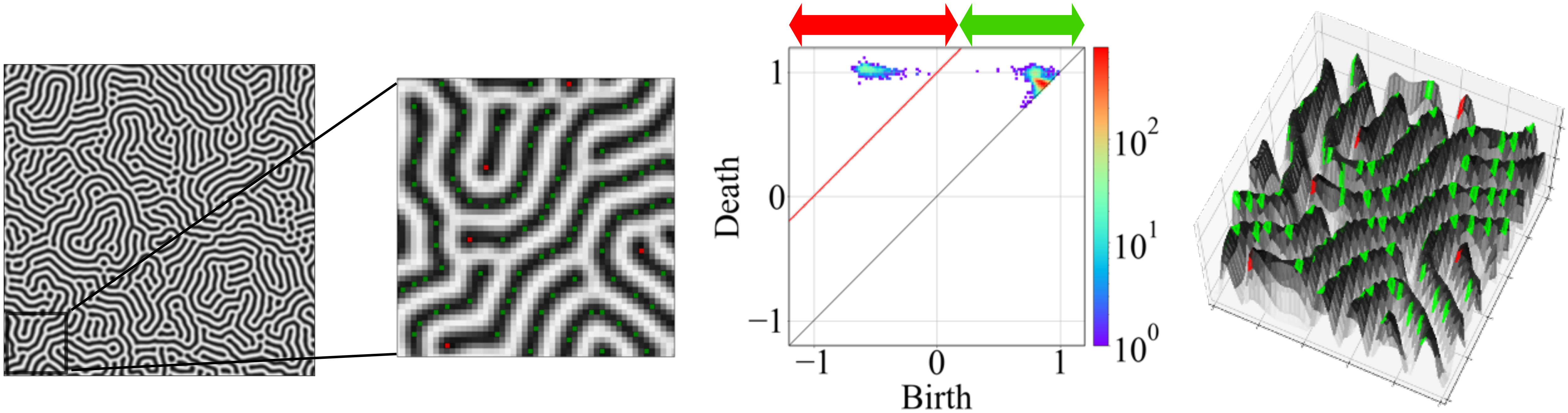


(a1) (a2) (a3)

Red: strong intensity peaks around 0.8 (= **Domain structure**)
Green: intermediate intensity peaks (= **Intermediate structure**)
Blue: weak intensity peak around 0.1 (= **Inter-domain structure**)

Inverse analysis

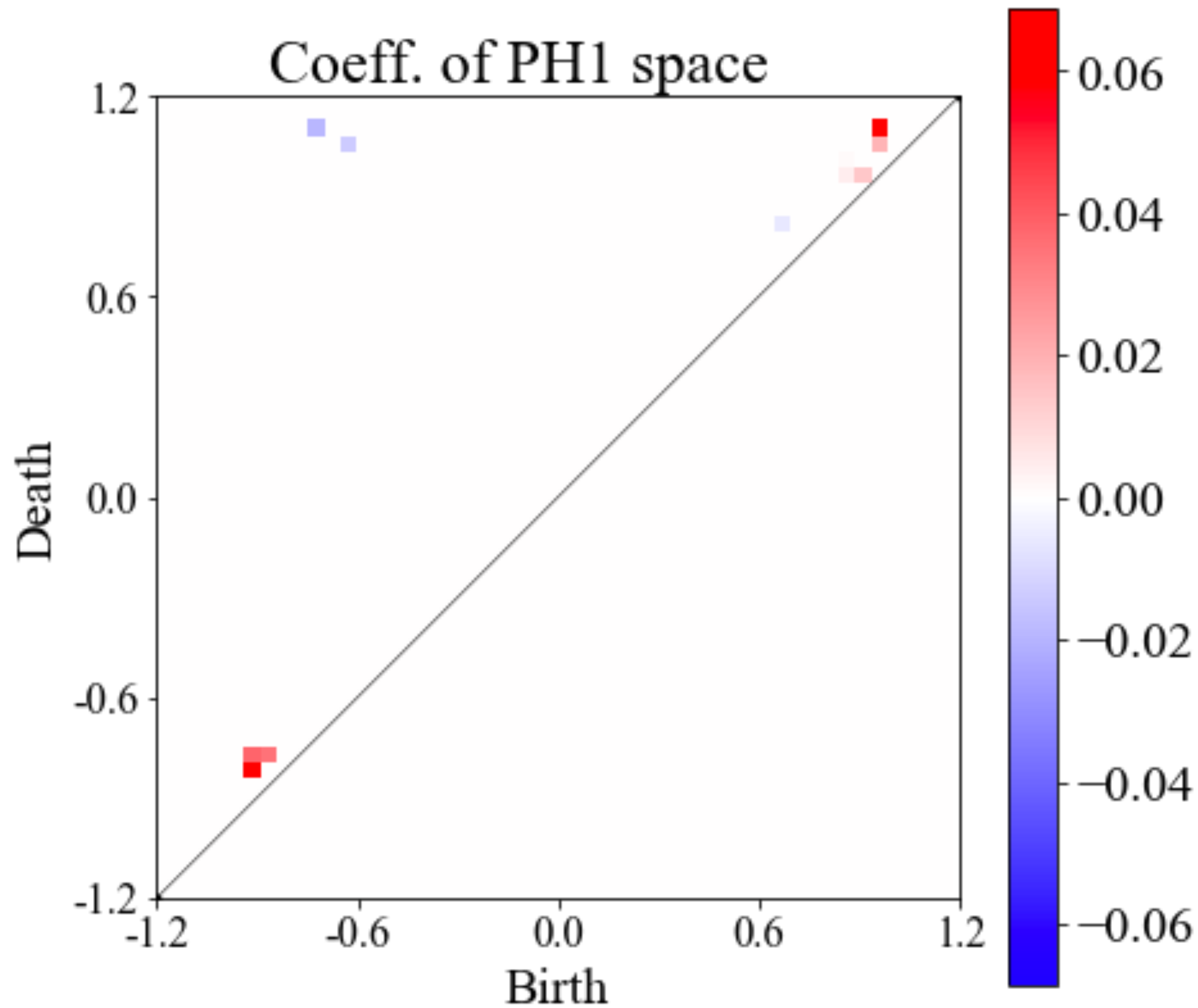
Death position of the hole

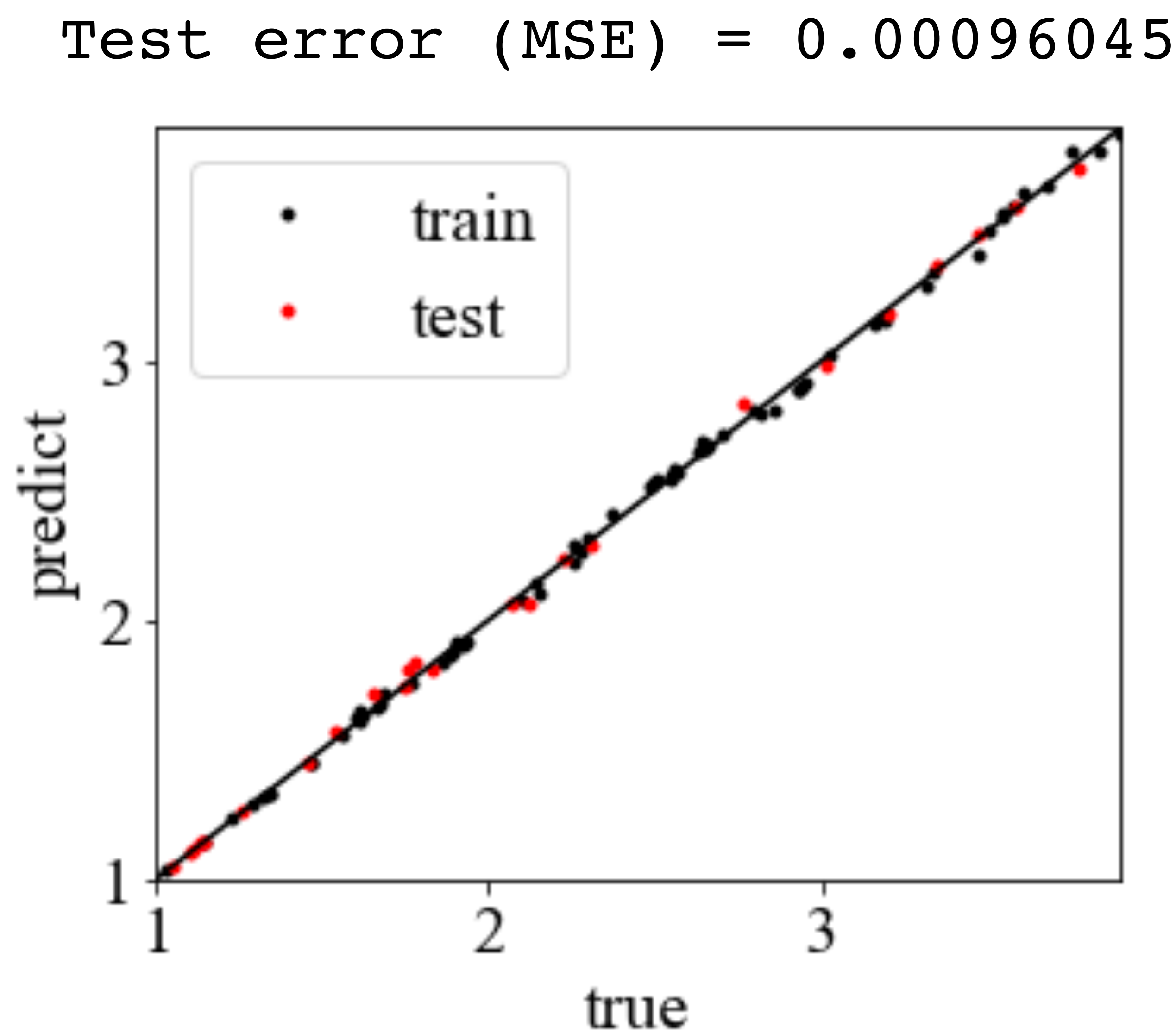


(b1) (b2) (b3)

The upper right area of the PD diagram corresponds to intra-domain fluctuations.

Interpret the obtained results

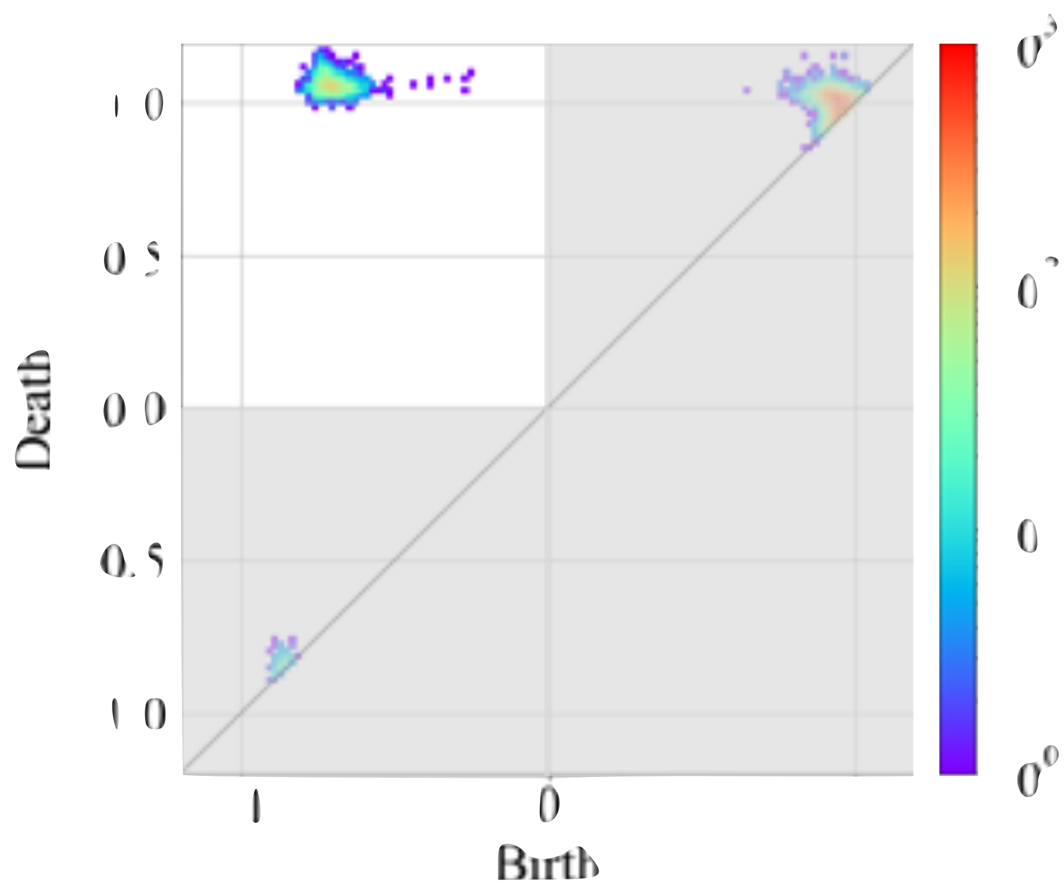




➡Do intra-domain fluctuations contain useful information for regression?

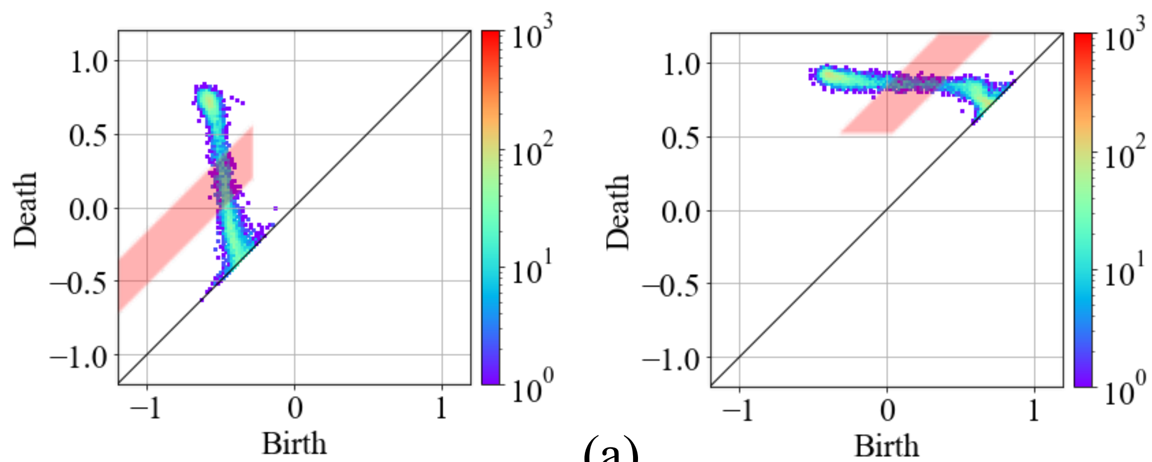
Interpret the obtained results

The effect of the internal structure of the domain

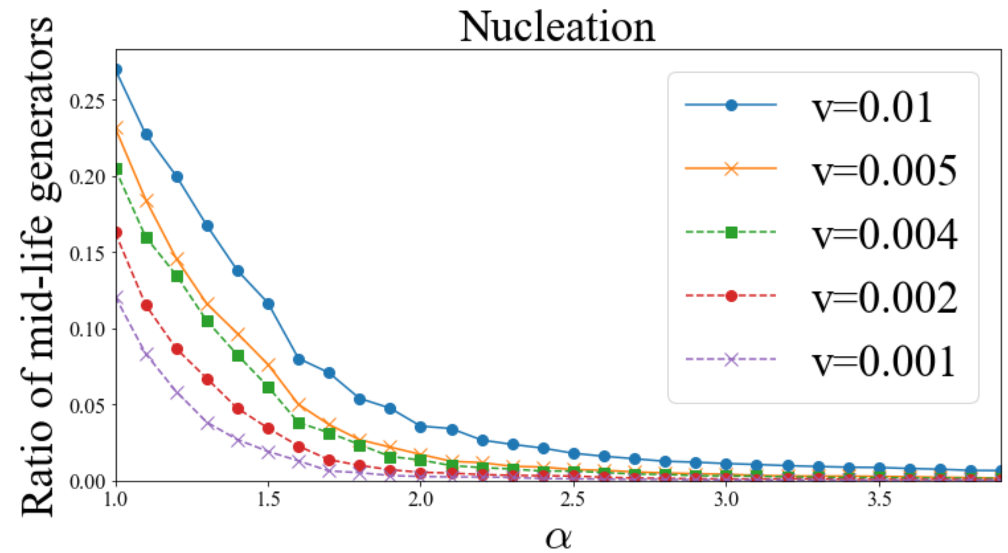


➡Erasing the information on the intra-domain structure greatly impaired the predictive accuracy of the regressions.

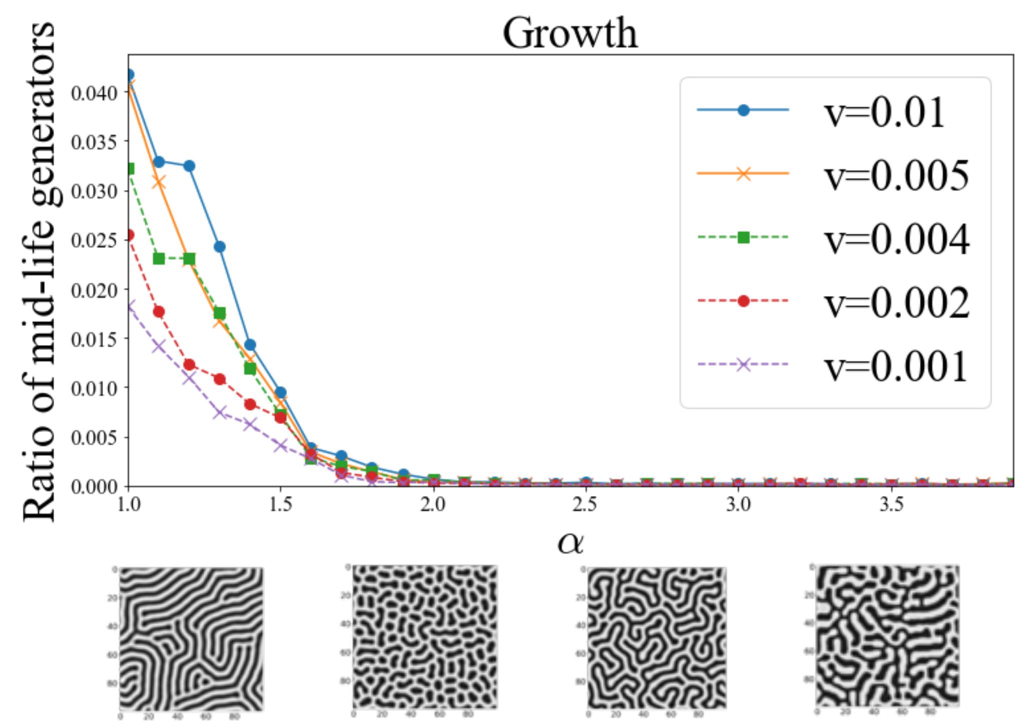
Interpret the obtained results



(a)



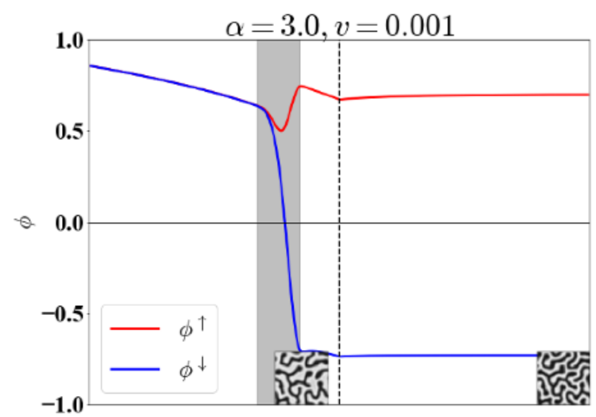
(b)

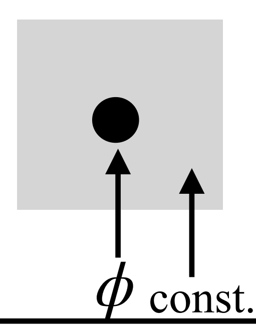


(c)

Interpret the obtained results

$$\frac{\partial\phi(\mathbf{r})}{\partial t} = -\frac{H}{\delta\phi(\mathbf{r})} = -\frac{\delta\left[\alpha\int d\mathbf{r}\lambda(\mathbf{r})\left(-\frac{\phi(\mathbf{r})^2}{2}+\frac{\phi(\mathbf{r})^4}{4}\right)+\beta\int d\mathbf{r}\frac{|\nabla\phi(\mathbf{r})|}{2}+\gamma\int d\mathbf{r}d\mathbf{r}'\phi(\mathbf{r})\phi(\mathbf{r}')G(\mathbf{r},\mathbf{r}')+-h(t)\int d\mathbf{r}\phi(\mathbf{r})\right]}{\delta\phi(\mathbf{r})}$$





$$\phi(\boldsymbol{r}) = \begin{cases} \phi & (\boldsymbol{r}\in D^{\downarrow}_{T_{\max}}) \\ C & (\boldsymbol{r}\in D^{\uparrow}_{T_{\max}}) \end{cases}$$

$$H(\phi(\boldsymbol{r})) = w_0(\beta) + w_1(\beta,\gamma,h(t))\phi + w_2(\alpha,\beta,\gamma)\phi^2 + w_4(\alpha)\phi^4$$

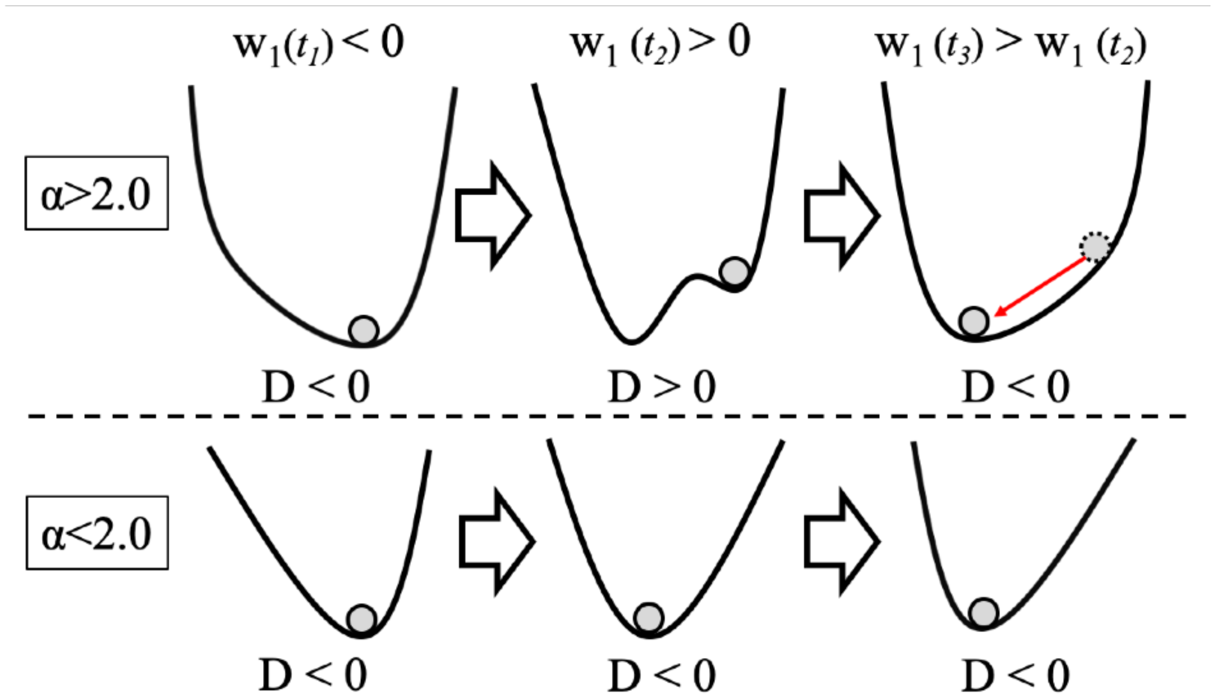
$w_1 \propto -h(t) \propto t,\ w_2 \propto -\alpha$、 $w_4 = \alpha S\lambda > 0$

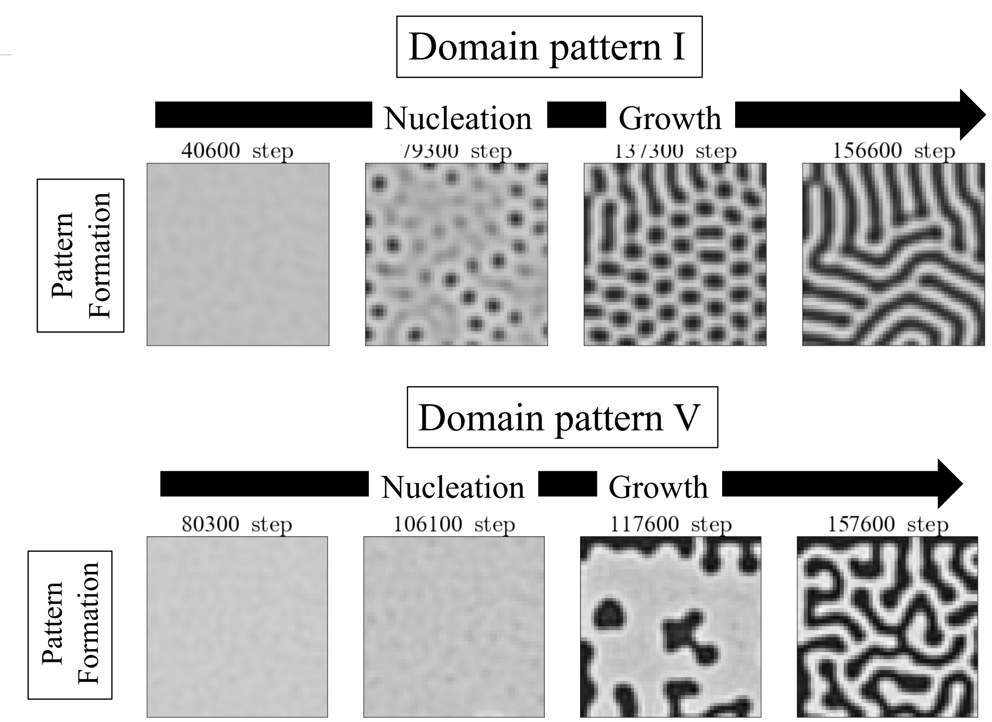
Interpret the obtained results

$$H(\phi(\boldsymbol{r})) = w_0(\beta) + w_1(\beta, \gamma, h(t))\phi + w_2(\alpha, \beta, \gamma)\phi^2 + w_4(\alpha)\phi^4$$

$$w_1 \propto -h(t) \propto t,\ w_2 \propto -\alpha、\ w_4 = \alpha S \lambda > 0$$

$$D = -\left(\frac{w_2(\alpha, \beta, \gamma)}{2w_4(\alpha)}\right)^3 - 27\left(\frac{w_1(\alpha, \beta, \gamma)}{4w_4(\alpha)}\right)^2$$

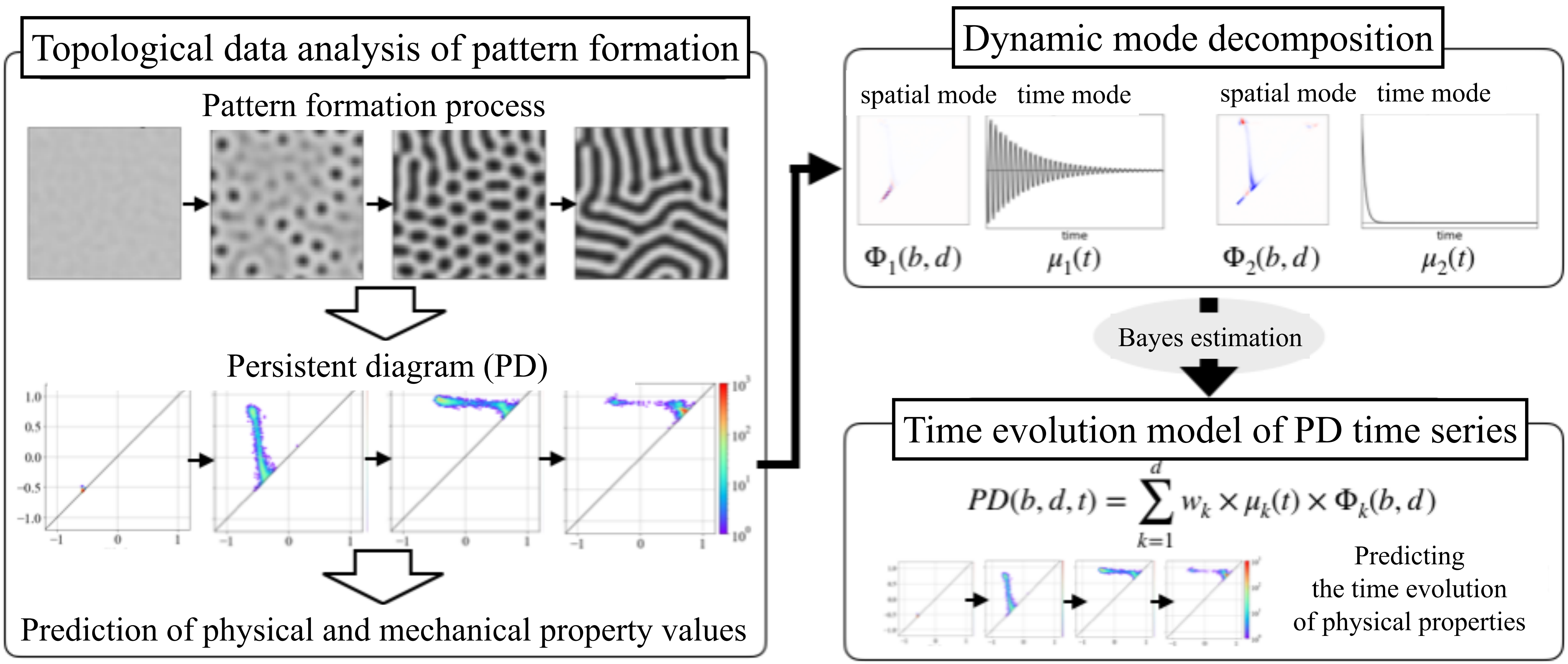




➡Differences in the time evolution of potential structures underlie the differences in the pattern formation process.

Model the time evolution of PD

Toward the modeling of the time evolution of PD



It seems possible to model time evolution by dynamic mode decomposition.

4. Summary

Summary

From the analysis of magnetic domain structure using persistent homology:

- Achieved high predictivity of material property value.(also found that the intradomain structure improves the estimation accuracy)
- Reasonably classify the domain patterns.
- Found the differences in the mechanisms of the domain formation process and model the mechanism.
- It could be possible to model the dynamics in the feature space of PD.

This research continue to be developed into the following project:

さきがけ PRESTO

PRESTO SAKIGAKE

“Extraction of mathematical structure of pattern dynamics by interpretable AI and its application to material informatics”
「解釈可能 AI によるパターンダイナミクスの 数理構造抽出と材料情報学への応用」

Research 4

Topological data analysis of microdomain patterns of block copolymer

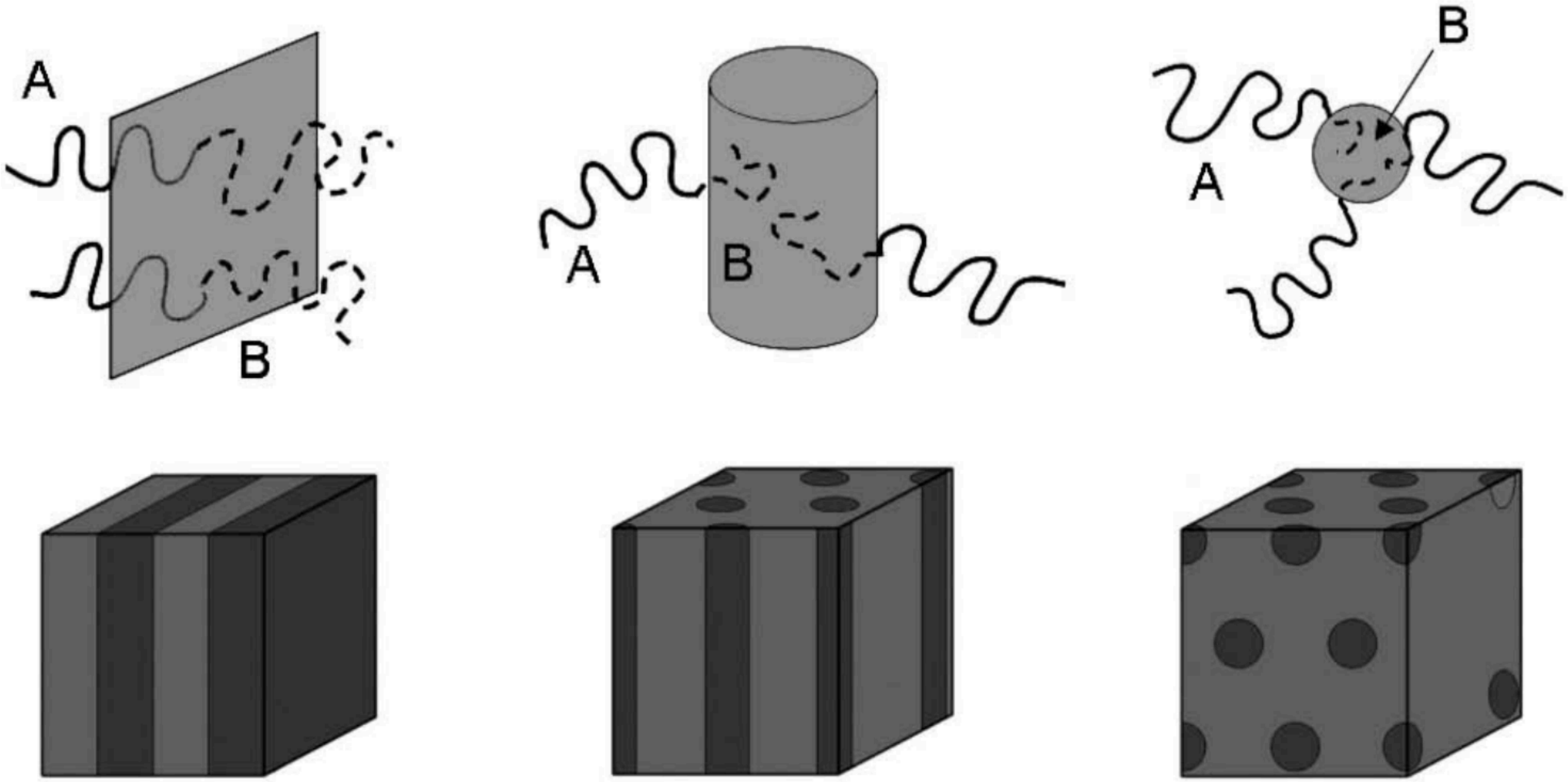
Yoh-ichi Mototake*, Sadato Yamanaka**, Takeshi Aoyagi**,
Takaaki Ohnishi*** and Kenji Fukumizu*

*The Institute of Statistical Mathematics,
** National Institute of Advanced Industrial Science and Technology (AIST),
***Rikkyo University

1. Background

Microphase separation structure

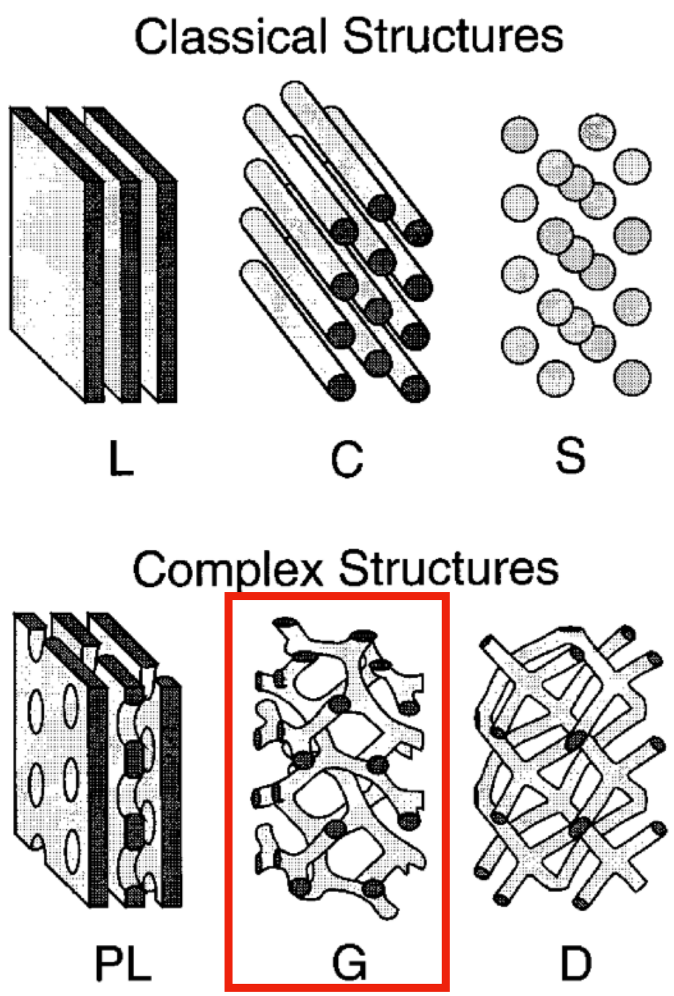
- A structure formed by the attracting and repulsive force between substructures of one polymer.



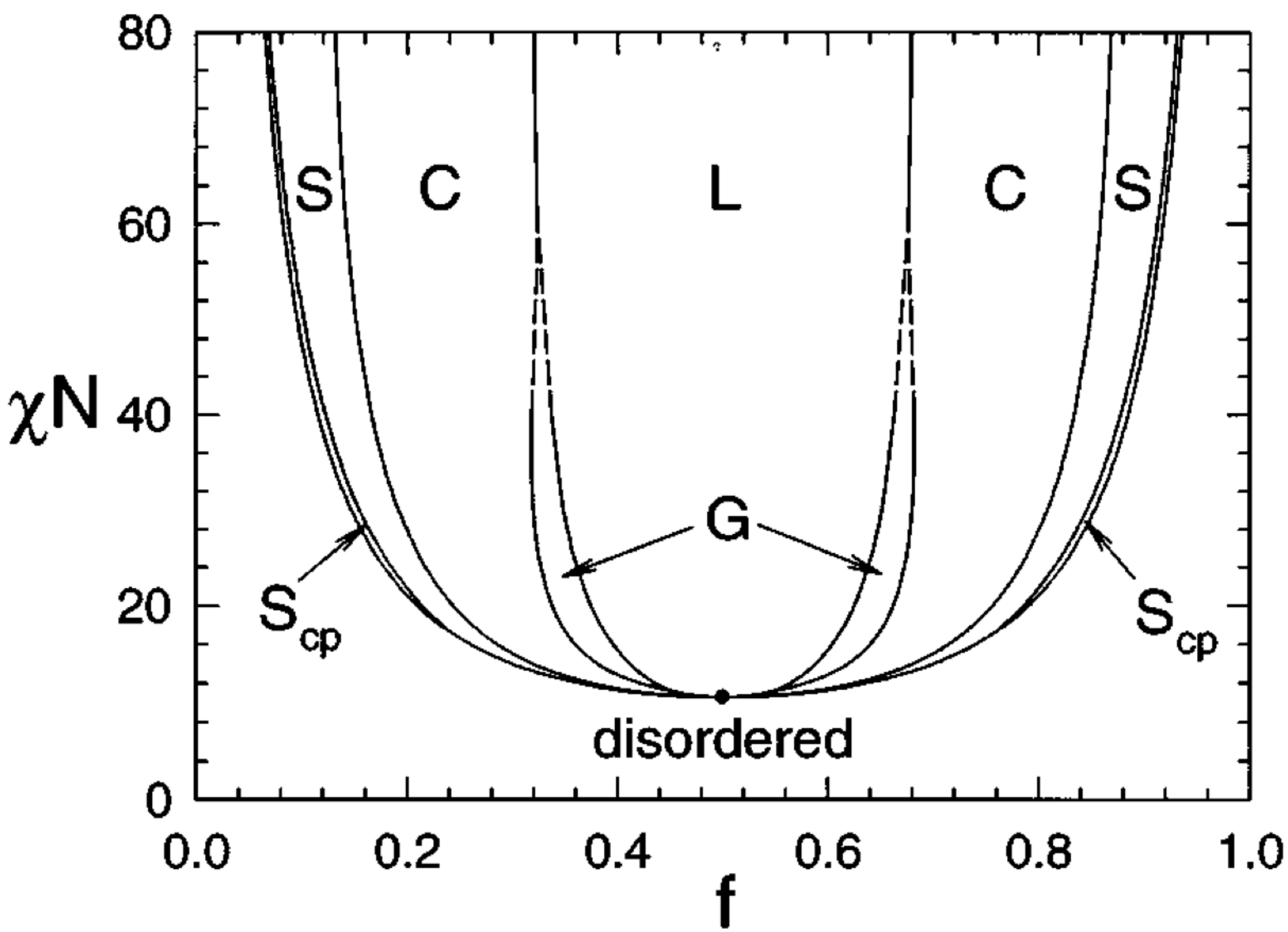
[Yushu Matsushita, Materia Japan, 48.2, 2009]

Microphase separation structure

- Forming microphase separation structure



Intersegment repulsion interaction strength



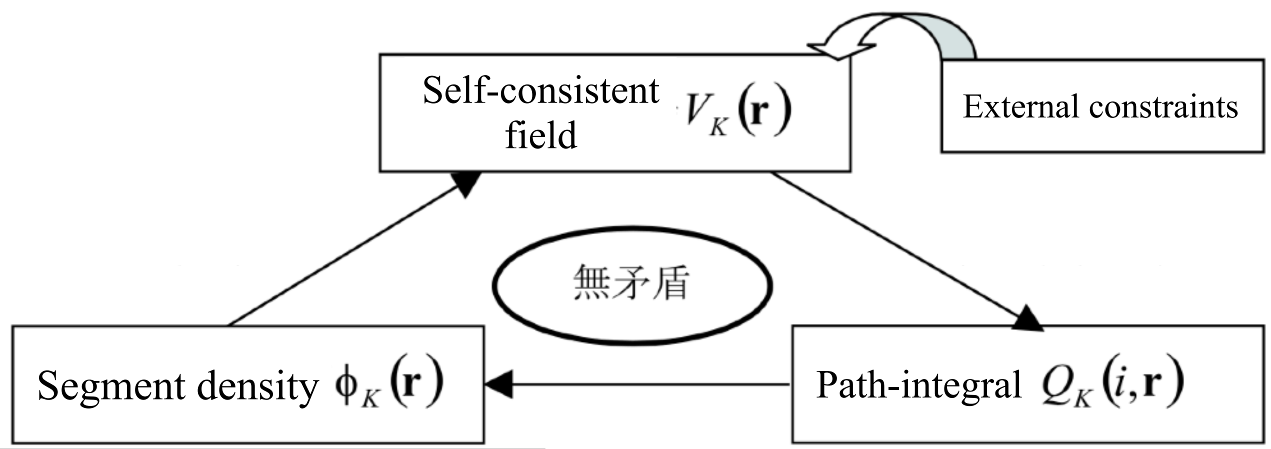
Ratio of A phase

[M. W. Matsen and F. S., J. Chem. Phys. 106, 2436 (1997)]

2. Pattern formation model

Self-consistent field theory

Pattern estimation of block copolymers using "self-consistent field theory"



(2.17) 式

[K. M. Hong and J. Noolandi, Macromolecules 1981, 14, 727-736]

[E. Helfand and Z. R. Wasserman, Macromolecules, 9,879, 1976]

Simulated by

SUSHI [SIMULATION UTILITIES FOR SOFT AND HARD INTERFACES]

[Japan Association for Chemical Innovation, "Computer simulation of polymeric materials: Application of the OCTA system," Springer, Singapore, Imprint:Springer, 2016]

$$F\left[\{\phi_k\},\{V_k\}\right] = -k_bT\sum_p M_p \ln Z_p + w\left[\{\phi_k(\mathbf{r})\}\right] - \sum_k \int d\mathbf{r} V_k(\mathbf{r})\phi_k(\mathbf{r}) + k_BT\sum_p M_p \ln M_p$$

Configuration entropy of molecular chains | **Interaction between segments** | **constraint condition** | **mixing entropy**

[Honda, Takashi, and Toshihiro Kawakatsu. "Computer Simulations of Nano-Scale Phenomena Based on the Dynamic Density Functional Theories: Applications of SUSHI in the OCTA System." *Nano structured Soft Matter*. Springer, Dordrecht, 2007. 461-493.]

2. Pattern formation model

Self-consistent field theory

$$F\left[\{\phi_k\},\{V_k\}\right] = -k_bT\sum_p M_p \ln Z_p + w\left[\{\phi_k(\mathbf{r})\}\right] - \sum_k \int d\mathbf{r} V_k(\mathbf{r})\phi_k(\mathbf{r}) + k_BT\sum_p M_p \ln M_p$$

Configuration entropy of molecular chains | **Interaction between segments** | **constraint condition** | **mixing entropy**

M_p :Total number of partial polymer chains p

k :index of segments

$\epsilon_{kk'}$:intersegment interaction energy

$\mu(\mathbf{r})$:Potential for uncompressed condition

$$\chi_{kk'} := z\beta\left[\epsilon_{kk'} - \frac{1}{2}(\epsilon_{kk} + \epsilon_{k'k'})\right]$$

→Flory's χ parameter

$$Z_p := \sum_{\text{all conformation of chain}} \exp\left[-\beta \sum_{\text{all segment } i} V_{k(i)}(\mathbf{r}_i)\right]$$

$$w\left[\{\phi_k\}\right] := \frac{1}{2}\sum_k\sum_{k'}\int d\mathbf{r}\,\epsilon_{kk'}\phi_k(\mathbf{r})\phi_{k'}(\mathbf{r})$$

$$V_k(\mathbf{r}) := W_k(\mathbf{r}) + \mu(\mathbf{r})$$

$\mu(\mathbf{r})$: Potential field representing the constraints

$$W_k(\mathbf{r}) := \sum_{k'} \chi_{kk'}\phi_{k'}(\mathbf{r})$$

→Mean Field Potential for intersegment interactions

Double gyroid structure

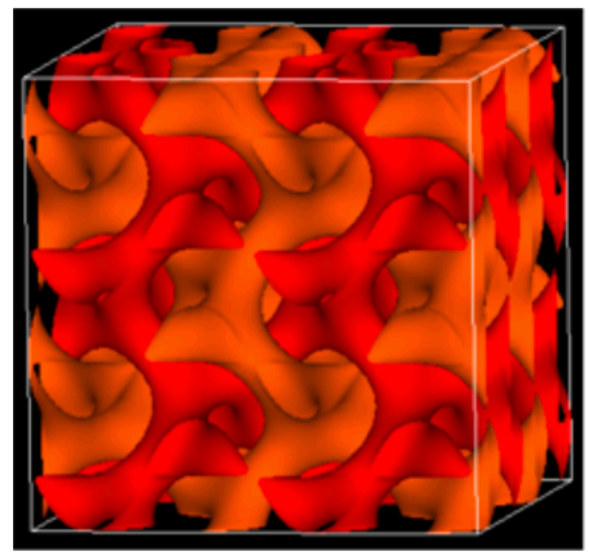


Figure: by Drs. Aoyagi and Yamanaka

[Importance of block copolymer structure]

To understand the self-organization of polymers.

Application for the polymer battery .

Application for the Surfactant .

Etc…

[Shinichi Yamazaki, Lecture note of Okayama Univ.]
[Wikipedia]

Double gyroid structure

The free energy landscape of double gyroid has a large number of **metastable** states.

→Elucidating the relationship between those metastable states and geometric features of the structure will help us **understand the physical mechanisms of the double-gyroid system.**

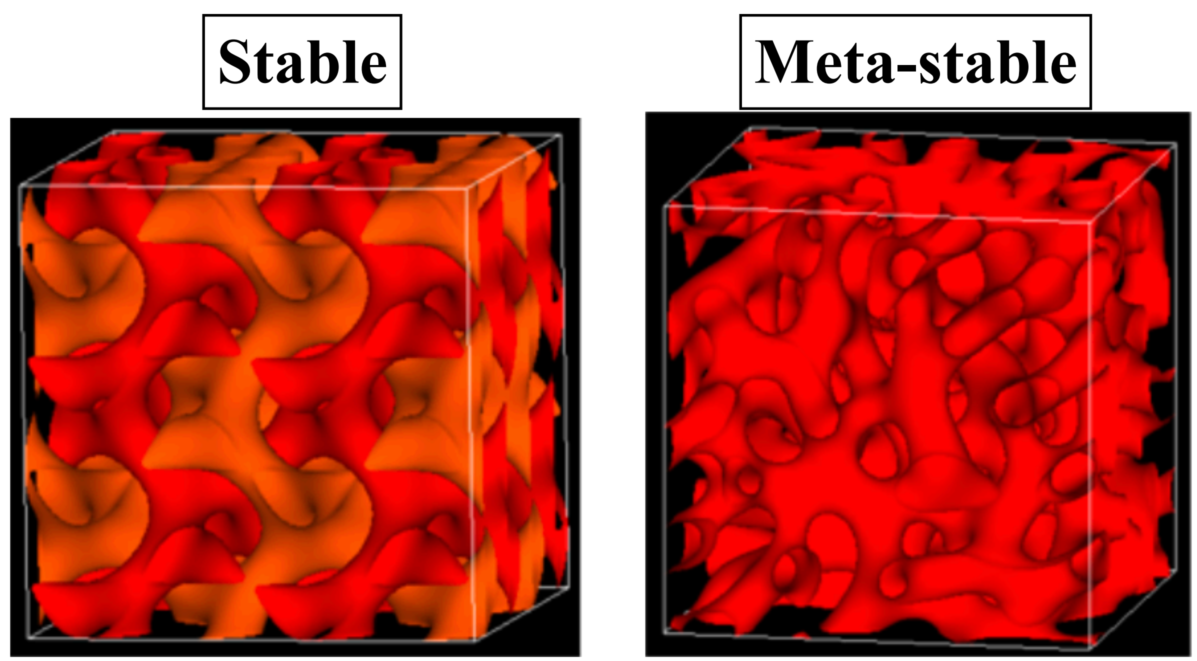


Figure: by Drs. Aoyagi and Yamanaka

Finding structural features characterizing metastable states in double gyroid systems
= Find **predictable structural features for the free energy** of meta-stable states

Minkowski functionals (MFs)

If the boundary ∂B of the body B is sufficiently smooth, for convex bodies the Minkowski functionals can be also written in the following form:

体積 $V(B) = \int_B d\lambda^{(3)}(x)$

表面積 $A(B) = \int_{\partial B} d\lambda^{(2)}(x)$

平均曲率 $M(B) = \int_{\partial B} H(x)\, d\lambda^{(2)}(x)$ (5)

オイラー数 $C(B) = \frac{1}{4\pi} \int_{\partial B} G(x)\, d\lambda^{(2)}(x)$

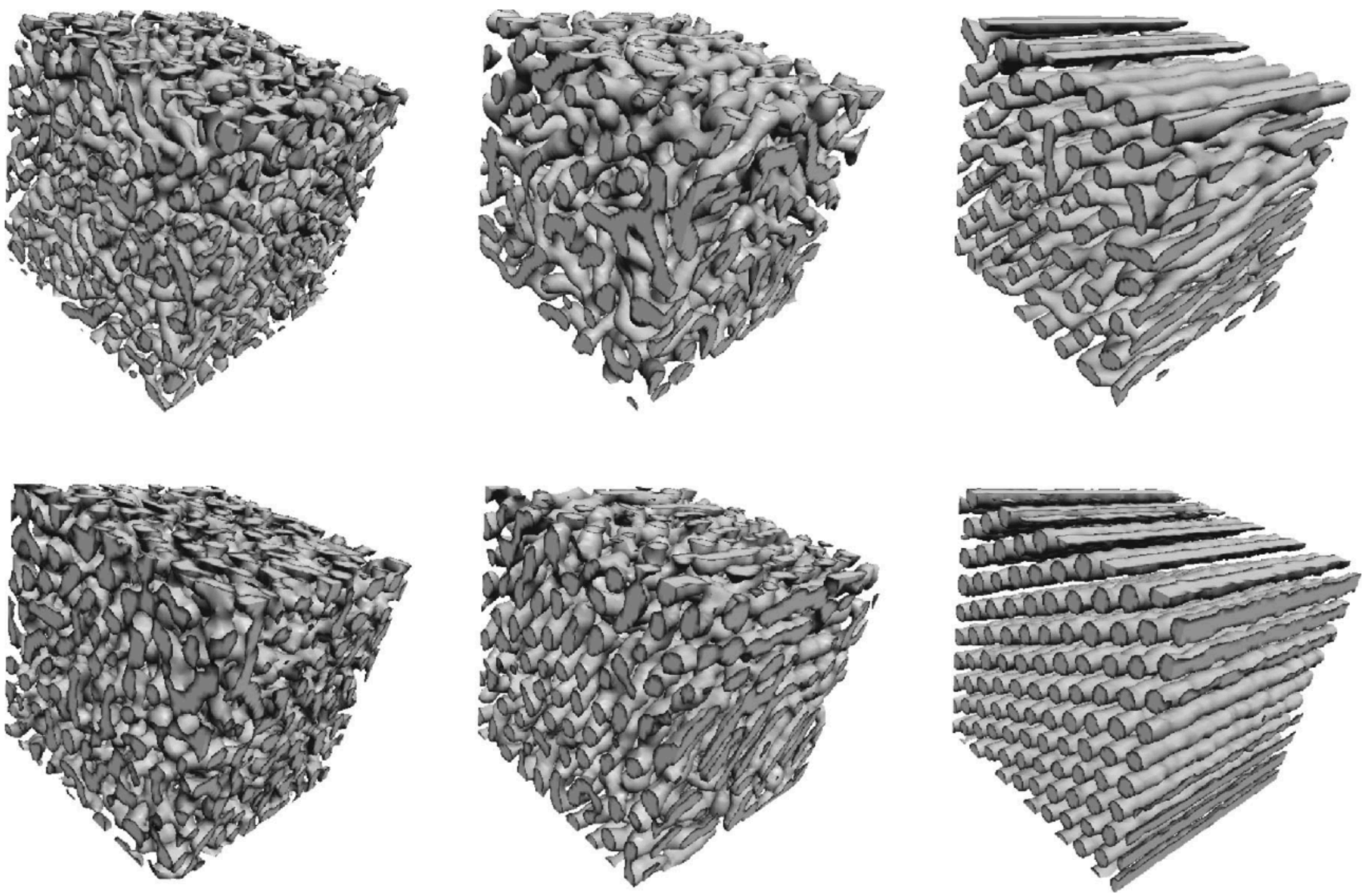
In these formulae $\lambda^{(3)}$ and $\lambda^{(2)}$ are the usual Lebesgue measures in the 3- and 2-dimensional space, measuring the volume of 3D objects and the area of 2D objects, respectively. Using the local principal radii of curvature R_1 and R_2, H and G are the local mean curvature and Gaussian curvature defined as

$$H(x) = \frac{1}{2}\left(\frac{1}{R_1(x)} + \frac{1}{R_2(x)}\right) \quad G(x) = \frac{1}{R_1(x)} \frac{1}{R_2(x)}. \qquad (6)$$

→Minkowski functionalによるブロックコポリマー の分析

G. J. A. Sevink and A. V. Zvelindovsky , The Journal of Chemical Physics 121, 3864 (2004)
G. J. A. Sevink and A. V. Zvelindovsky, Macromolecules 38, 7502-7513 (2005)
G. J. A. Sevink and A. V. Zvelindovsky, Mol. Sim. 33, 405-415 (2007)
M. Pinna, A. V. Zvelindovsky, S. Todd and G. Goldbeck-Wood, J. Chem. Phys. 125, 154905 (2006)

Minkowski functionals (MFs)



[G. J. A. Sevink and A. V. Zvelindovsky , The Journal of Chemical Physics 121, 3864 (2004)]

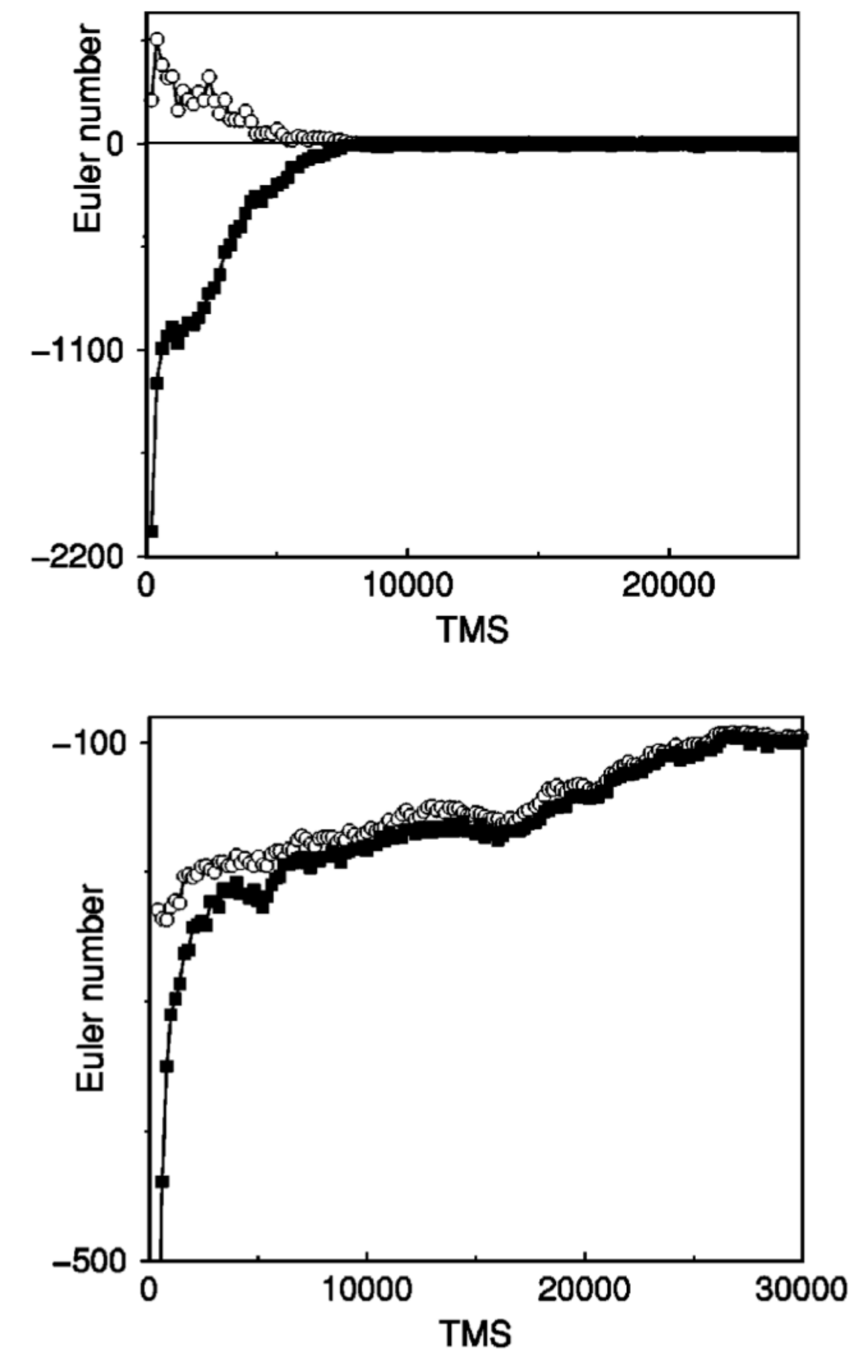


FIG. 4. The Euler characteristic as a function of time for the cylinder forming component in the solution (top) and in the melt (bottom). The shear was applied starting from TMS = 0. The Euler characteristics were calculated for two choices of the threshold parameter: $h=\rho^0$ (○), and an arbitrary one, $h=0.5$ (■).

Research Purpose

Find the geometrical features which characterize the metastable state of the double gyroid structure better than MFs.

OBJECTIVE: To characterize the **metastable states** of double gyroid structures using **persistent homology** and estimate the free energy.

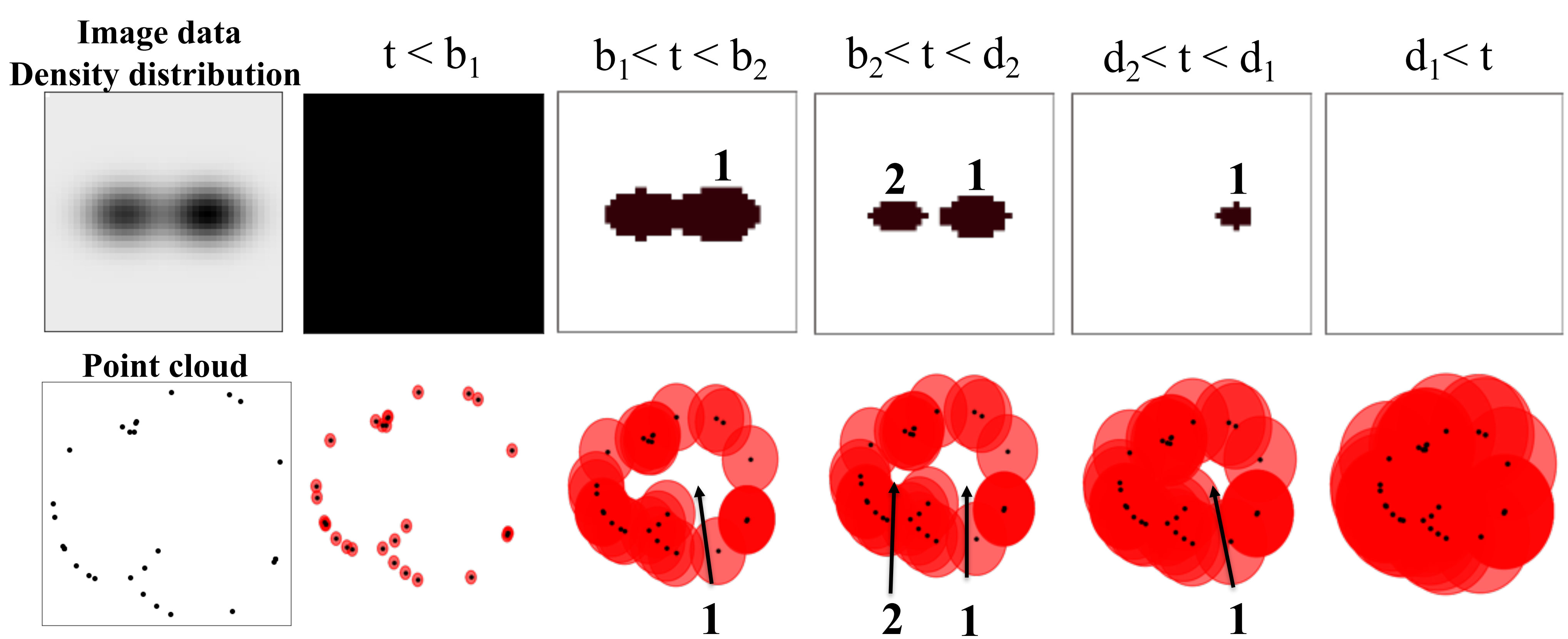
2. Analysis Method

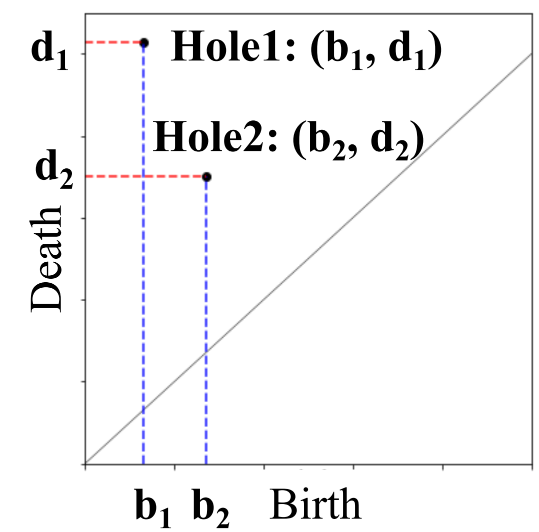
Calculation of Persistence Diagram (PD)

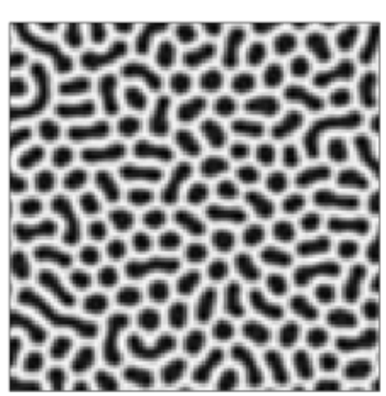
Persistent homology by level set filtration

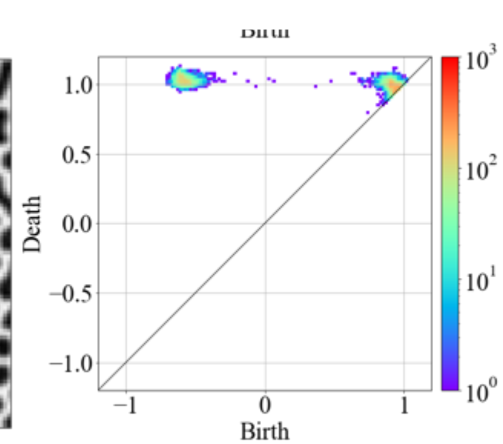
➡Persistent homology using the threshold of the continuous field $\phi(r)$ for the filtration.

[H. Wagner, C. Chen, and E. Vucini, “Mathematics andVisualization,” Springer, Berlin, Heidelberg]

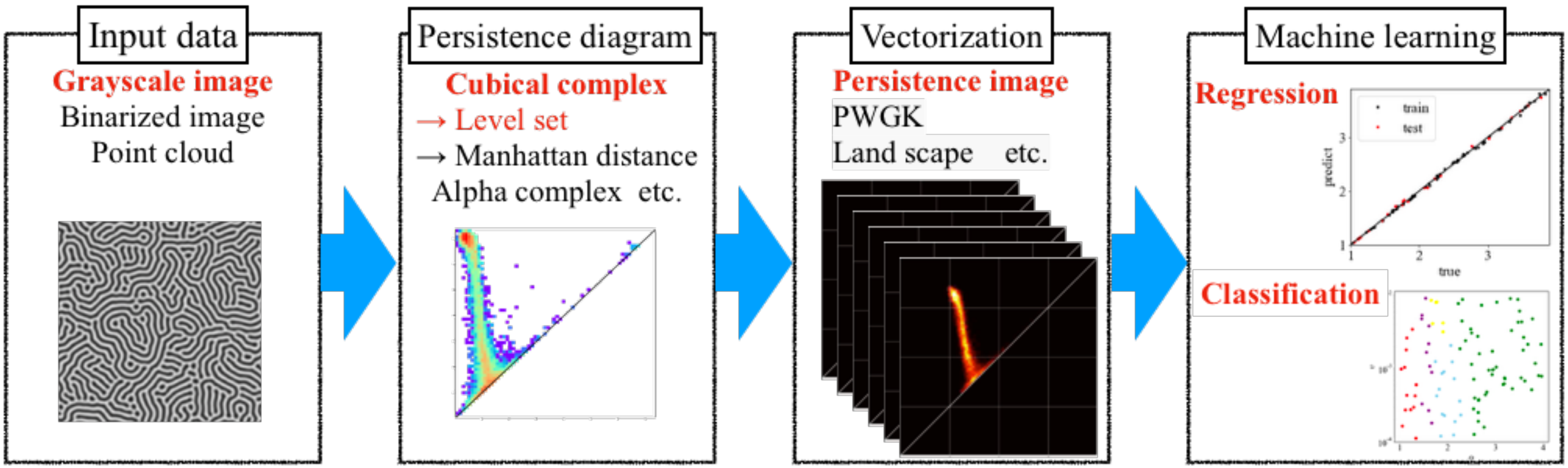








Analysis procedure of PD

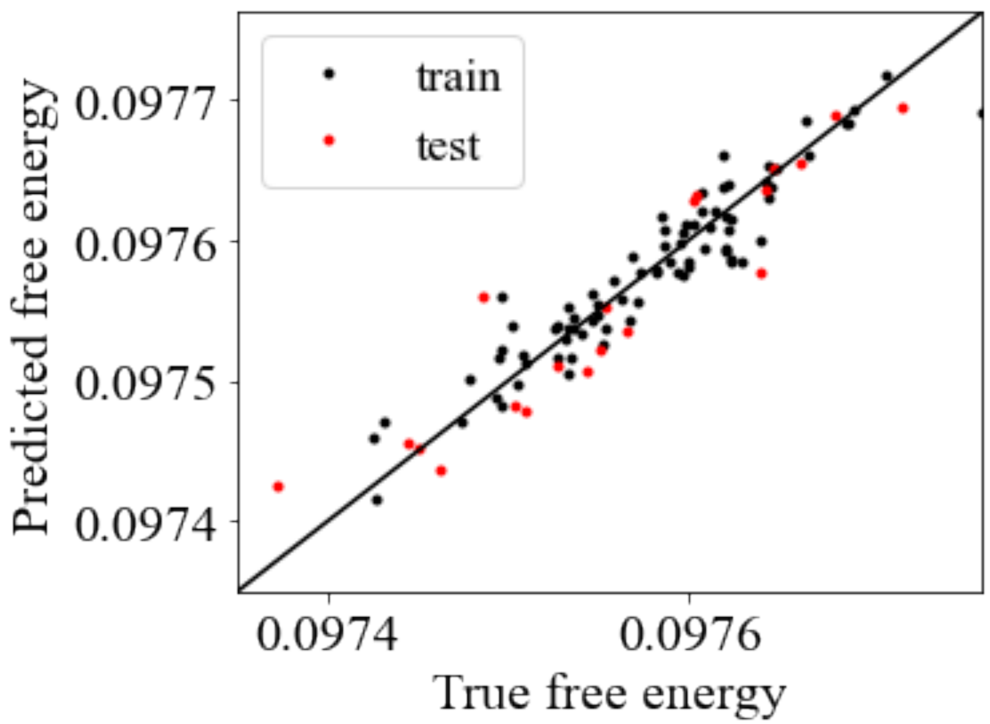


➡PDをベクトル化してLASSO回帰によって
自由エネルギー予測モデルを構築

3. Results and discussion

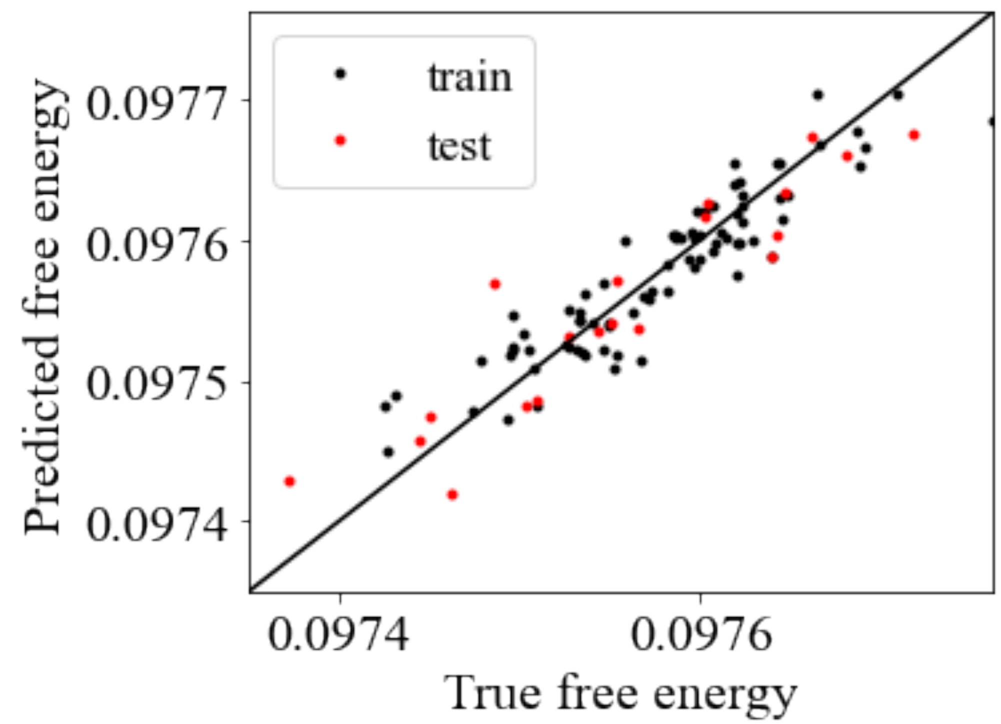
Prediction of the free energy

Persistent homology



mean R^2-value as 0.82
(0.91 for correlation coefficient)

Minkowski functionals



mean R^2-value as 0.78
(0.88 for correlation coefficient)

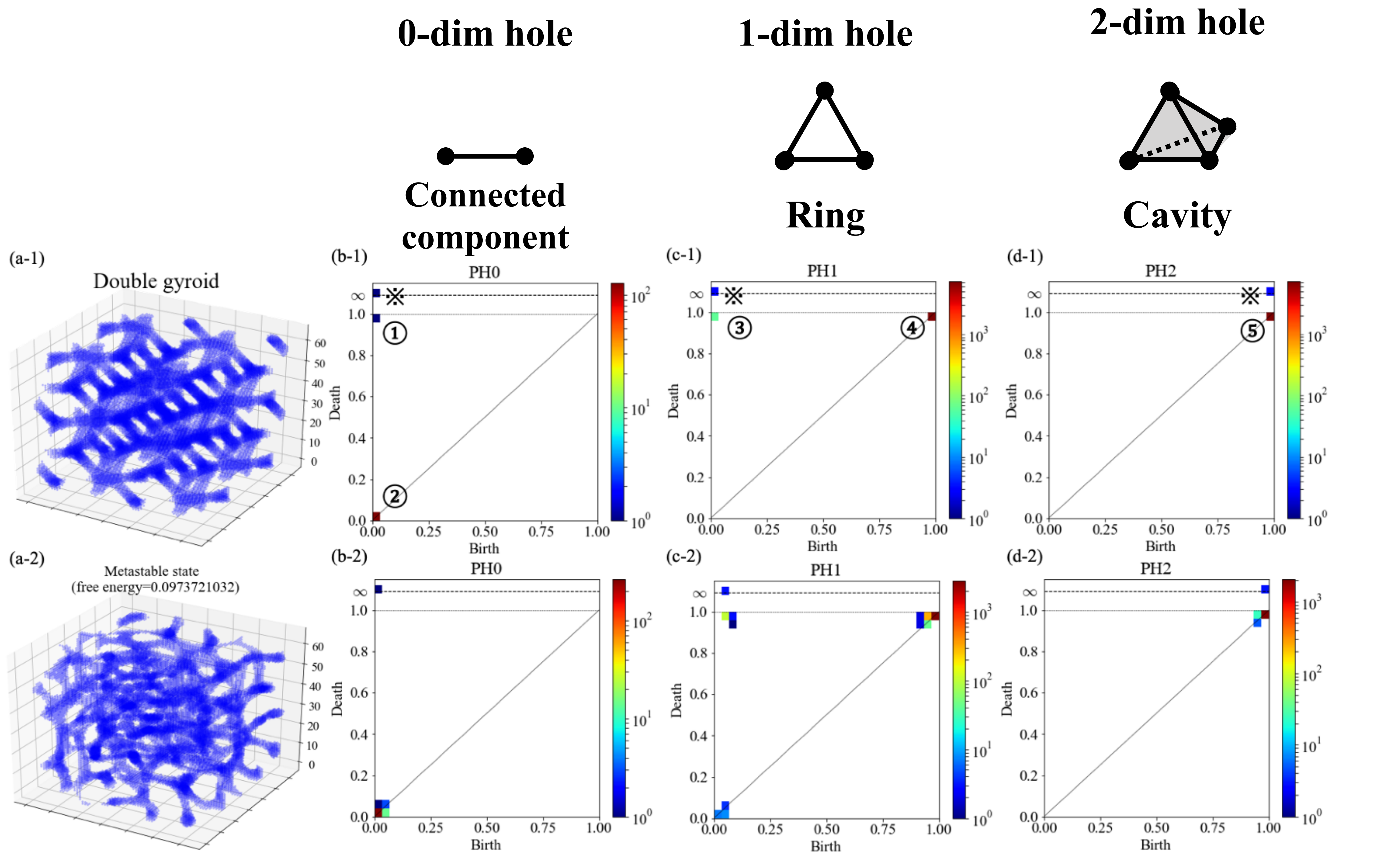
交差検証法でハイパーパラメータ（カーネル幅、LASSOの係数）を最適化

訓練-テストデータ分割をランダムに100回繰り返して平均R^2値を算出

→**有意な性能差が確認された**：pvalue<0.001

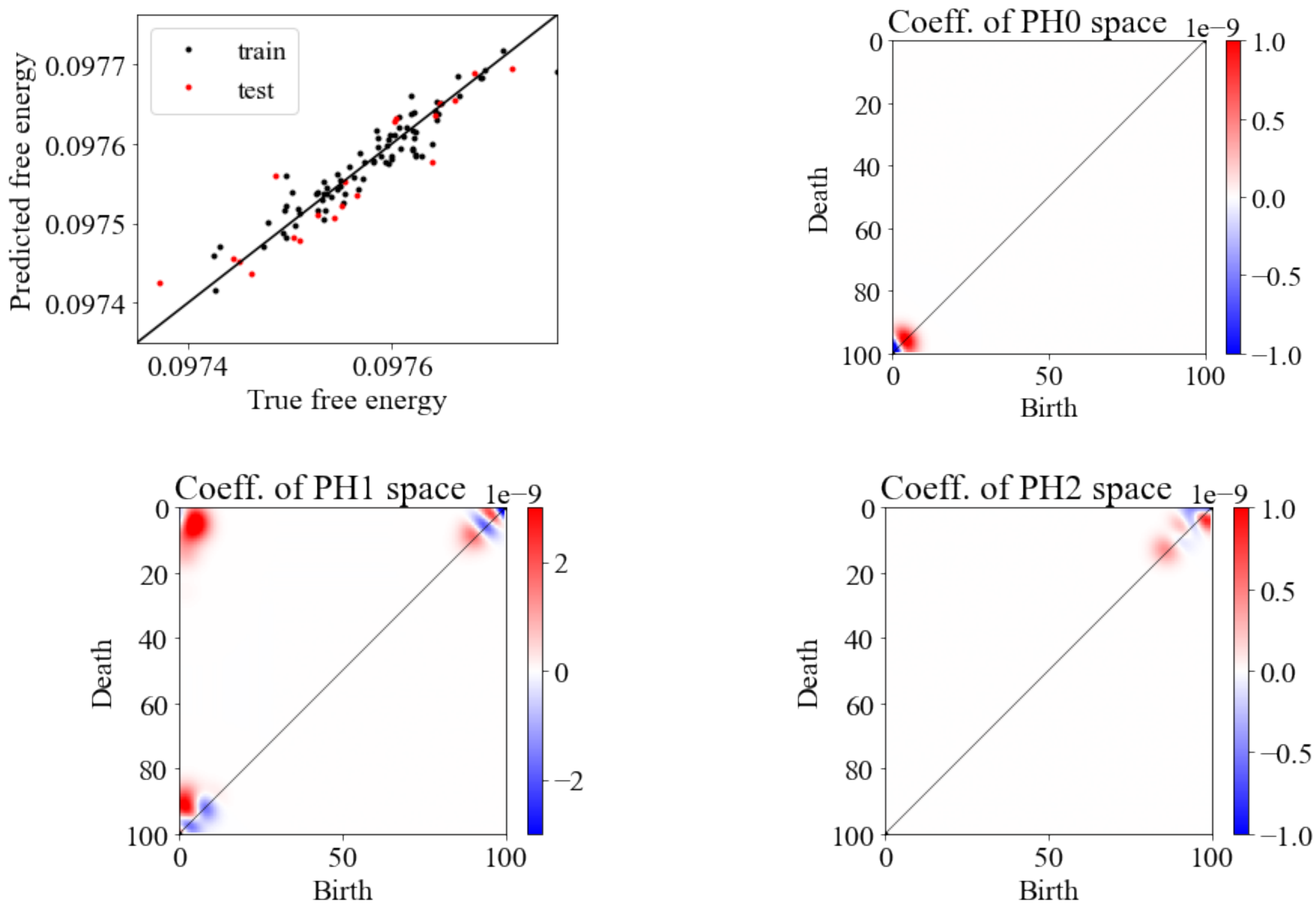
3. Results and discussion

Persistence diagram



3. Results and discussion

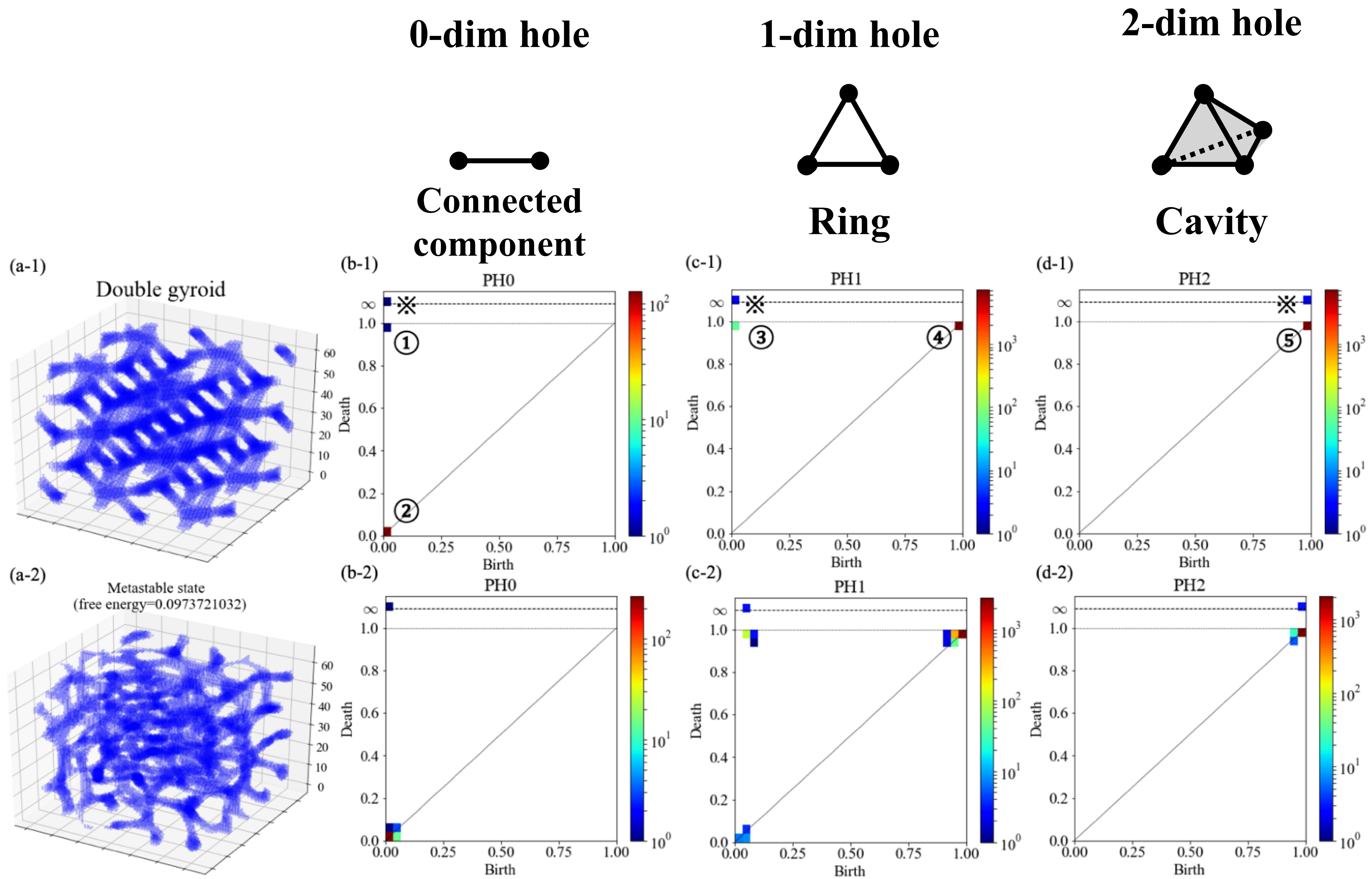
Regression analysis



PD上の②③④⑤周辺が回帰性能に寄与している可能性

3. Results and discussion

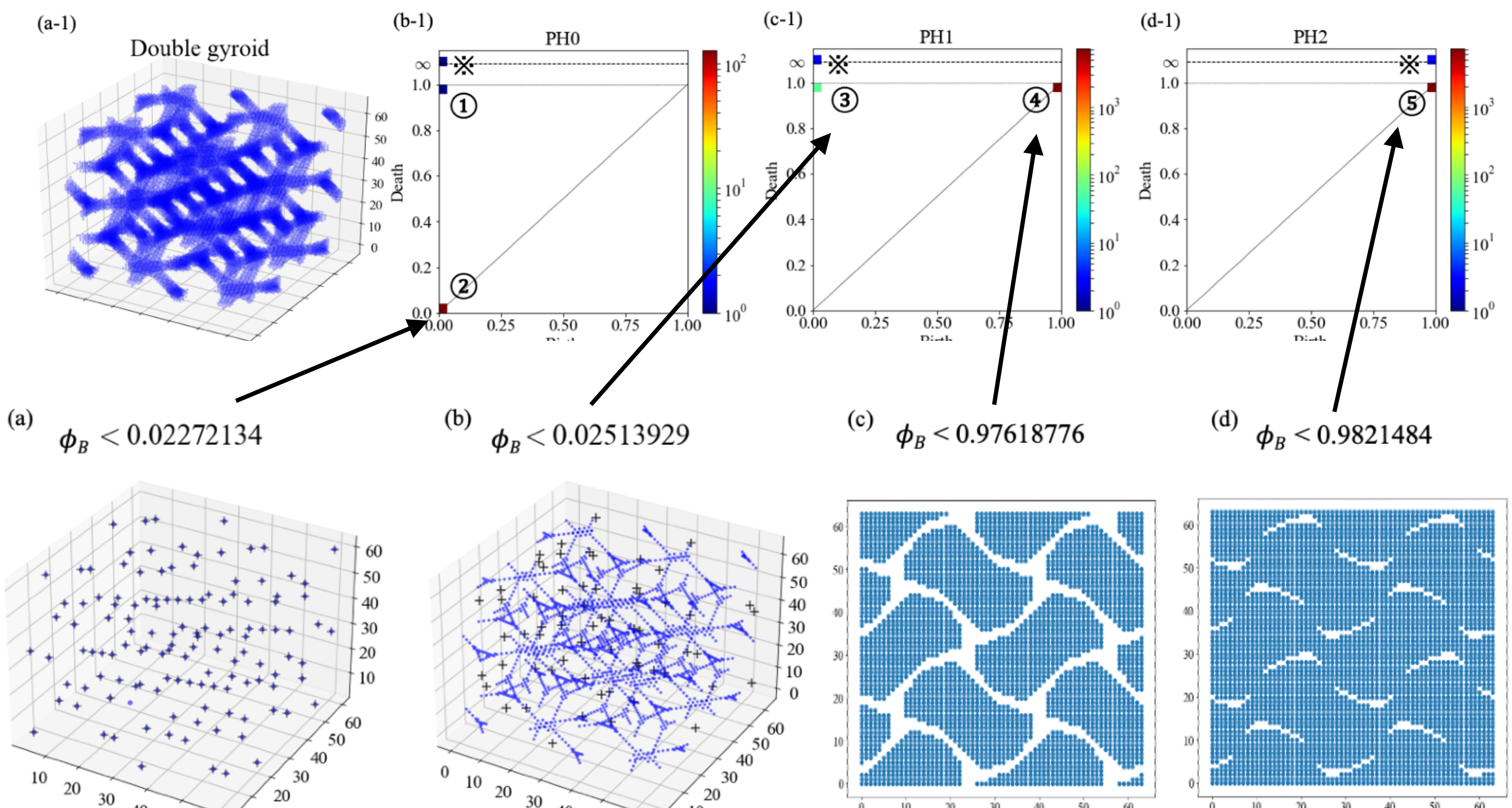
Inverse analysis of PDs



→**The PD in the metastable state can be interpreted as the scattered PD of DG.**
→**Analyze PD of DG to understand the metastable state of PD**

3. Results and discussion

Inverse analysis of PDs



① Two independent domains of the double-gyroid are connected at this death-time. As a result, the number of connected components, which are one-dimensional holes, is reduced by one at this birth--death point.

② One-dimensional holes (connected components) are generated corresponding to those shown in Fig. 4(a). The holes dead when the connected components are connected and form a network (Fig. 4(b)).

③ As shown in Fig. 4(b), a two-dimensional hole (ring) is created by the connection of networks.

④The ring structures of a short lifetime are generated by connecting the domain at many points (Fig. 4(c)).

⑤The cavities are generated for a short time as a pore structure as shown in Fig. 4(d).

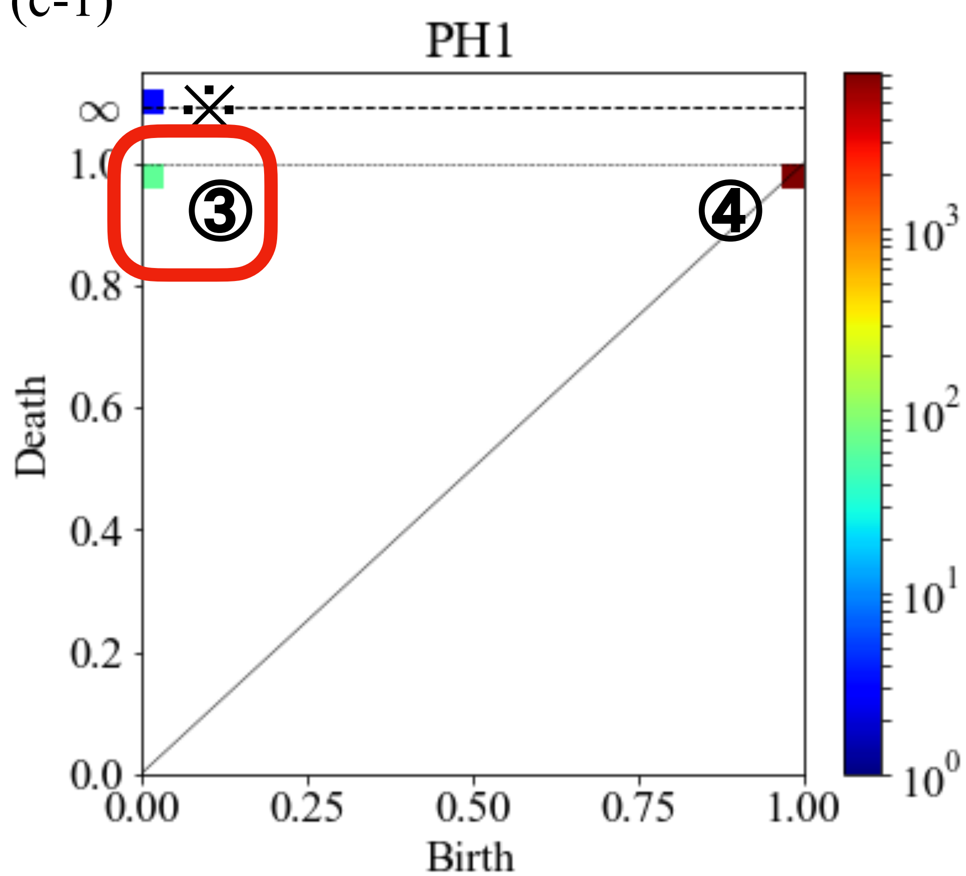
※These birth-death pairs correspond to the torus structure of the periodic boundary space.

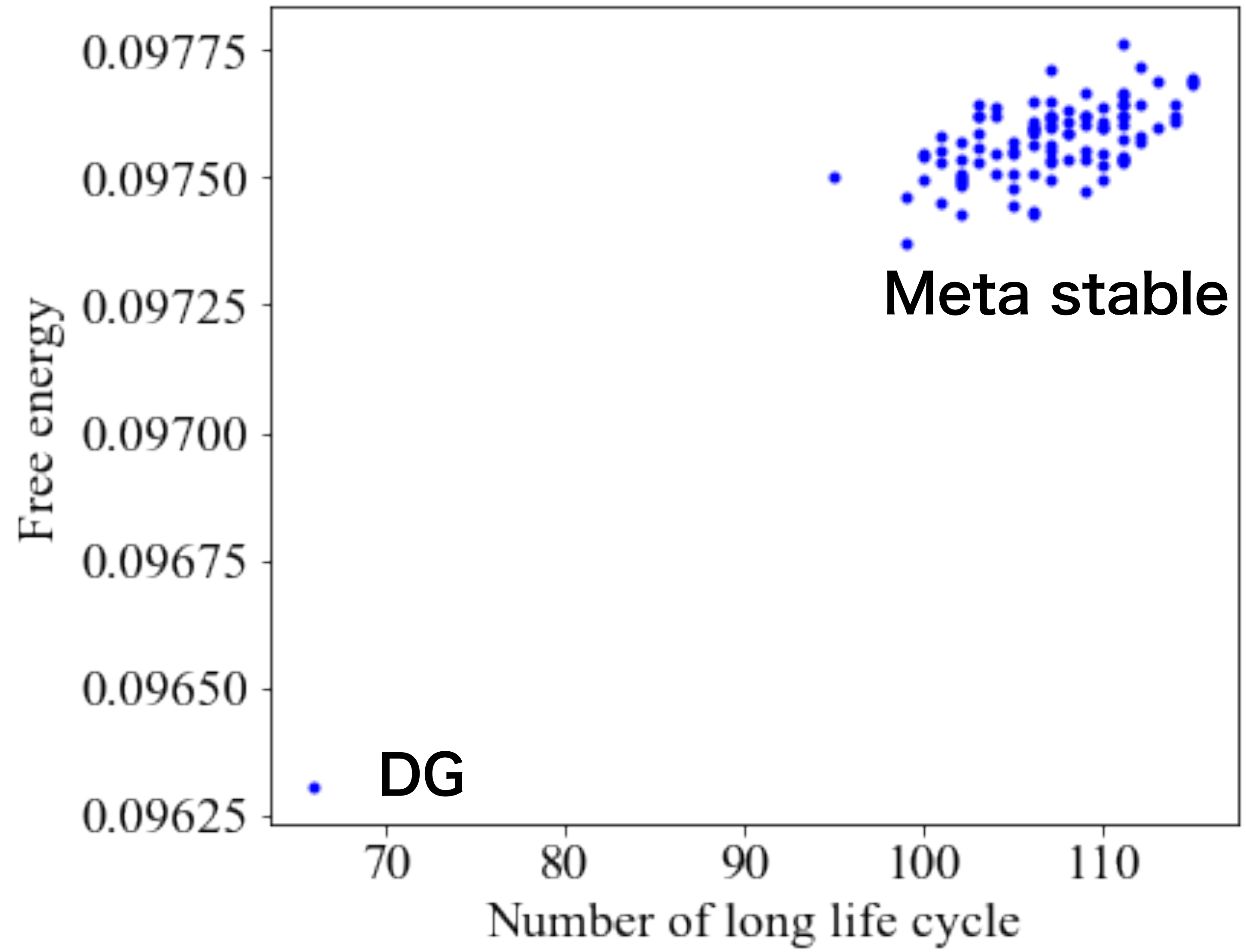
3. Results and discussion

Inverse analysis of PD

The relationship between the structure of polymer’s networks topology ③ and free energy

(c-1)





→**The number of rings suggests that the network's coupling structure is more complex**
→**The number of rings in ③ is correlated with the free energy**

→**<u>Extracting information other than curvature that can be estimated for free energy?</u>**

3. Summary

Summary

- The results obtained in this study suggest that PH is a good feature for using to estimate the free energy of the metastable structure of a double-gyroid.

- The analysis results suggest that the PDs characterize the **network structure** of the domain.

→The free energy is usually estimated from the interfacial structure, such as the interfacial curvature or its length, but it is suggested that other information is also useful.

- The analysis results would also suggest that **PDs include information about the curvature or length** of the interface structure indirectly.

→It is generally **computationally difficult** to estimate these features from the data. Thus, it is expected that it will generally be possible to easily extract features that can be used to estimate free energy using PH.