

MI²i 最終報告会

19-20 February 2020 @一橋講堂



Materials research
by Information Integration"
Initiative

Activity Summary of Topological Analysis Group

Kazuto Akagi
AIMR, Tohoku University/NIMS

トポロジカル解析グループ

トポロジカルデータ解析の
理論・計算手法開発・応用展開

赤木 和人 (GL、東北大学)

平岡 裕章 (SGL、京都大学)

小串 典子 (NIMS/京都大学)

実験と計算機シミュレーションによる
非晶質材料の作成・解析・モデリング

小原 真司 (SGL、NIMS)

小野寺 陽平 (京都大学)

田原 周太 (琉球大学)

増野 敦信 (弘前大学)

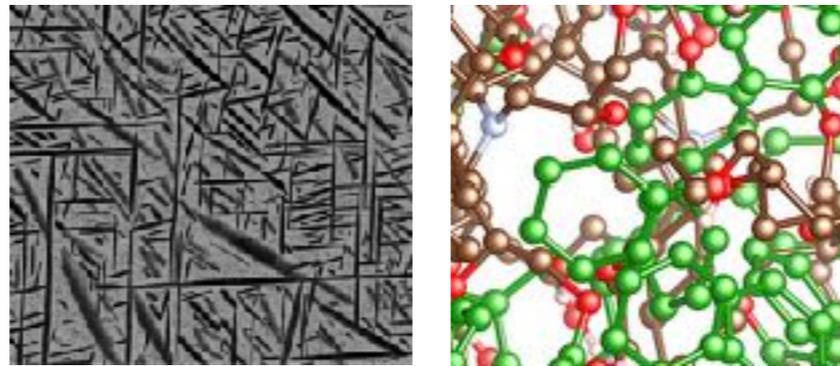
トポロジカル機械学習手法の
磁性材料課題への展開

小嗣 真人 (東京理科大学)

- 非晶質の物性を理解するための本質的な記述の発見
- 材料データベースの基盤デザイン
- 材料特性の支配要因の抽出
- HomCloud の開発、応用

目指しているもの

複雑な構造データ



組成

プロセス条件

環境の履歴

材料特性 1

材料特性 2

材料特性 3

新しい構造記述子

□□□□□□……□□ vector data

**定量的で検索性が良い構造記述子を生成して
「中身が見える」逆問題アプローチを行う**

Persistent Homology

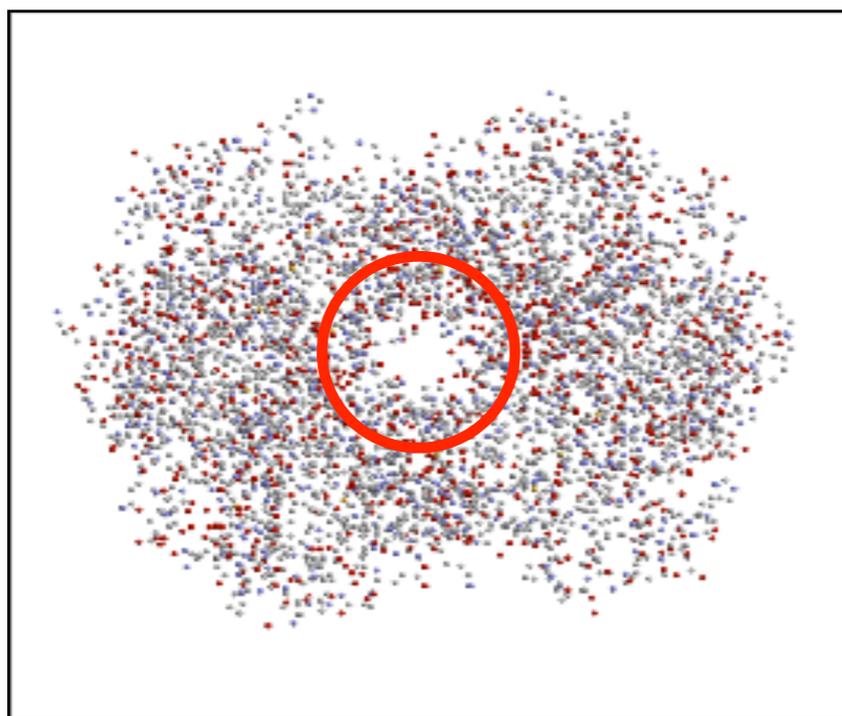
– Mathematical tool treating “shape” of discrete data



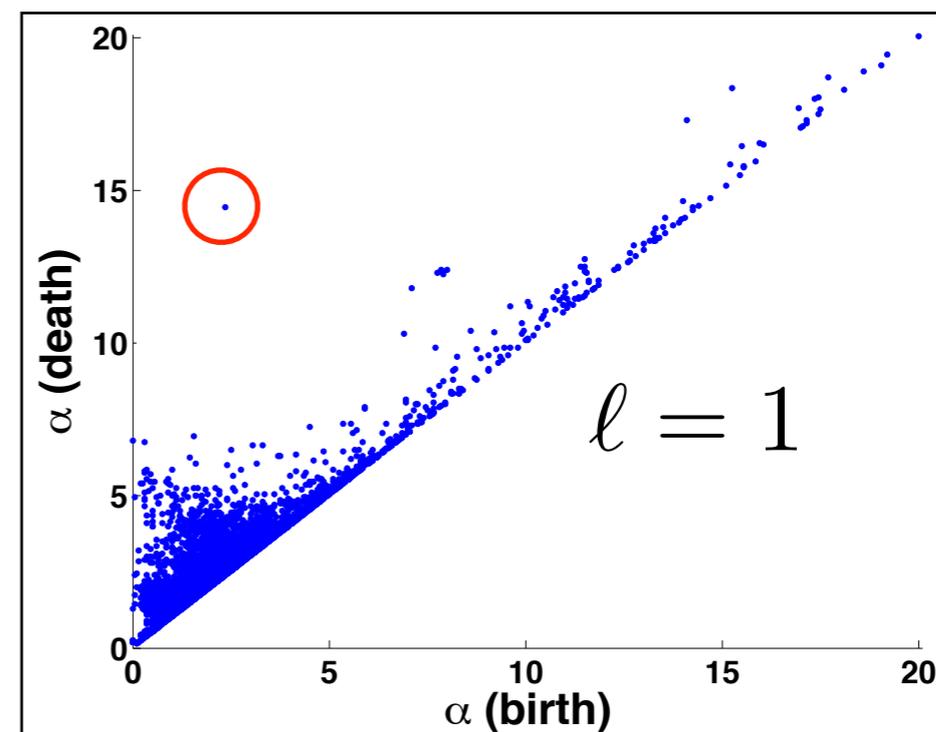
Yasuaki Hiraoka



input: hemoglobin

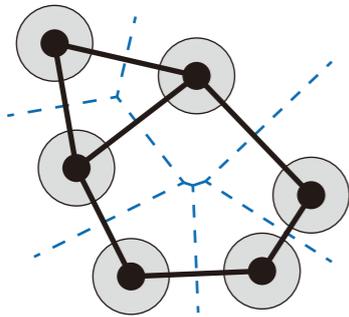


output: persistence diagram (PD)



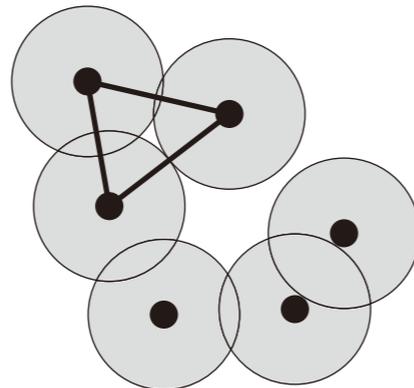
Persistent Homology

— Mathematical tool treating “shape” of discrete data

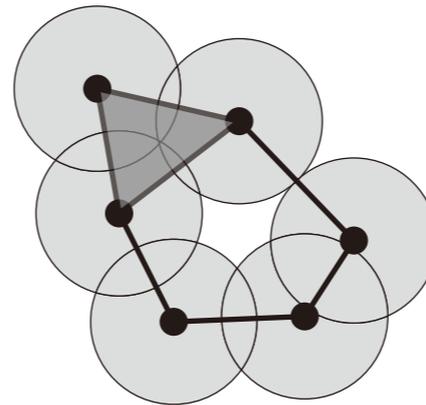


Voronoi division

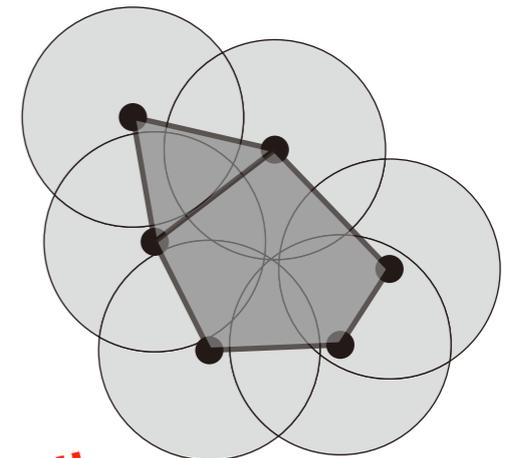
an example for $\ell = 1$ (ring)



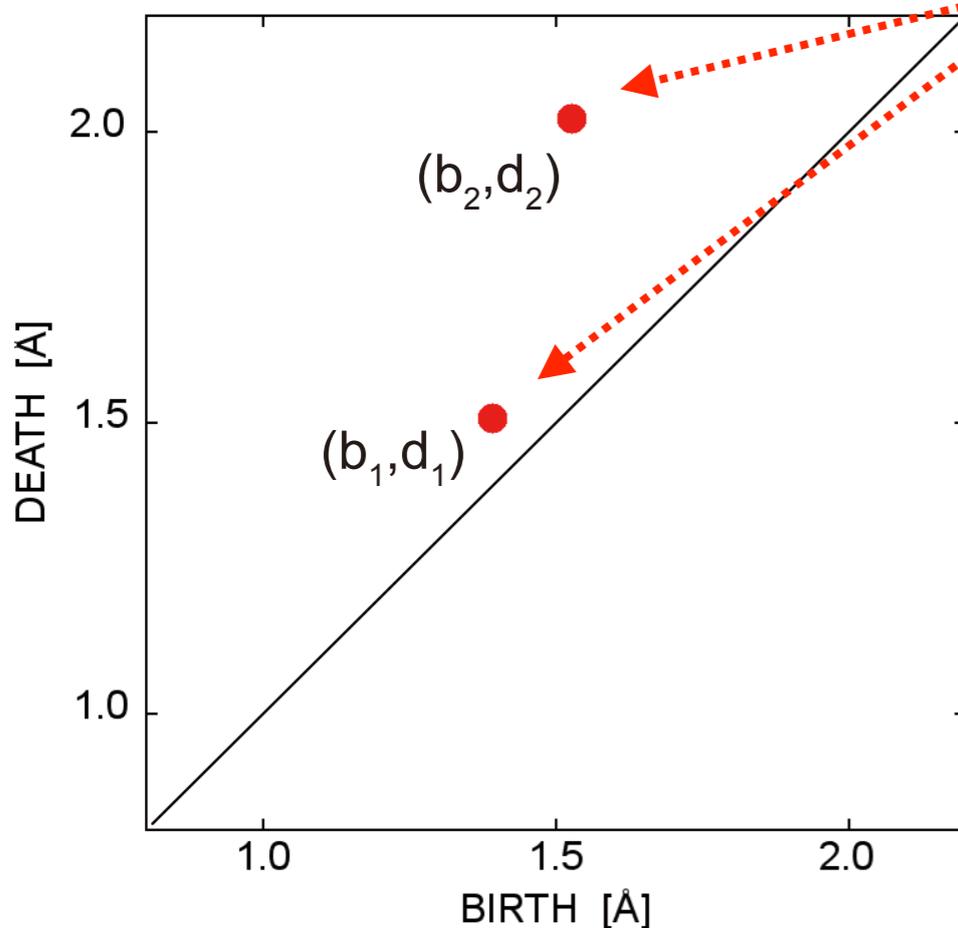
$$b_1 = 1.39 \text{ \AA}$$



$$d_1 = 1.51 \text{ \AA}$$
$$b_2 = 1.52 \text{ \AA}$$



$$d_2 = 2.02 \text{ \AA}$$

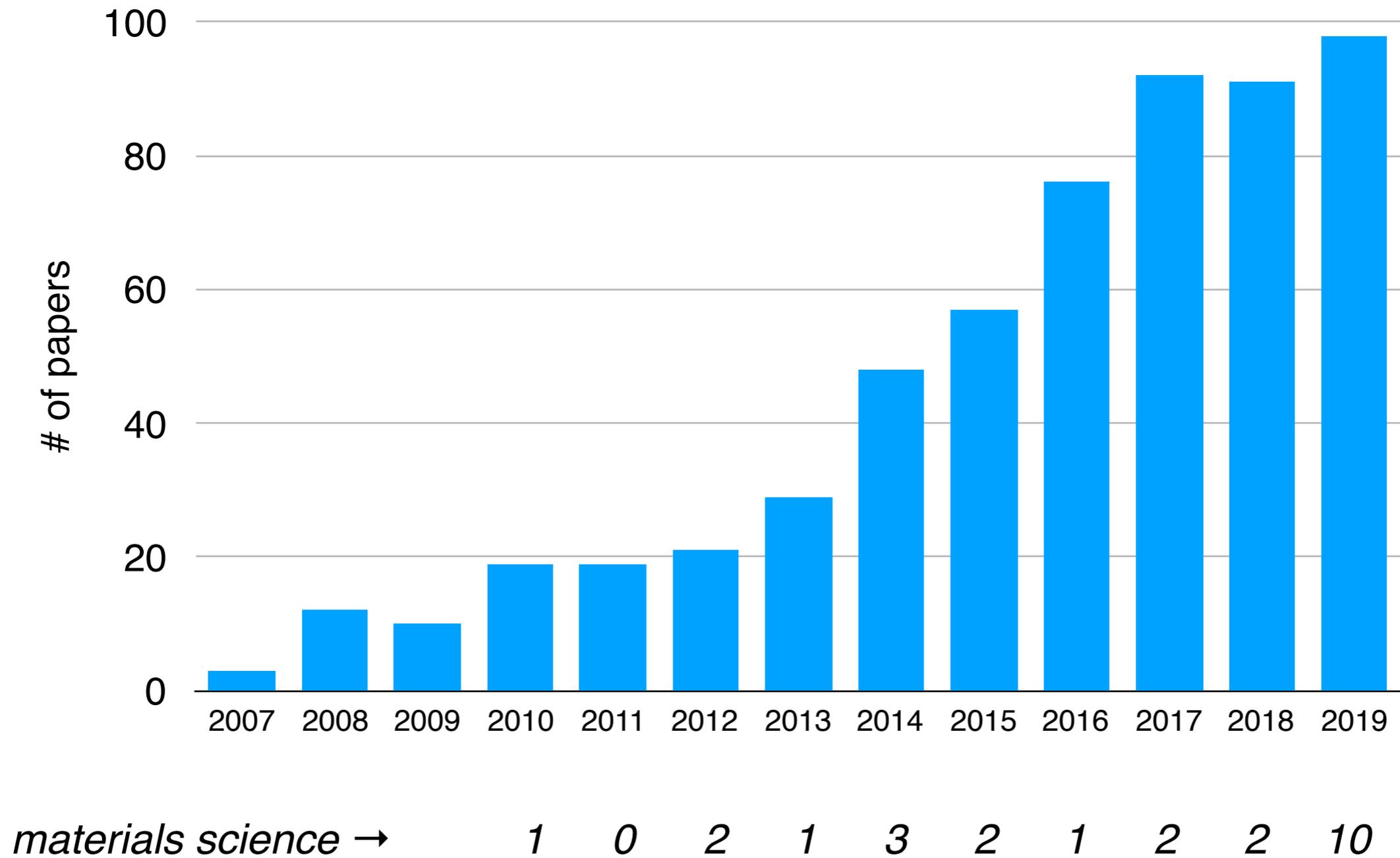


Persistence diagram

= Fingerprint of the "shape" in discrete data summarized as a 2-D histogram

- Born at $r=b$, dead at $r=d$
- Each (b,d) represents each "Hole"
- Robust "Hole" : apart from the diagonal line
- Noisy "Hole" : near by the diagonal line

Publication on "Persistent Homology" (Web of Science)



秩序に気づく

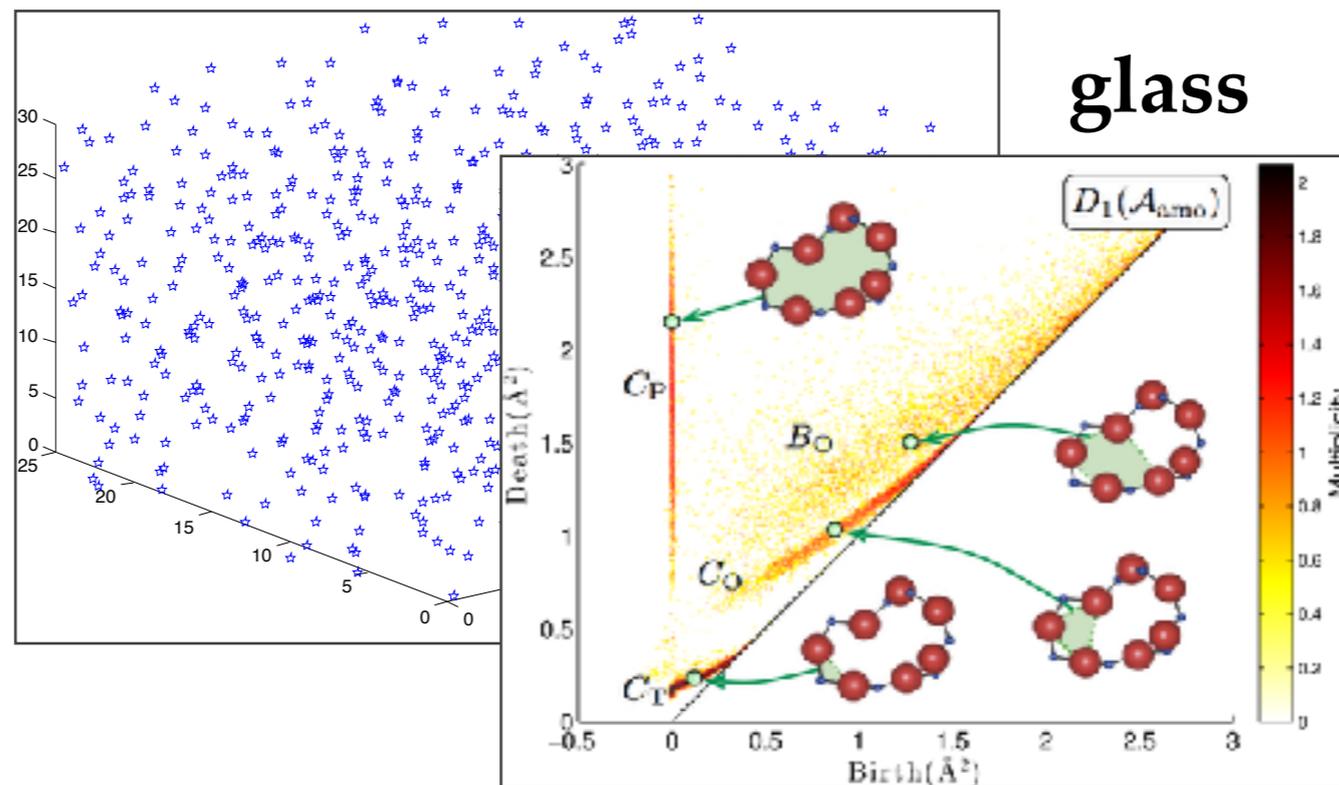
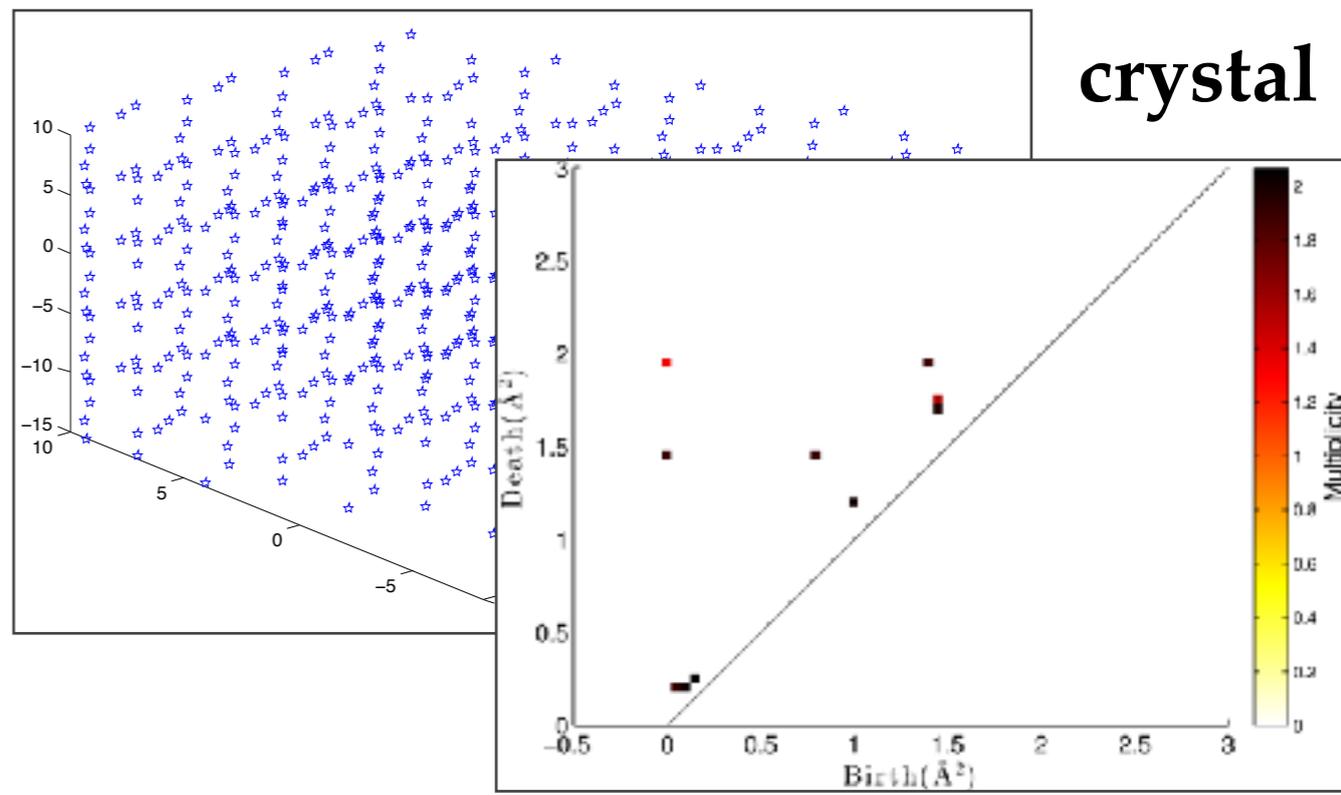
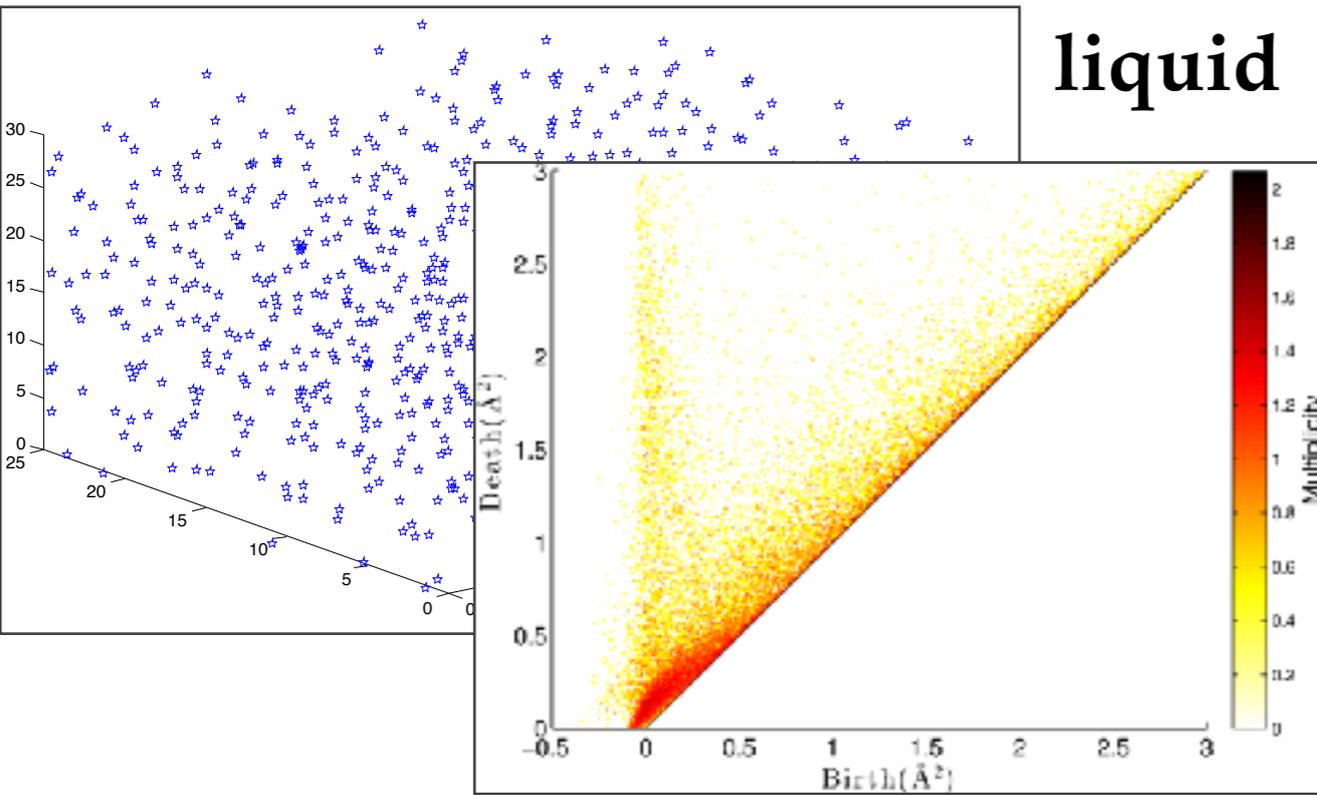
Application to SiO₂

Nakamura, H. *et al.* Nanotechnology 26 (2015)

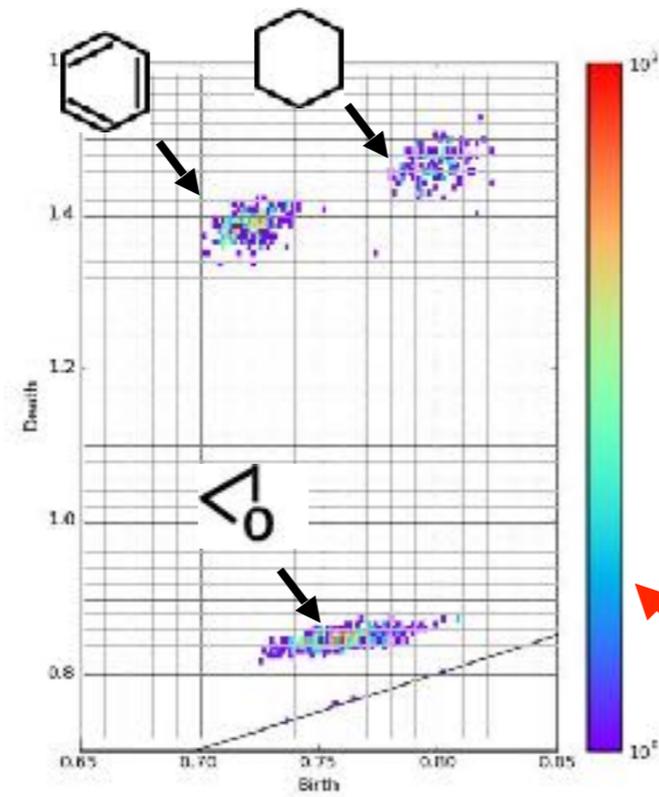
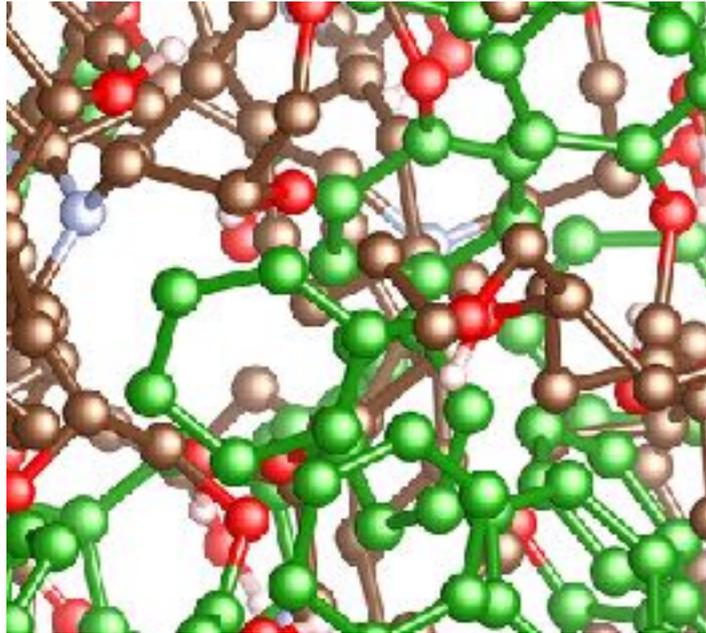
liquid

crystal

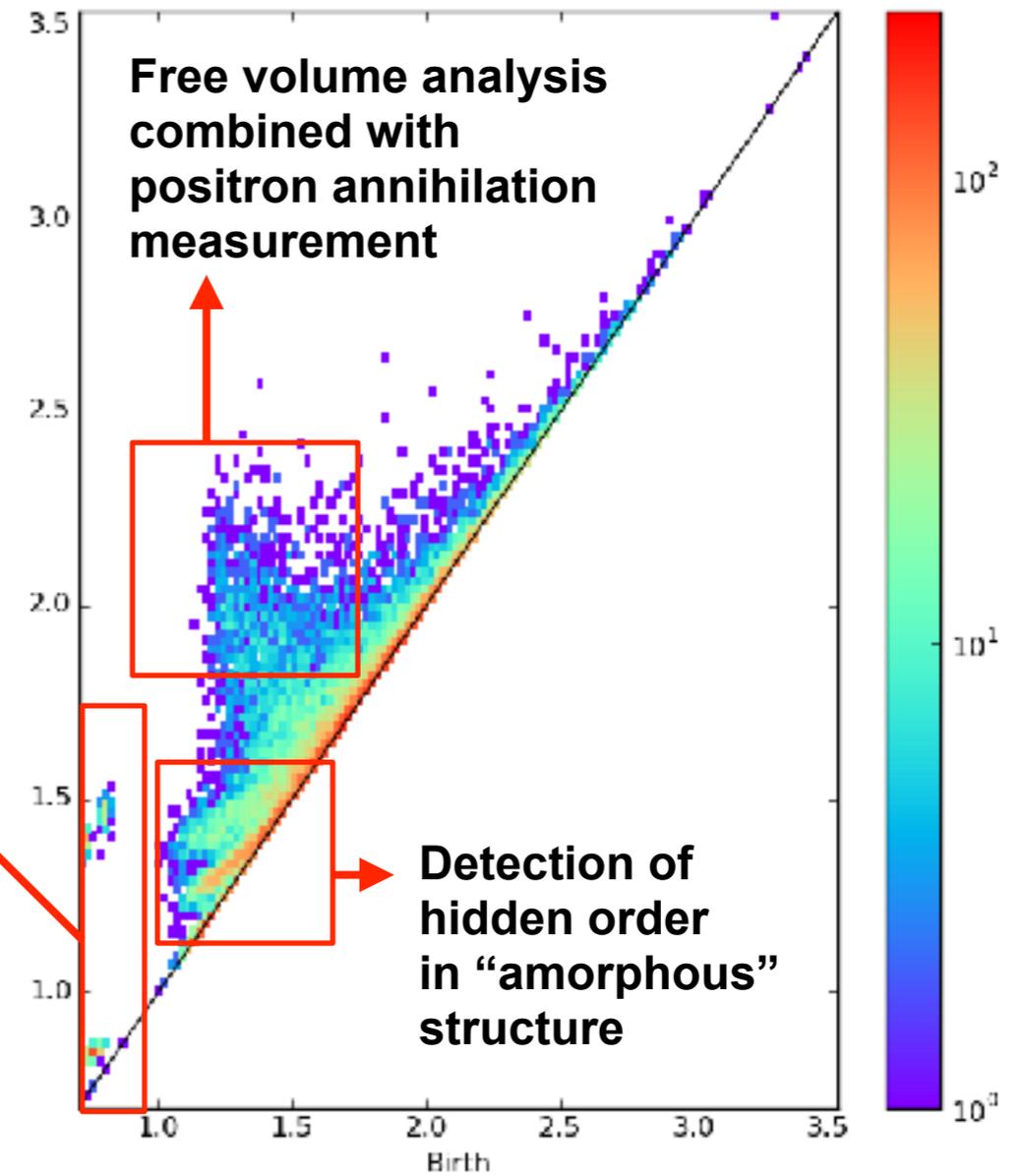
glass



Detection of "hidden" order

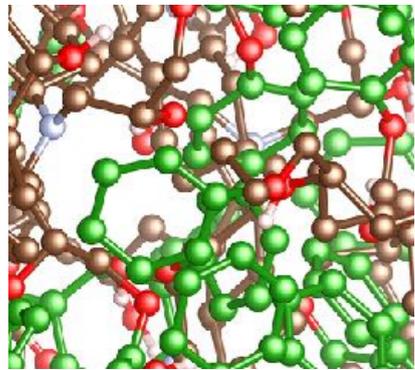


Spatial ordering analysis of specific atomic groups (a kind of coarse graining)



Forward and Inverse Analysis based on Persistent Homology

Input Data



Atomic Configuration

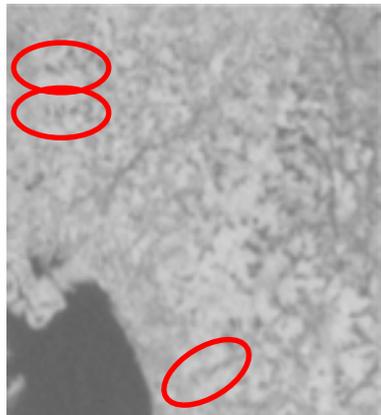
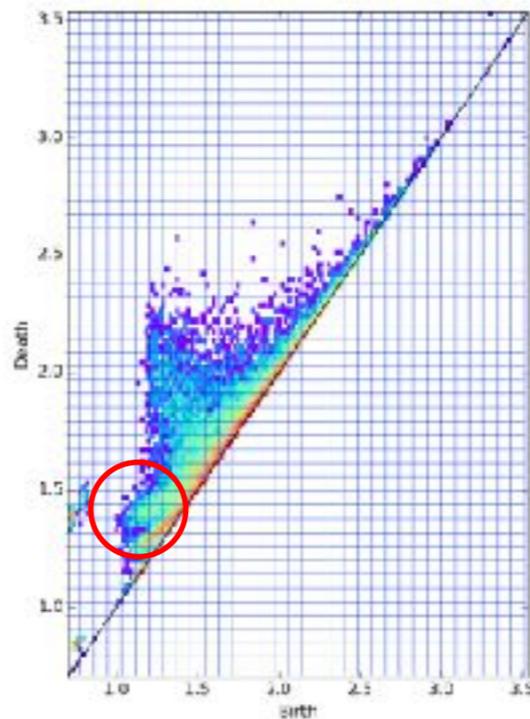


Image Data

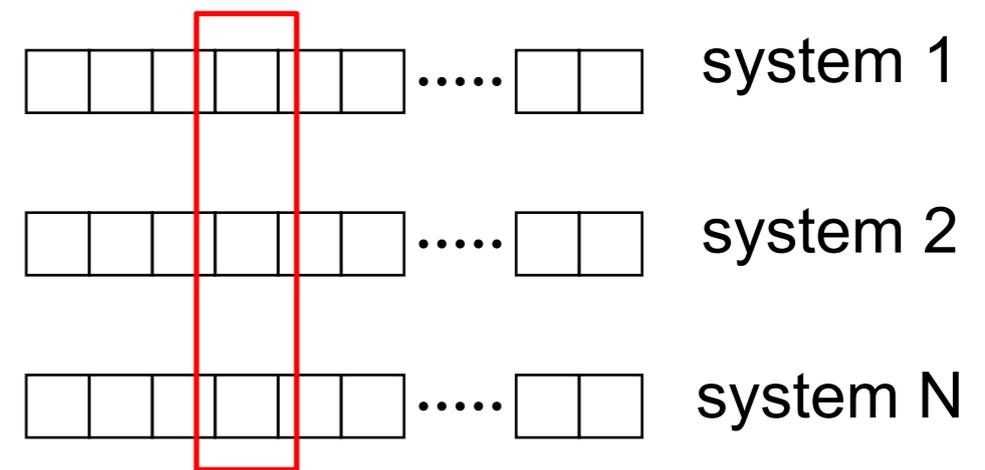
Persistence Diagram

- Extraction of hidden order



Descriptor

(properly translated vector data)



- Good affinity with machine-learning
- Database of complex systems

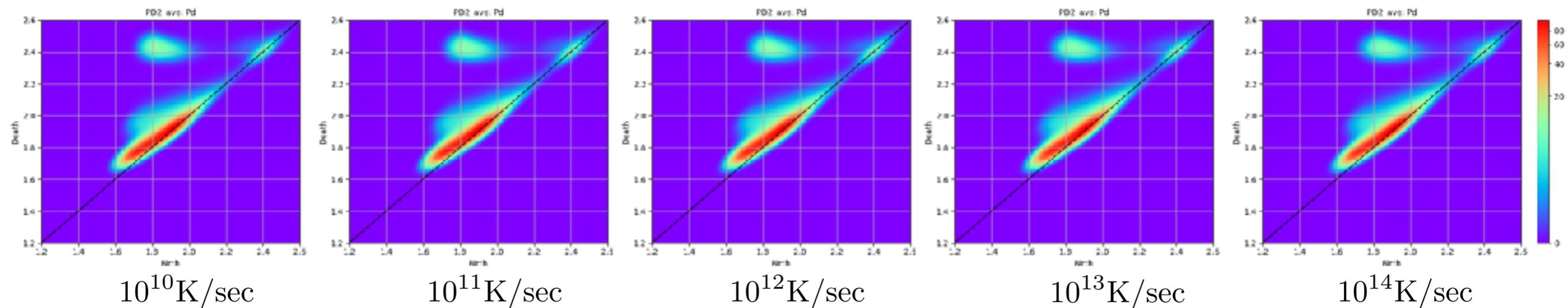
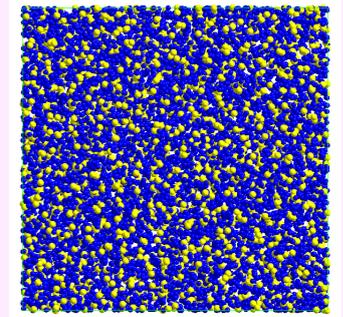
- Finding correlation with various properties
- Elucidation of key structures in original data

違いを調べる、分類する

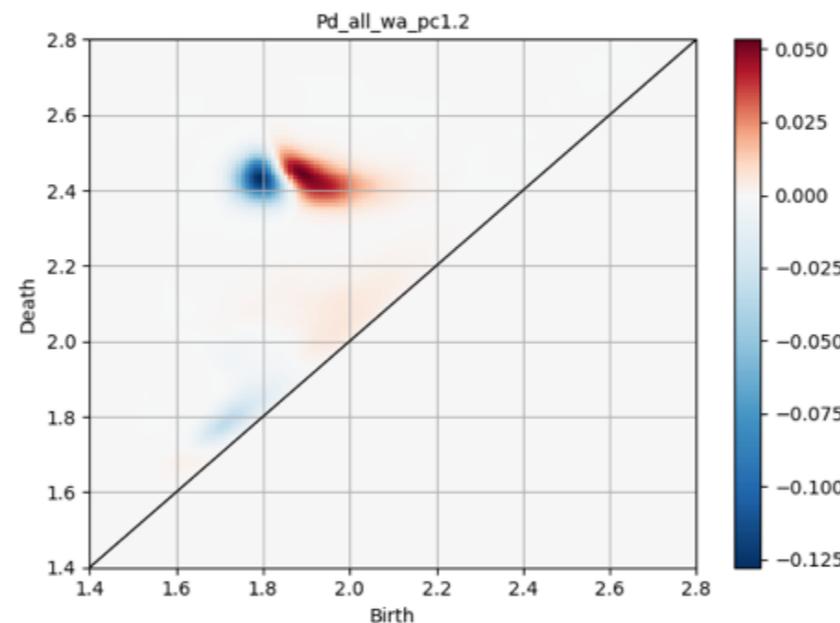
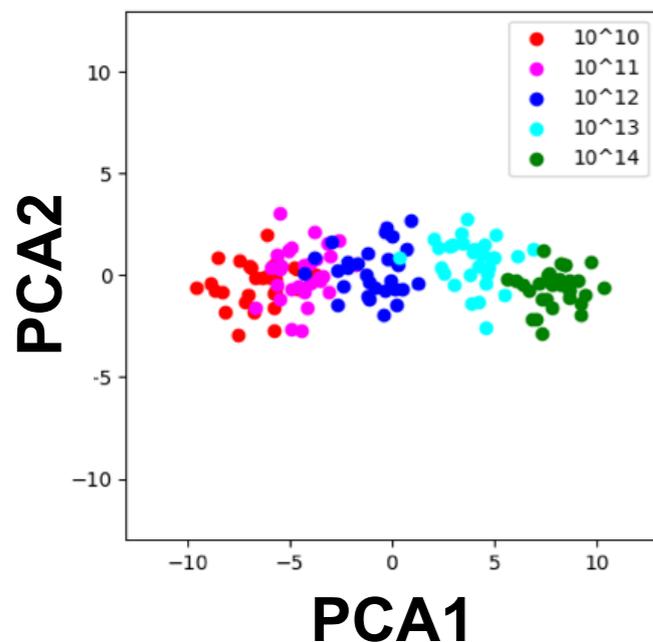
Metallic Glass: cooling rate effect on glass structures

(平岡、大林、平田)

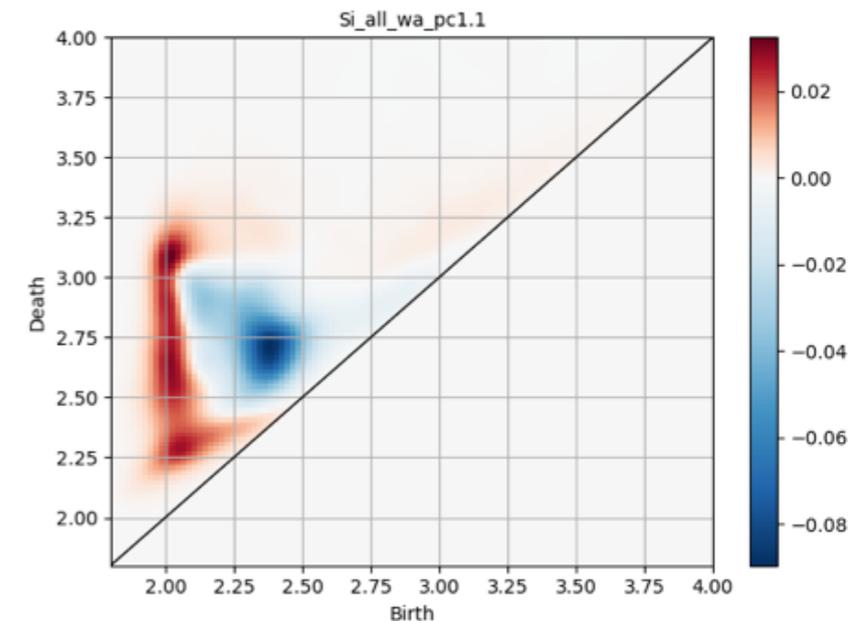
- target: metallic glass ($\text{Pd}_{80}\text{Si}_{20}$)
- identify structural changes induced from cooling rates
- apply PDs to MDs for describing structures
- combine ML and inverse analysis for explicitly identify those changes



Pd, dim=2



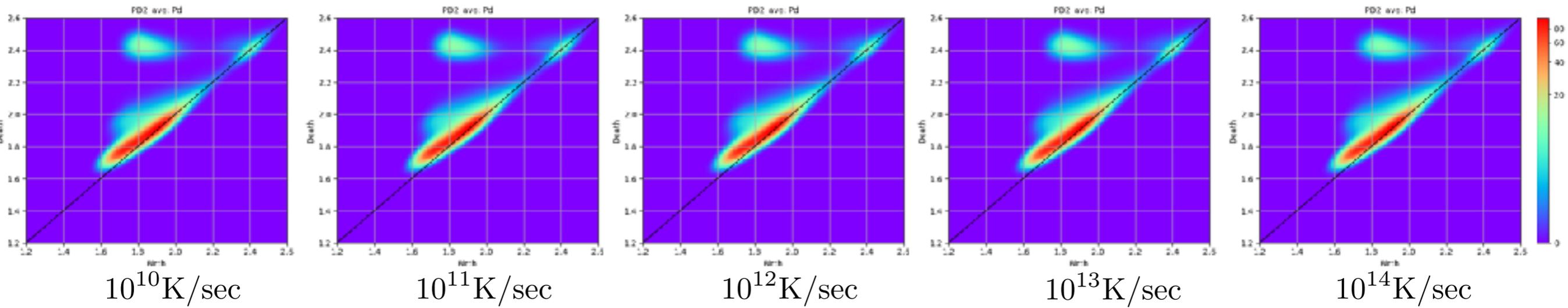
PD of PCA1 (Pd, dim=2)



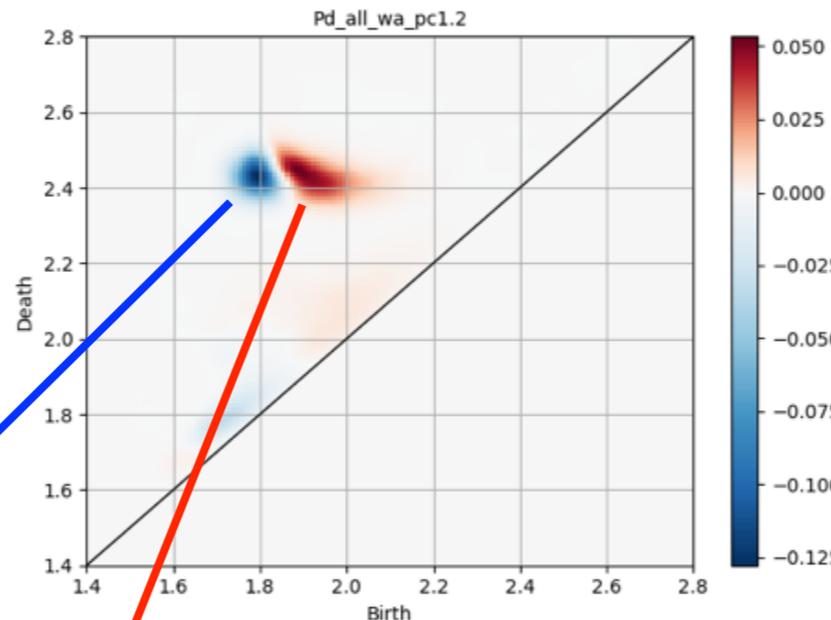
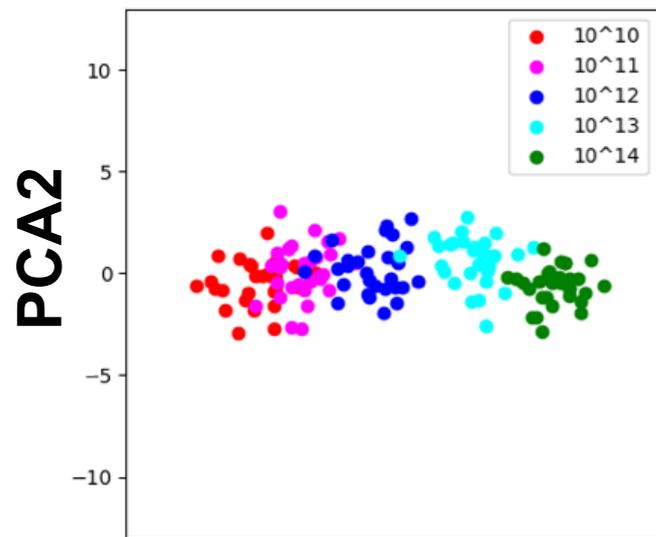
PD of PCA1 (Si, dim=1)

Metallic Glass: cooling rate effect on glass structures

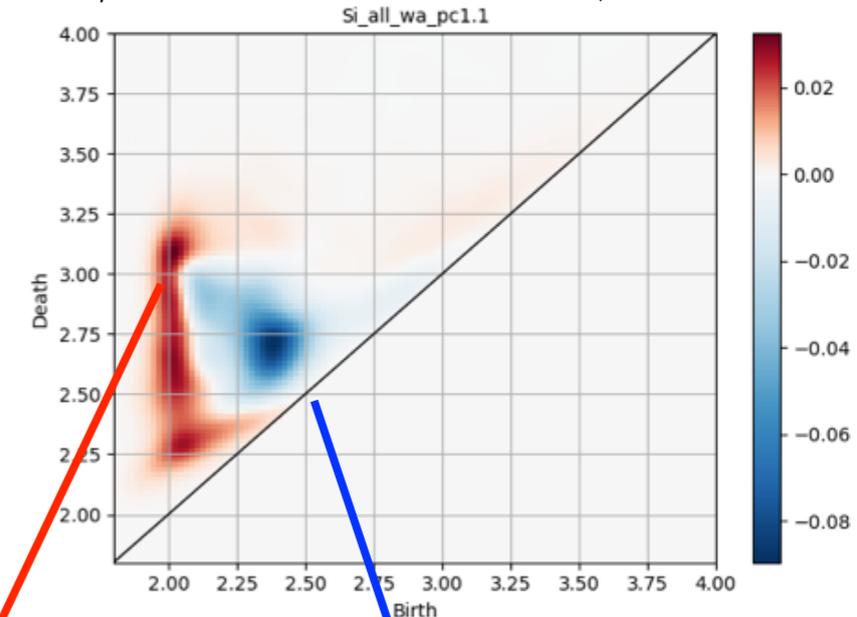
(平岡、大林、平田)



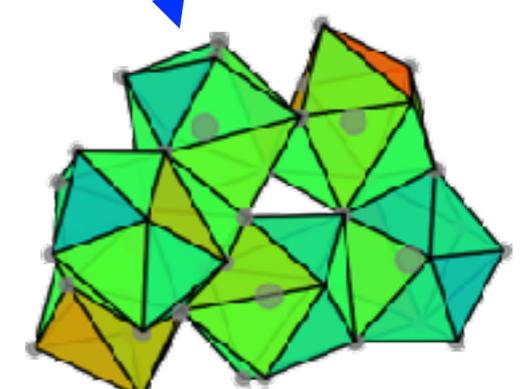
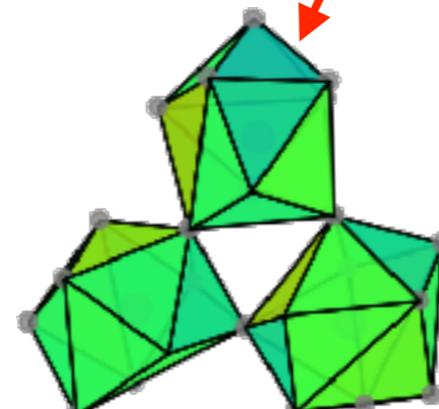
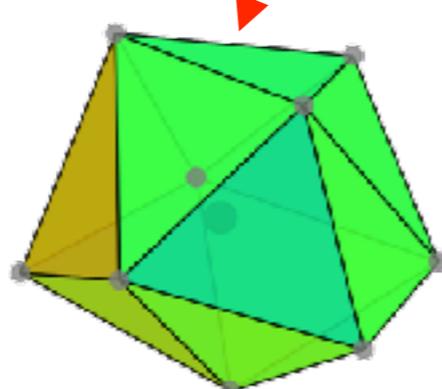
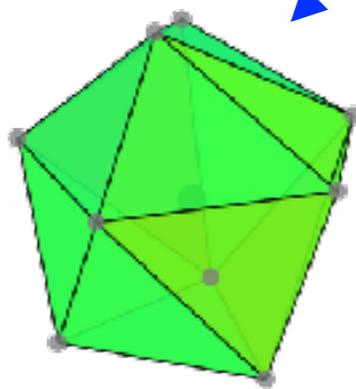
Pd, dim=2



PD of PCA1 (Pd, dim=2)



PD of PCA1 (Si, dim=1)



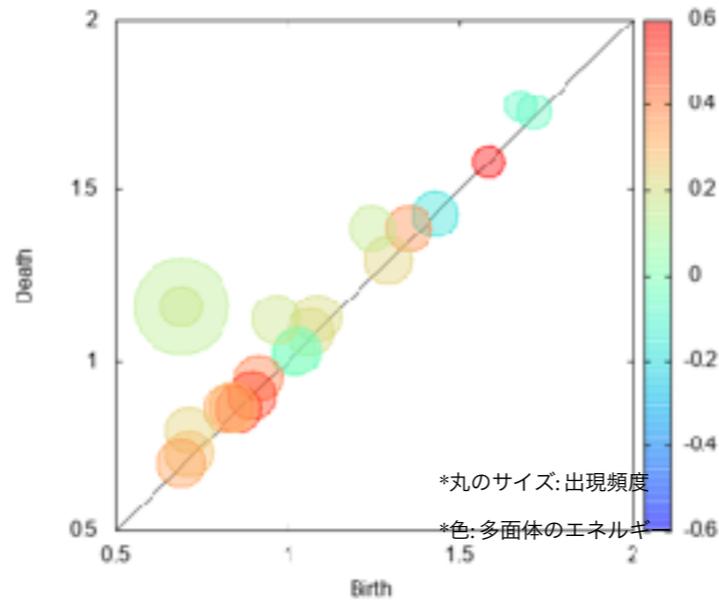
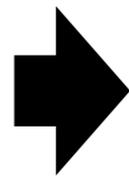
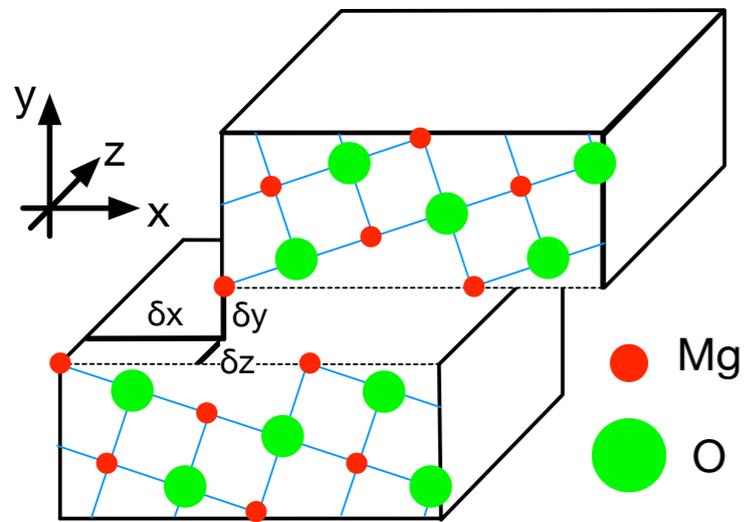
Inverse of PCA explicit identifies geometry affected by cooling rates!

Evaluation of Interface Structure

(小串)

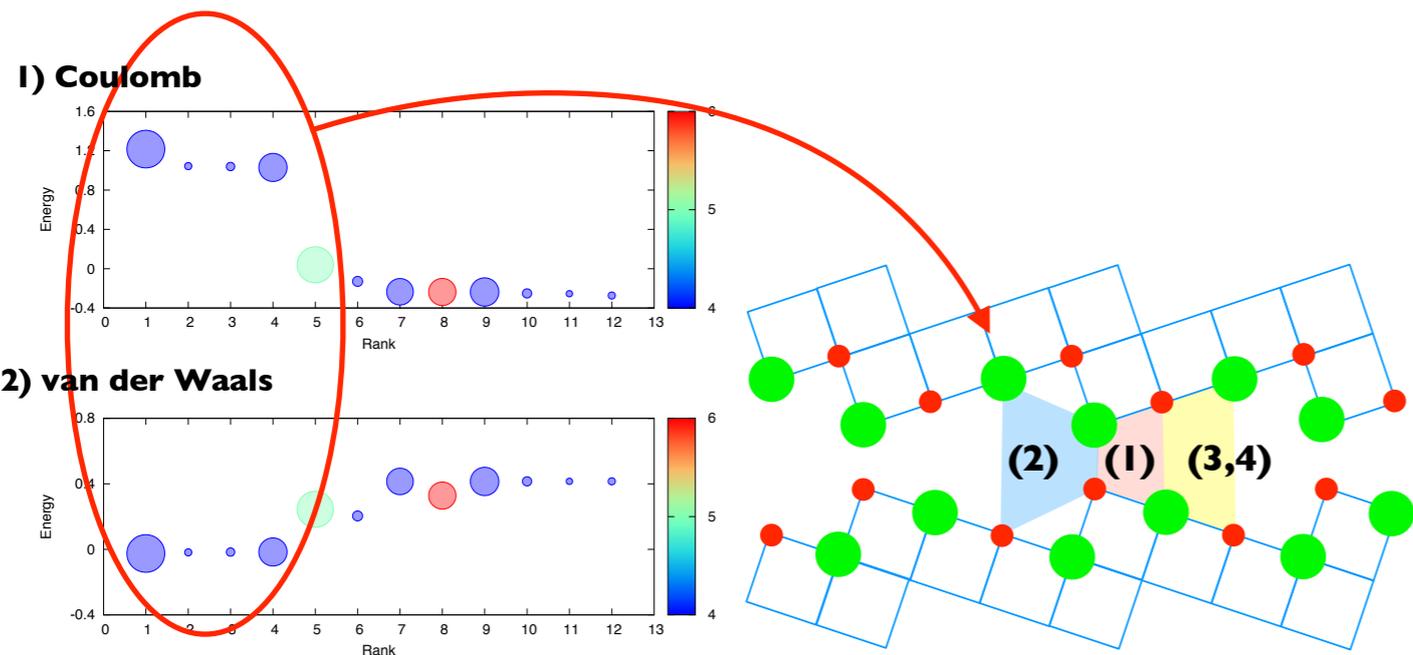
Model: MgO (310) $\Sigma 5$ Grain boundary

粒界構造を系統的に生成

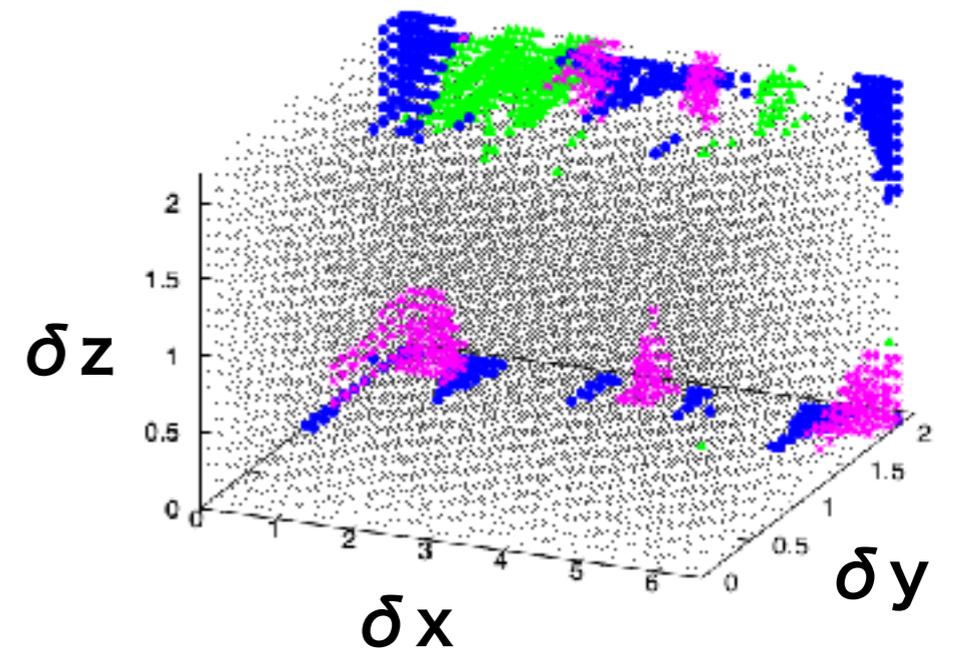


粒界のコストを各 (b_k, d_k) を与える
最小サイクル Z_k のエネルギー
(Coulomb & van der Waals) で評価

例) $(\delta x, \delta y, \delta z) = (0.0, 2.1, 1.7)$



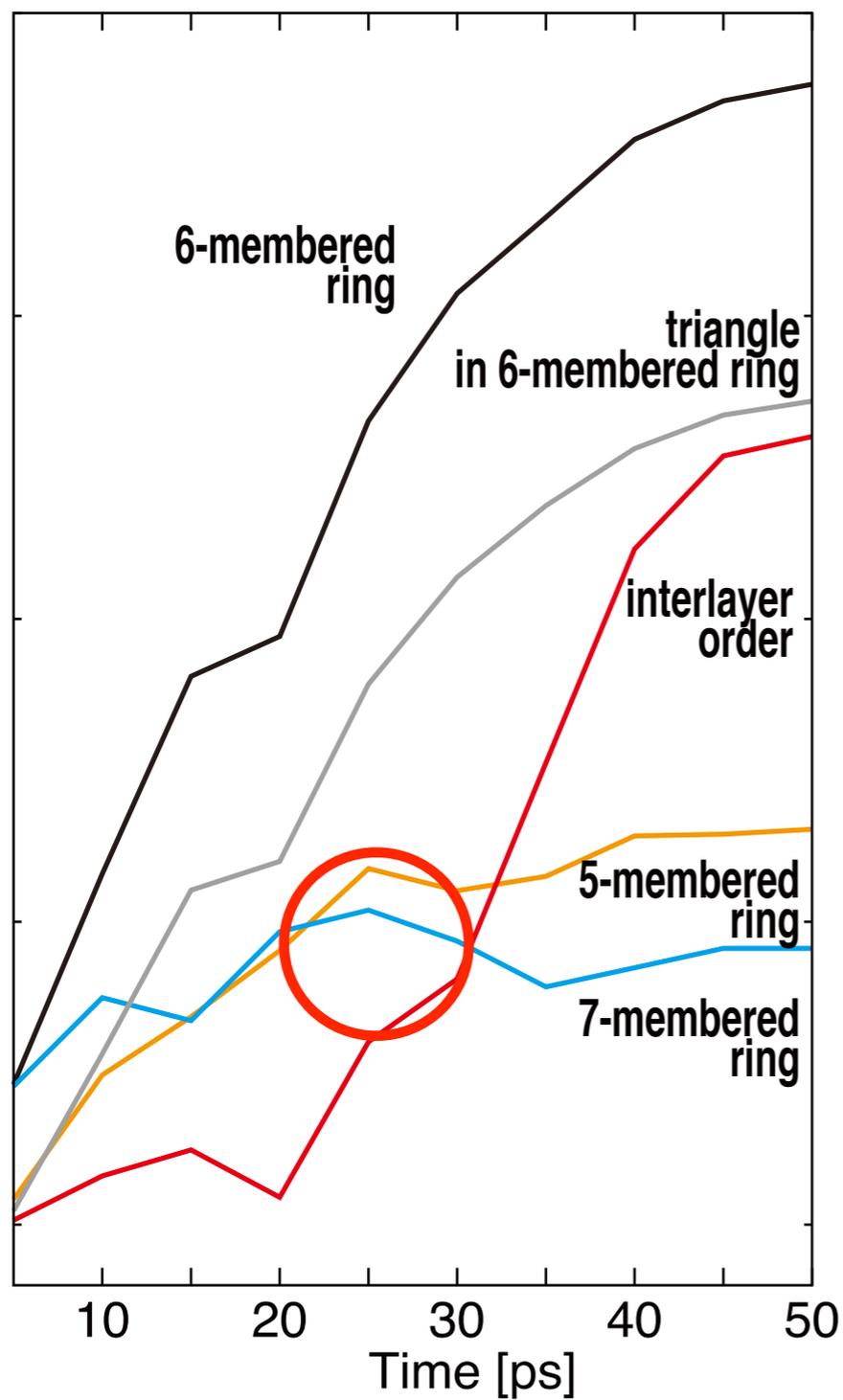
最安定構造の候補 (上位1%)



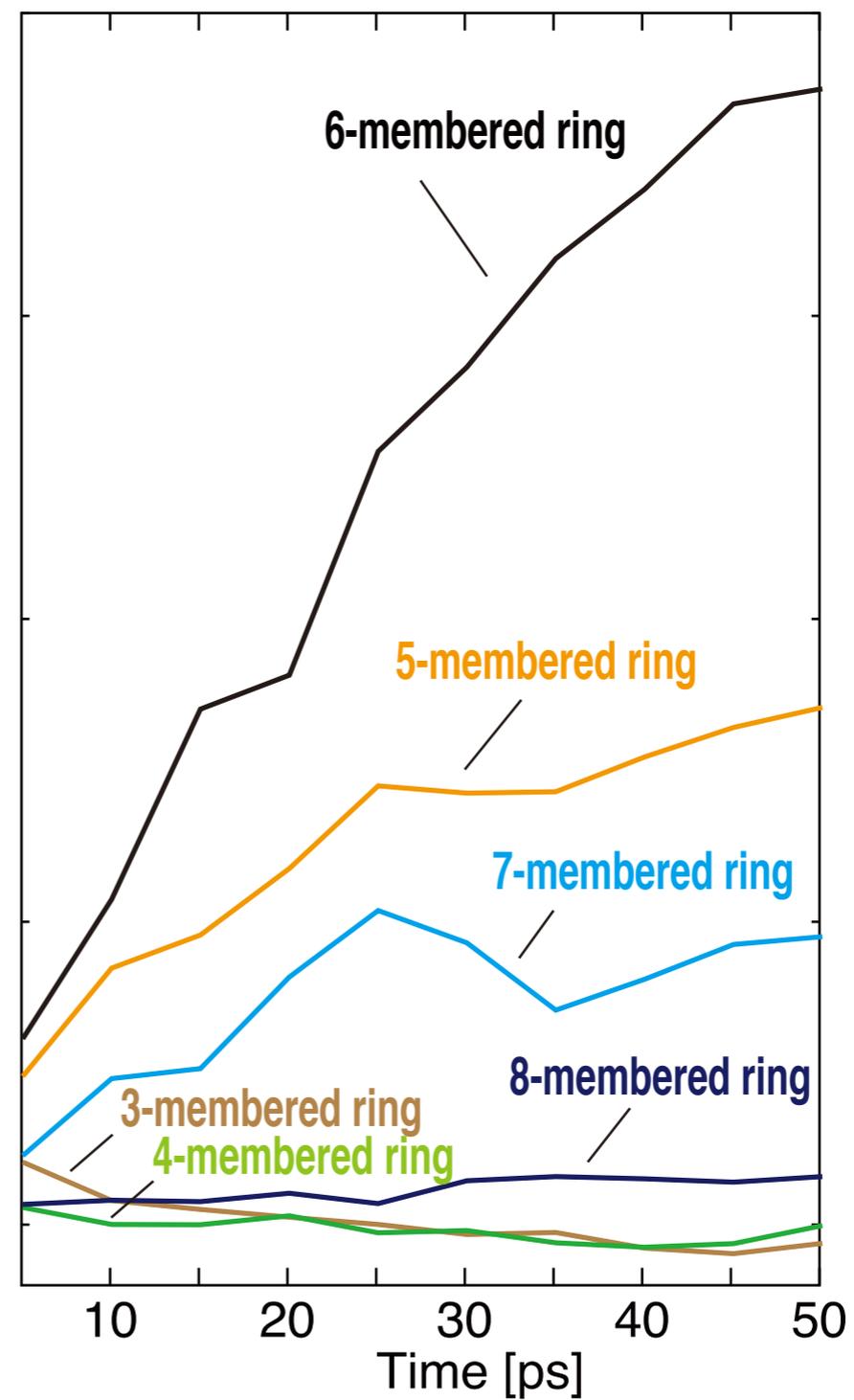
変化を捉える

Quantification of Structural Motifs

of generators in PD



conventional ring analysis

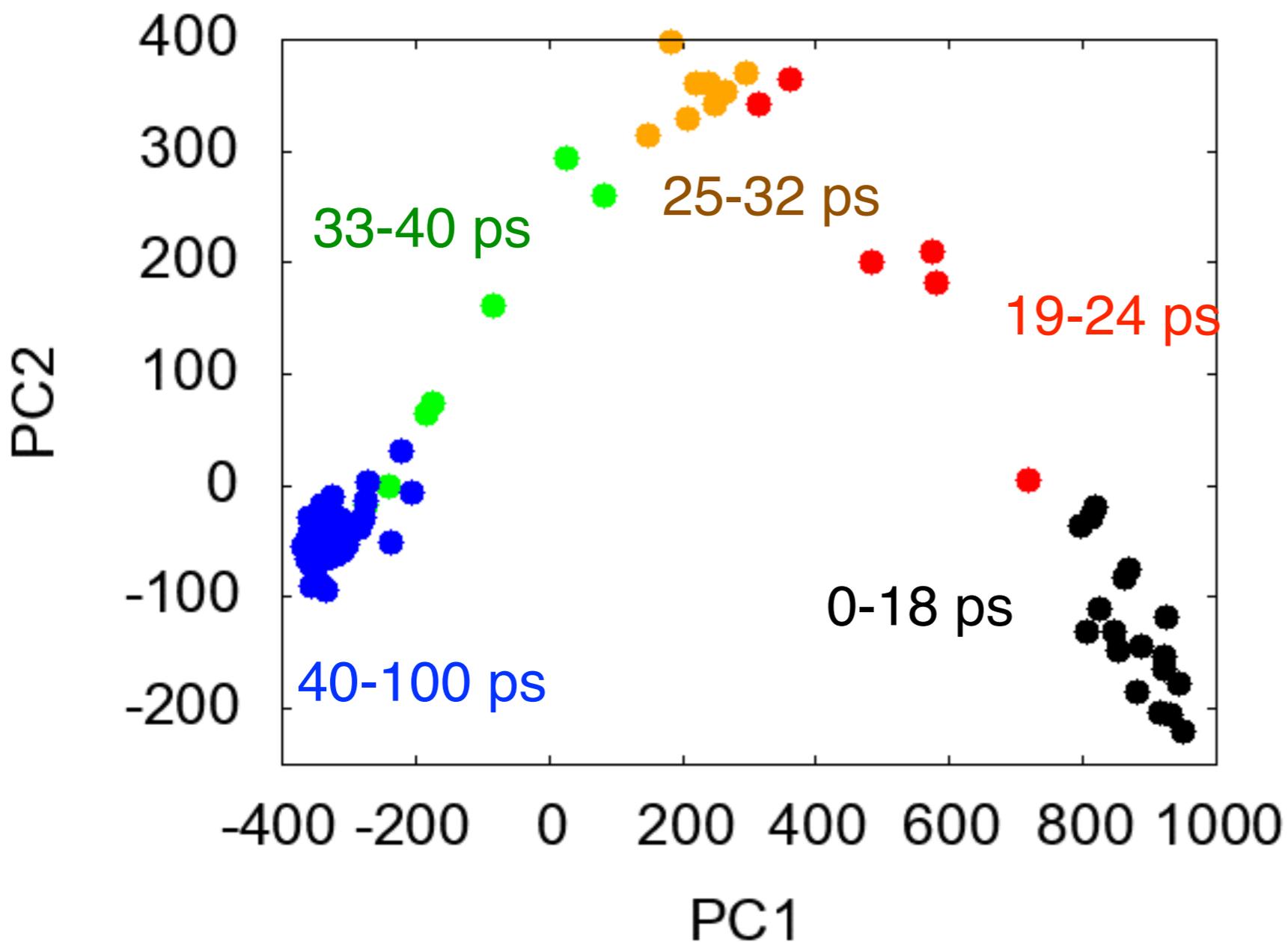


Interlayer order can also be quantified based on PD.

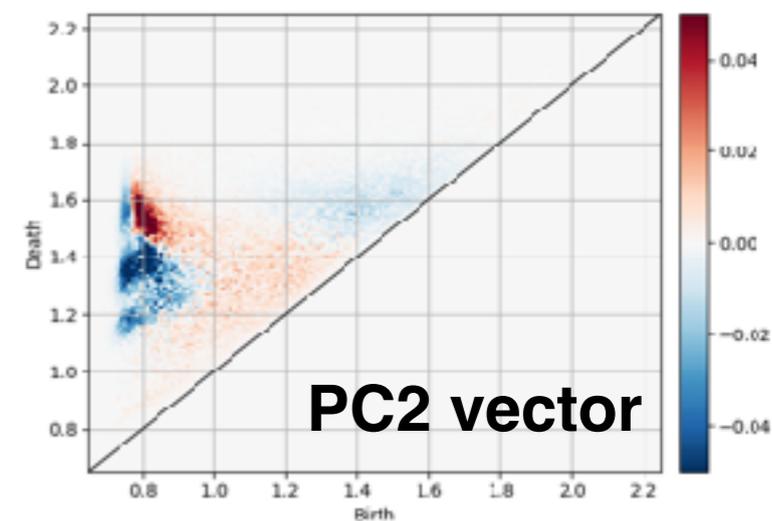
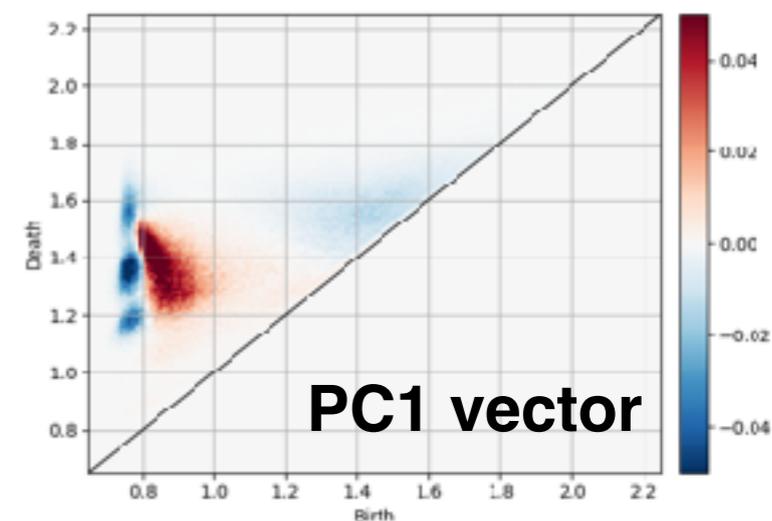
Detecting transformation of ring structures

7員環の増減

PCA of PD₁



6員環の増減

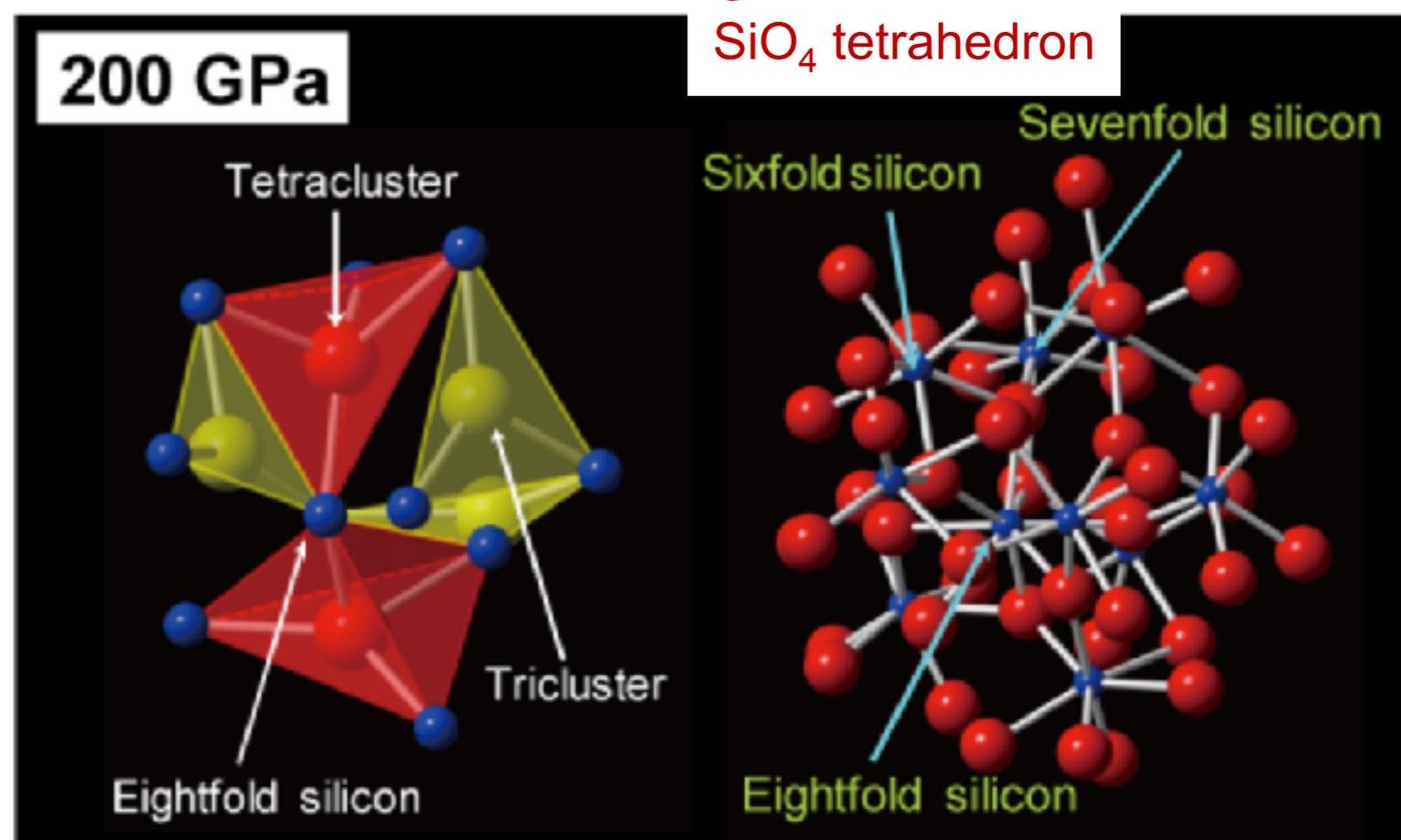
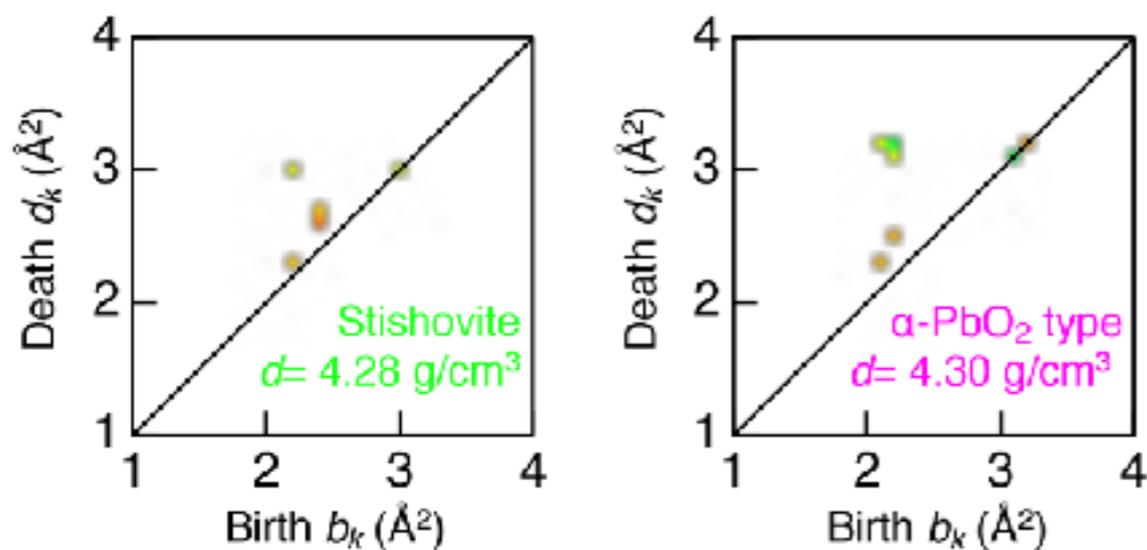
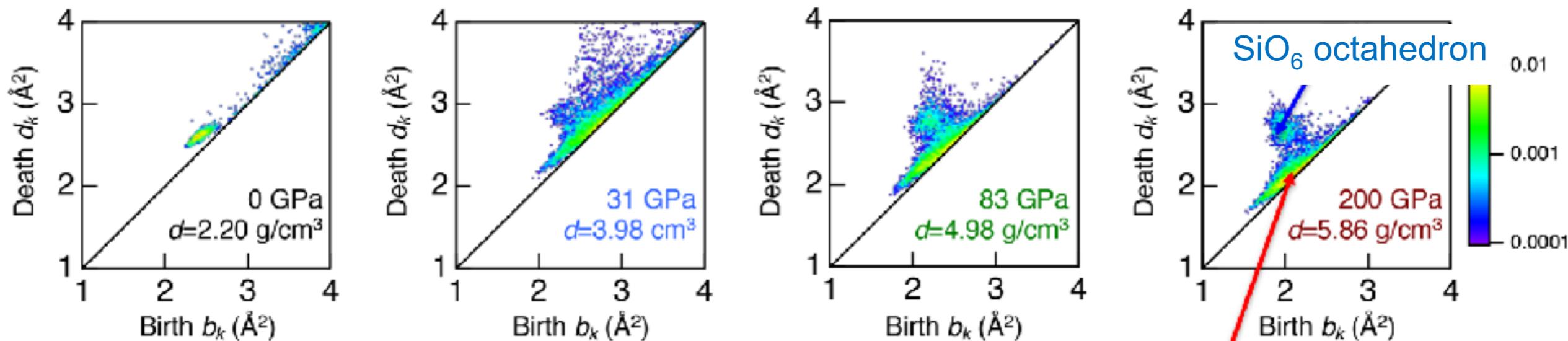


実材料の解析

ガラスの構造の本質を語る

Novel Structure in Oxide Glass

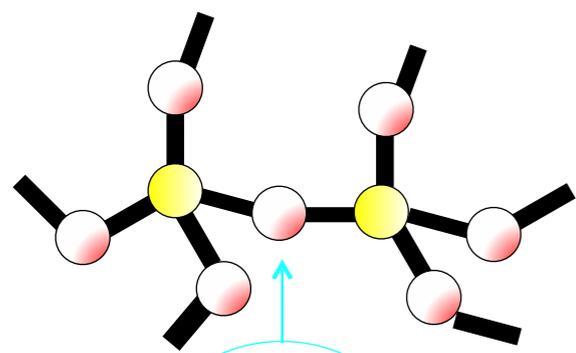
(小原、小野寺、増野、田原)



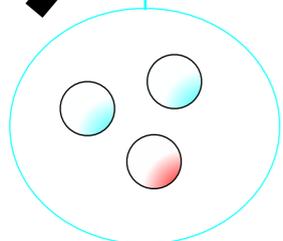
Transition from tetrahedral SiO₄ to octahedral SiO₆ (PD₂)

Structural origin of mixed alkali effect in alkali silicate glass

(小原、小野寺、増野、田原)

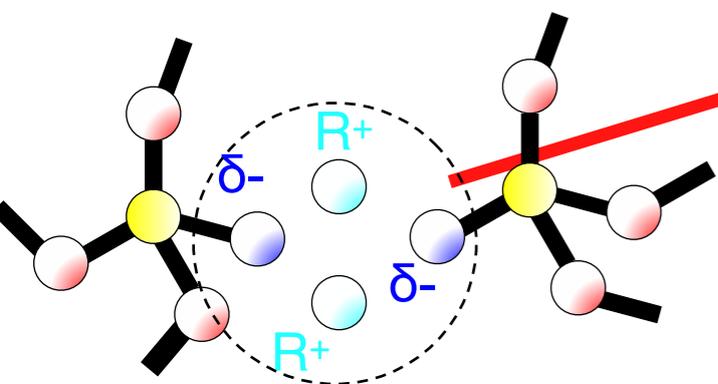


Yellow : Si
 Red : Bridging O (BO)
 Blue : Non-bridging O (NBO)
 Cyan : R = Na, K

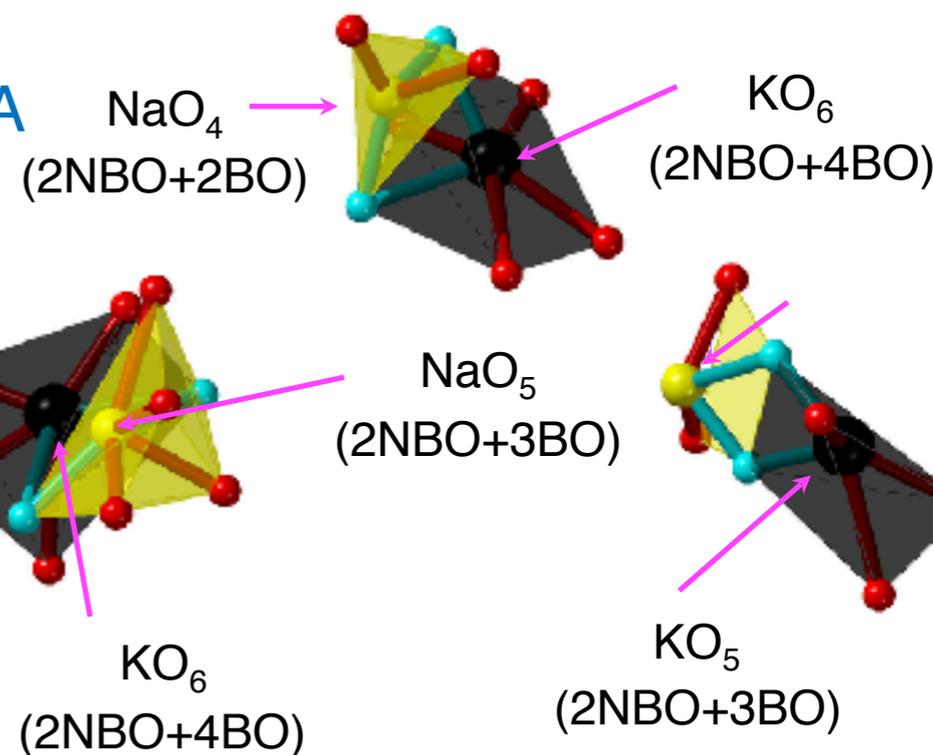
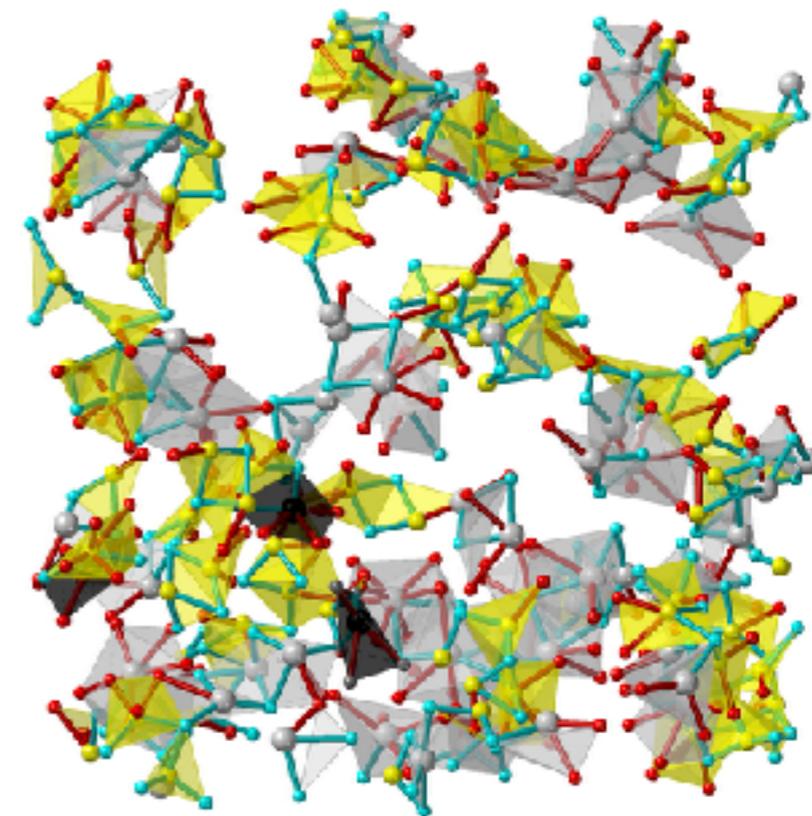


R_2O

remove one BO
 put two NBO



Four-membered rings with R_2NBO_2 are detected by TDA
 → Getting aware of hidden correlation between Na and K



Two alkali ions are trapped around these two NBO to compensate negative charge.

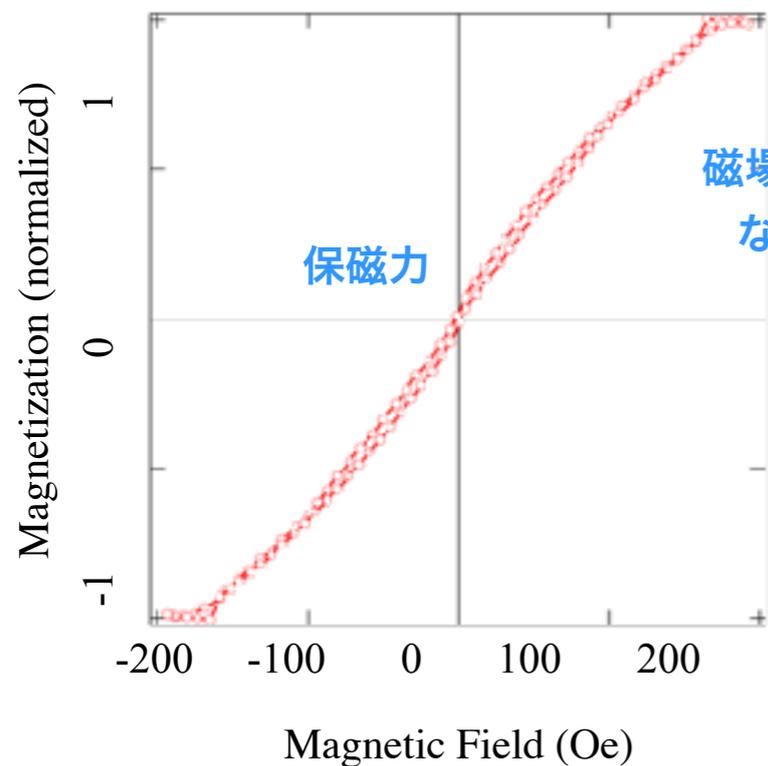
Information beyond “pair-correlation” plays an important role!

磁区構造から情報を取り出す

非平衡成分のマッピング

(小飼)

磁気ヒステリシスループ

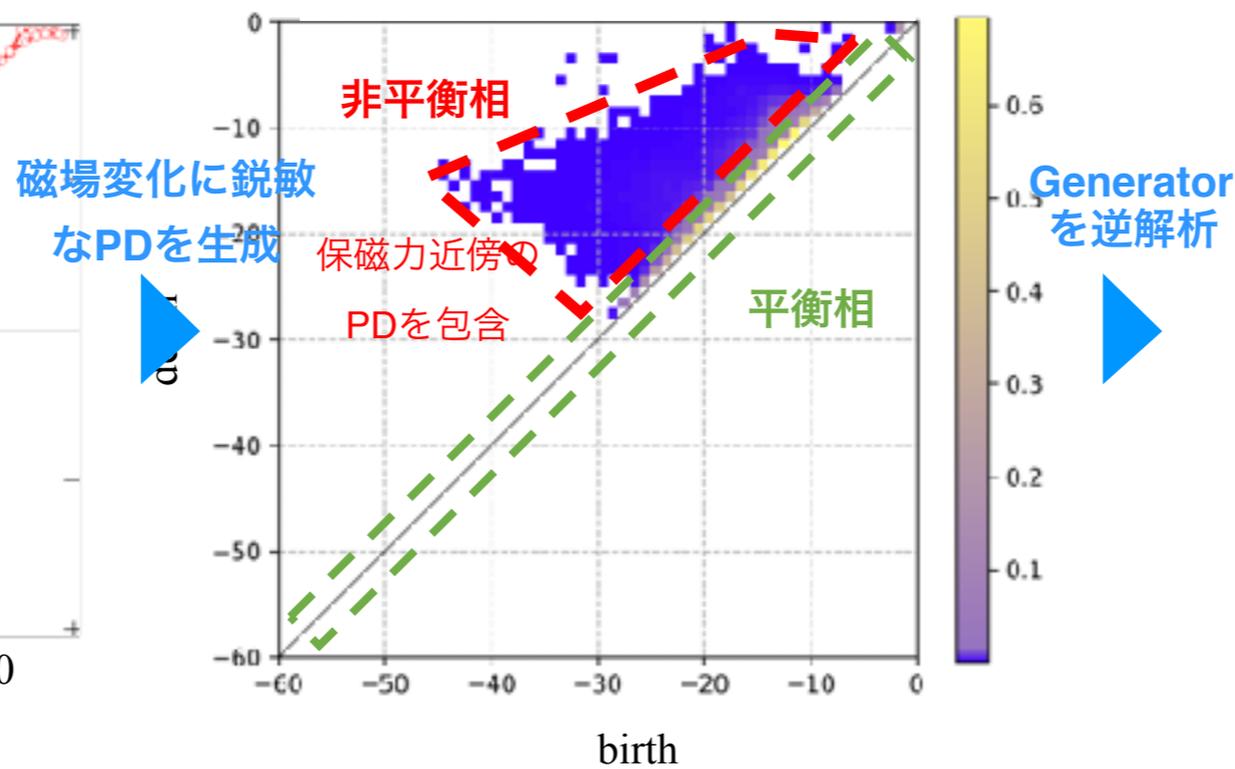


保磁力近傍

→ 磁化率が最も高い

→ 外部磁場変化に最も鋭敏

PCA loadingから作成したPD



PDにおいて保磁力に寄与する
非平衡相に相当する部分を同定

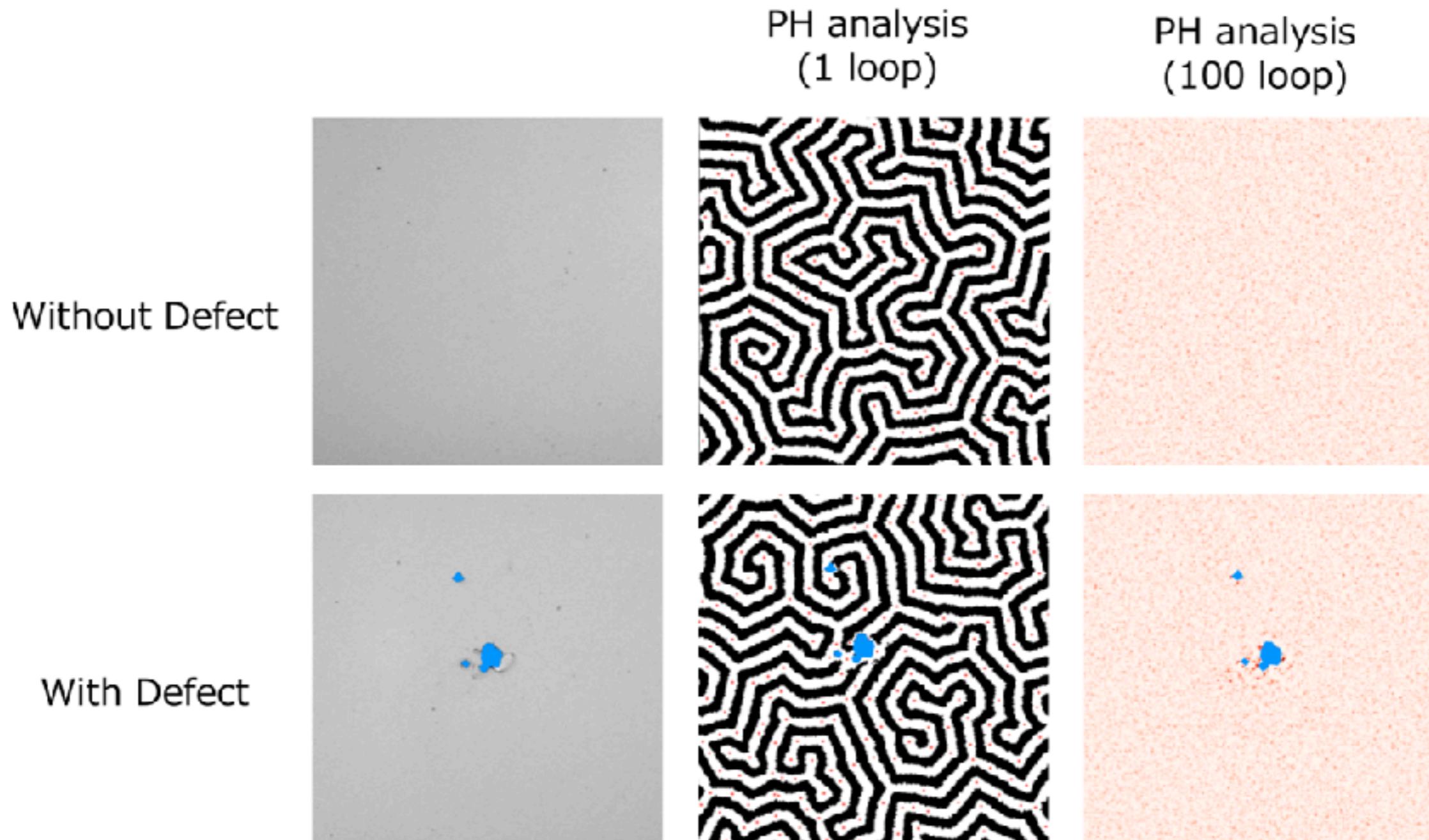
PDから元の磁区構造に逆解析



逆解析により迷路状磁区構造の
トポロジカル欠陥を可視化

パーシステンス図と主成分分析を用いたピンニングサイトの可視化

(小飼)

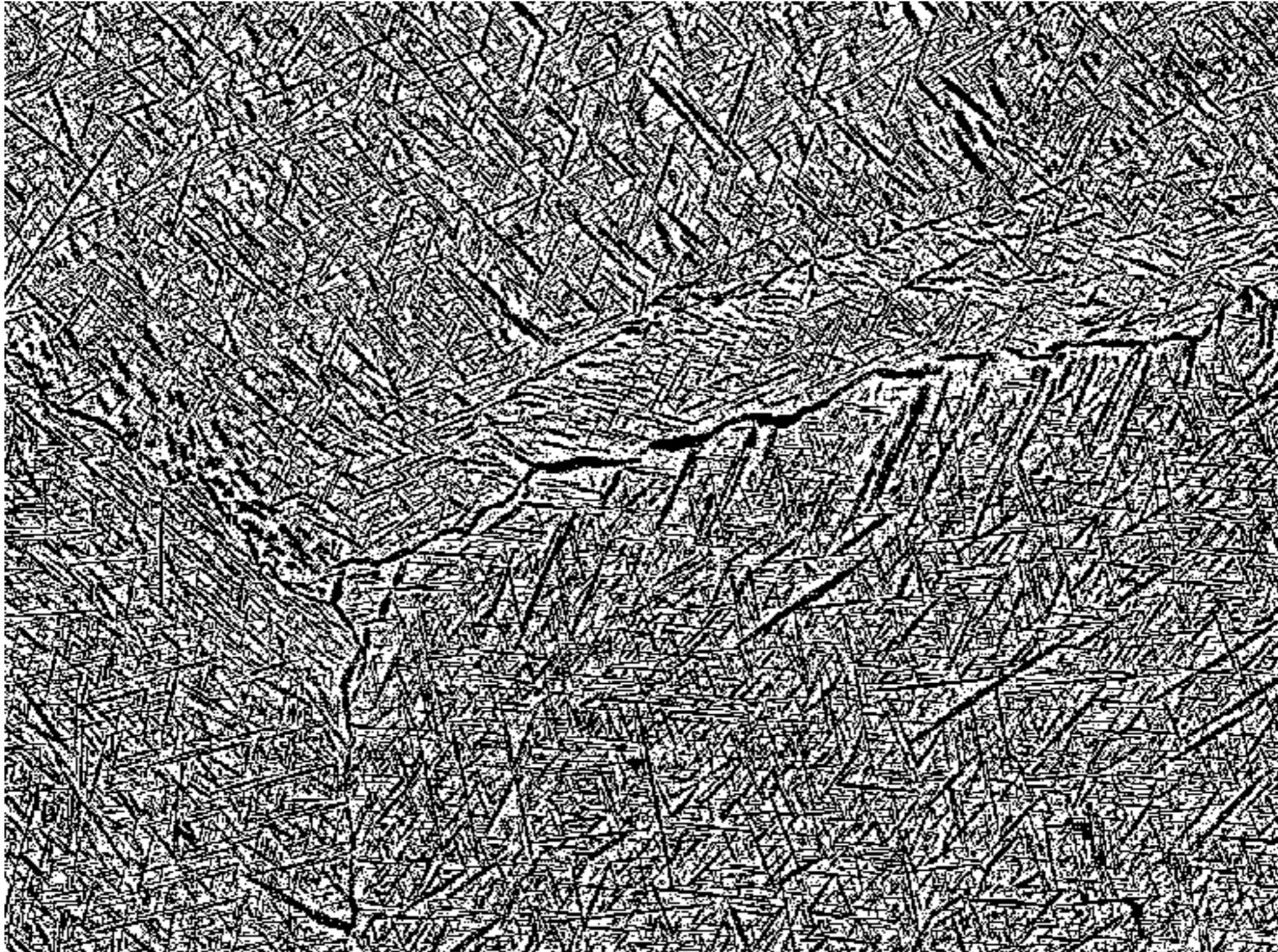


磁区構造のパターン自体は毎回異なるが、
「トポロジカル欠陥」の場所を積算してみると
格子欠陥の近傍がピンニングサイトになっている様子があった

構造を「測る」 I

SEM image of forged Ti alloy

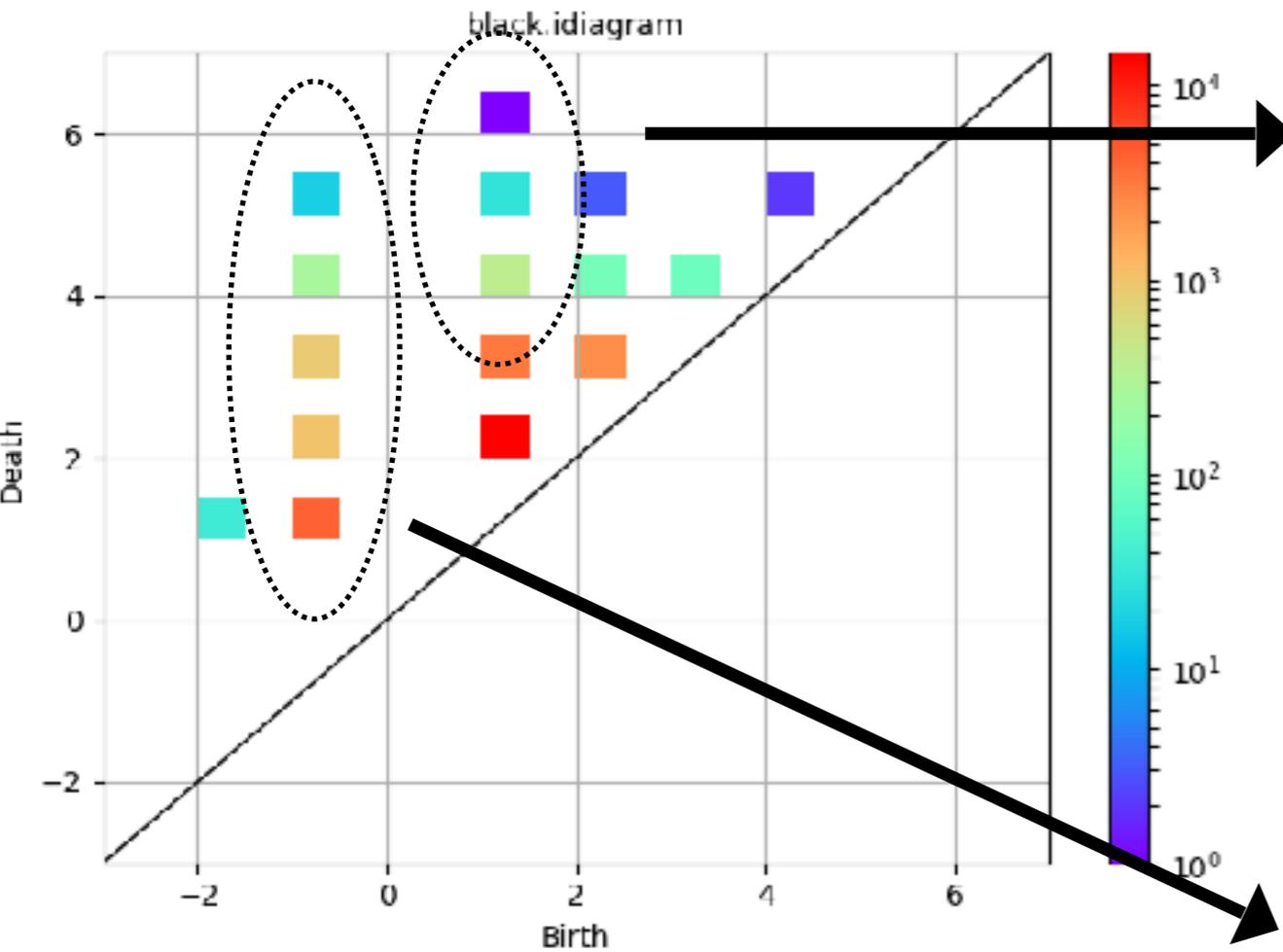
(provided by KOBELCO)



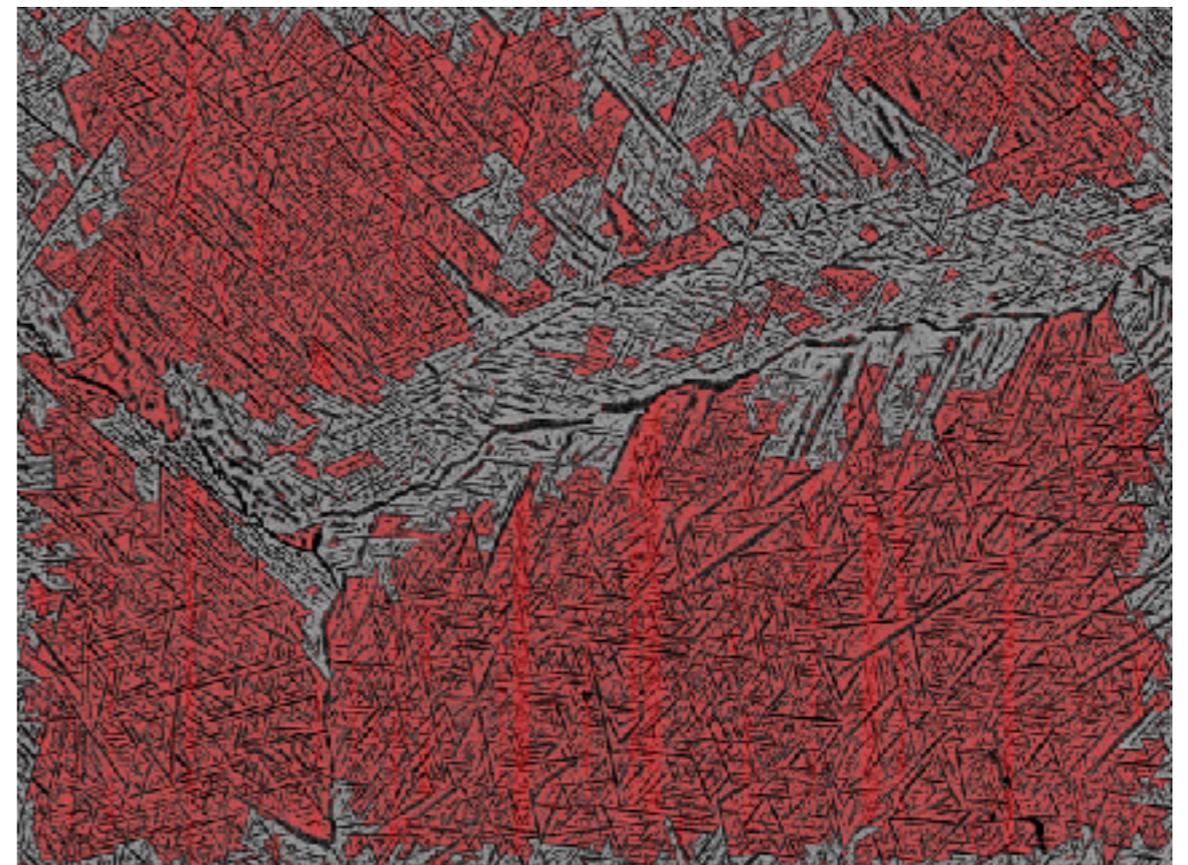
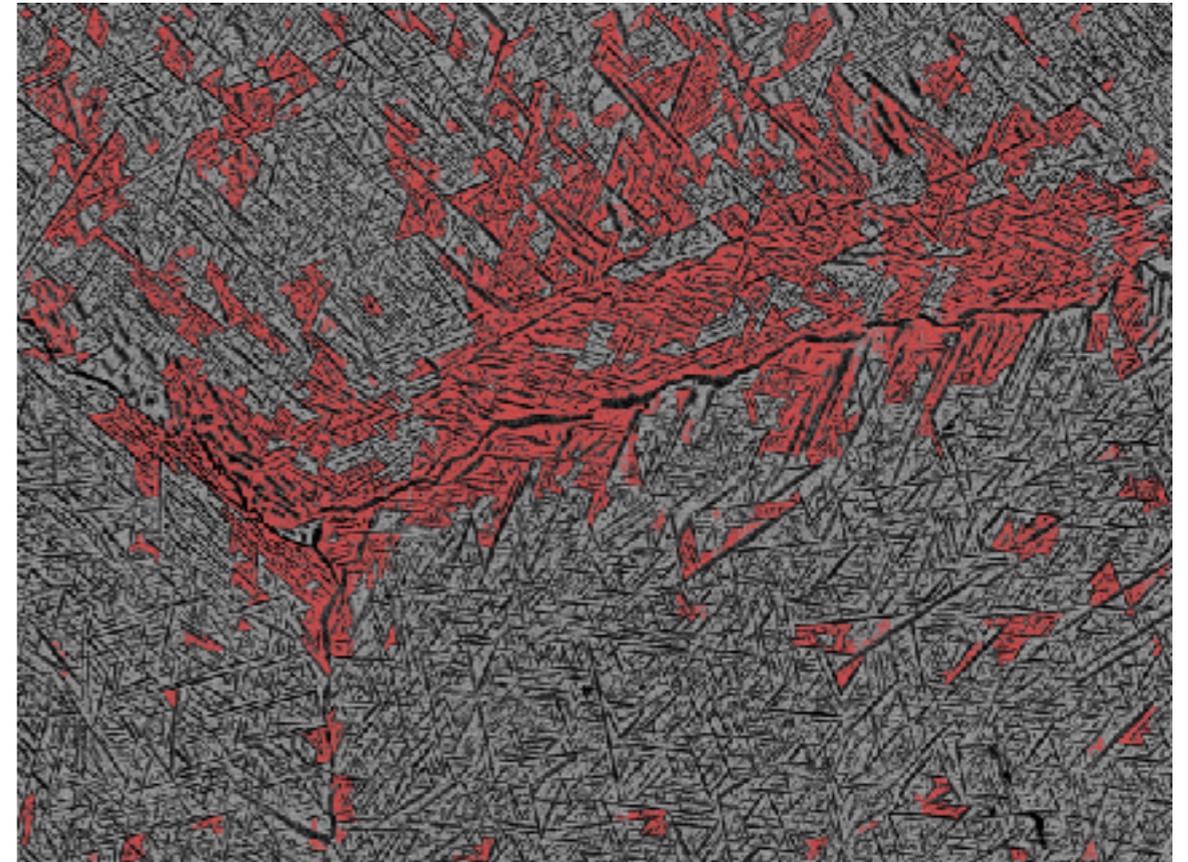
dark part : α -phase (hcp structure)

bright part : β -phase (bcc structure)

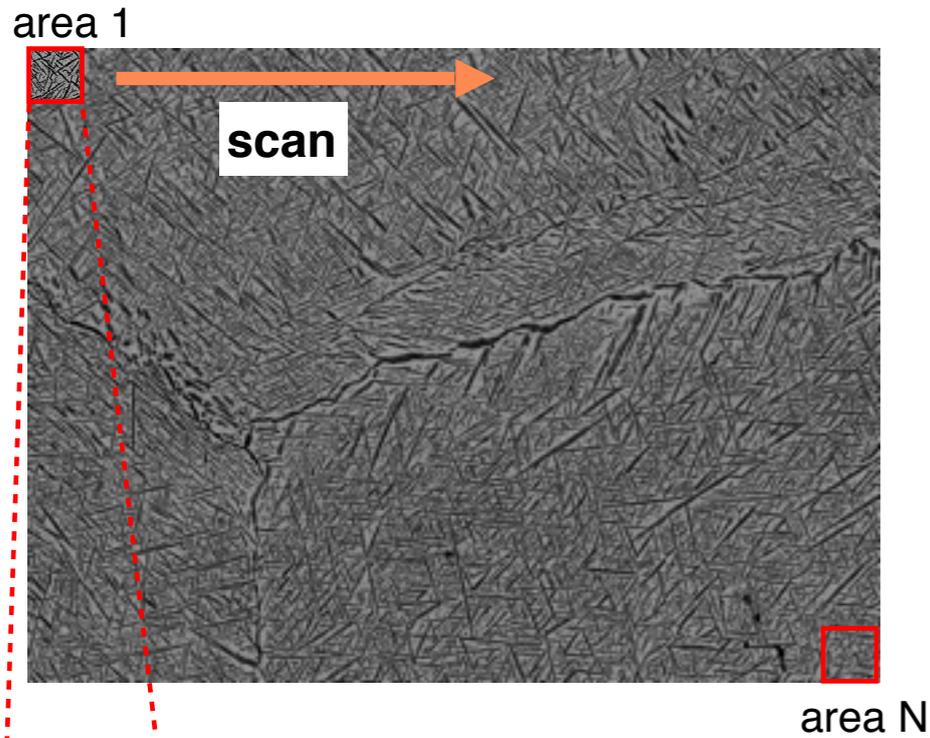
Quantitative characterization by inverse analysis of persistence diagram



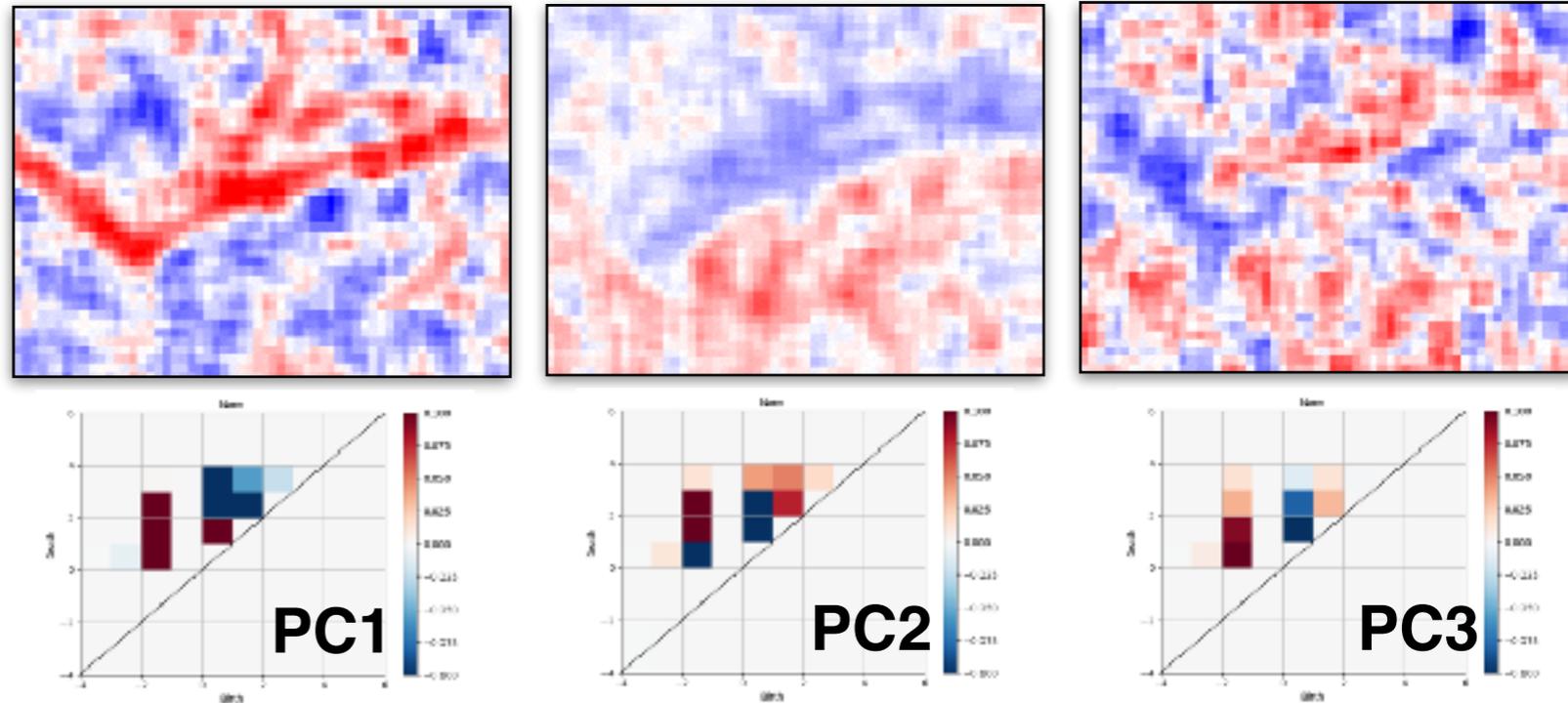
- 複雑な画像をコンパクトに記述
- 特徴ごとに定量化
- 不均一性の抽出



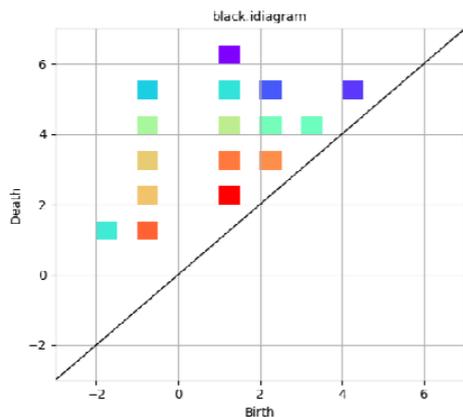
Quantitative characterization by PCA of local structures via persistence diagram



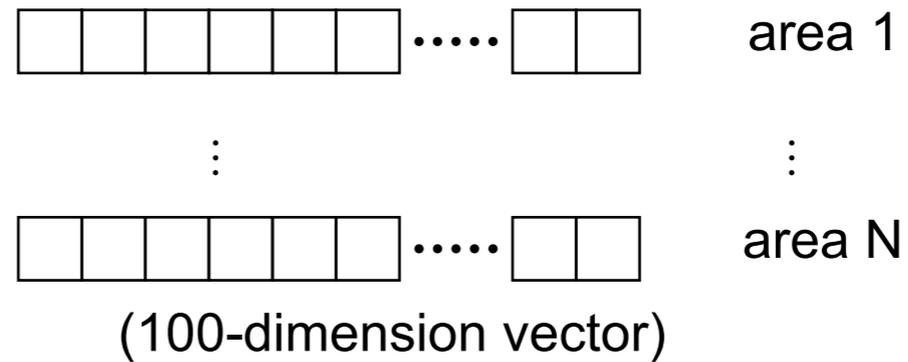
Different characterization by different feature values



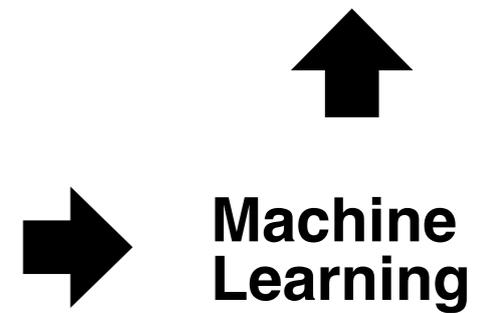
a set of PDs from massive small cells



Persistence Diagram (PD)



Primitive Descriptor



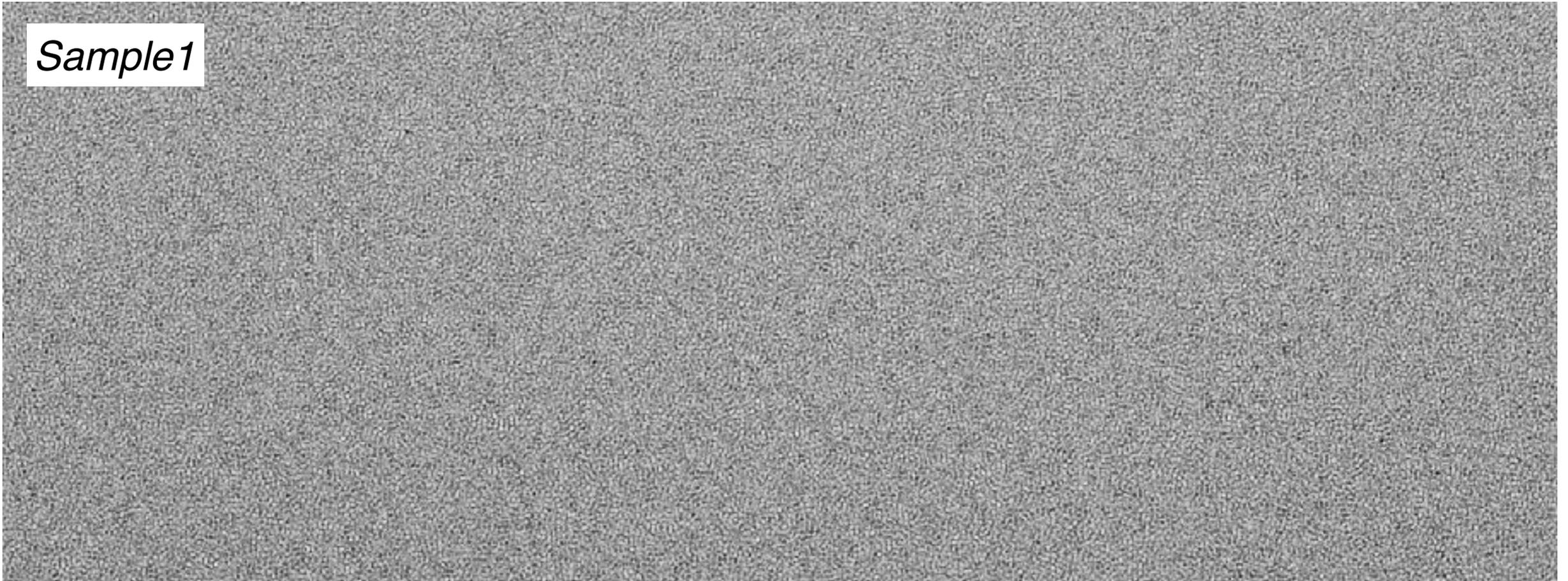
画像内の局所構造の分布を自動抽出&可視化

構造を「測る」 II

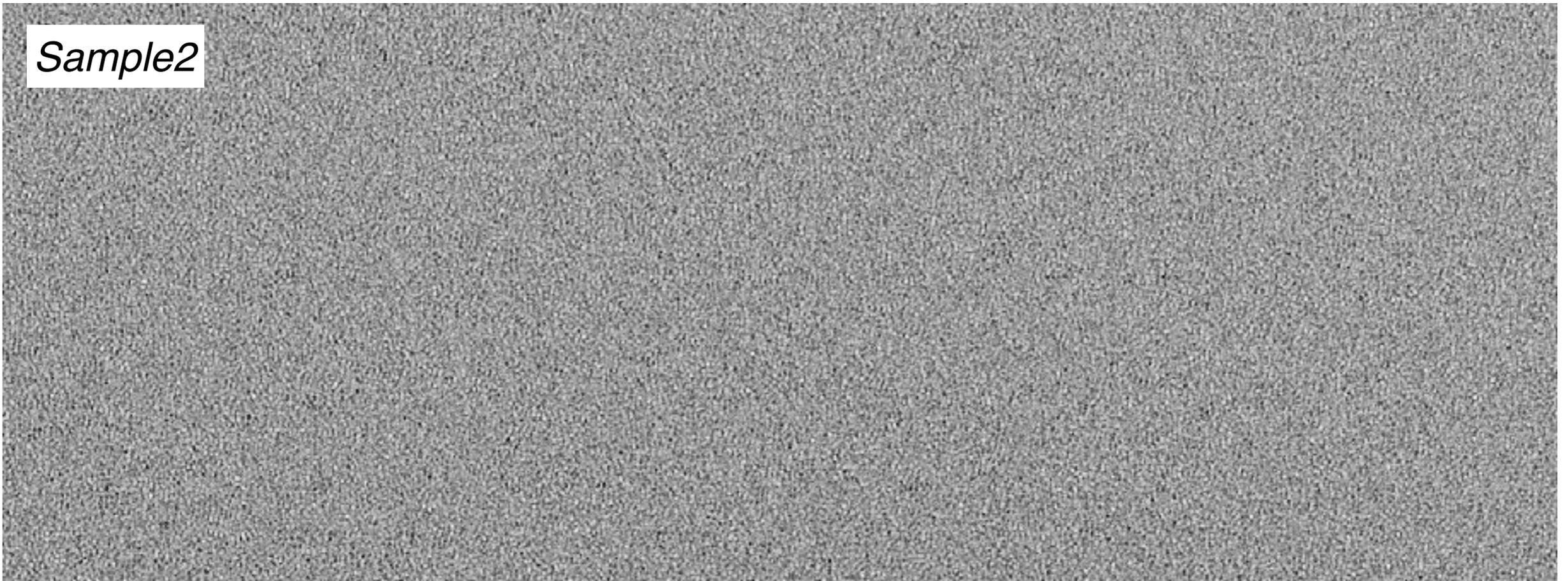
Can we distinguish TEM images of amorphous Ge?

(Xu)

Sample1

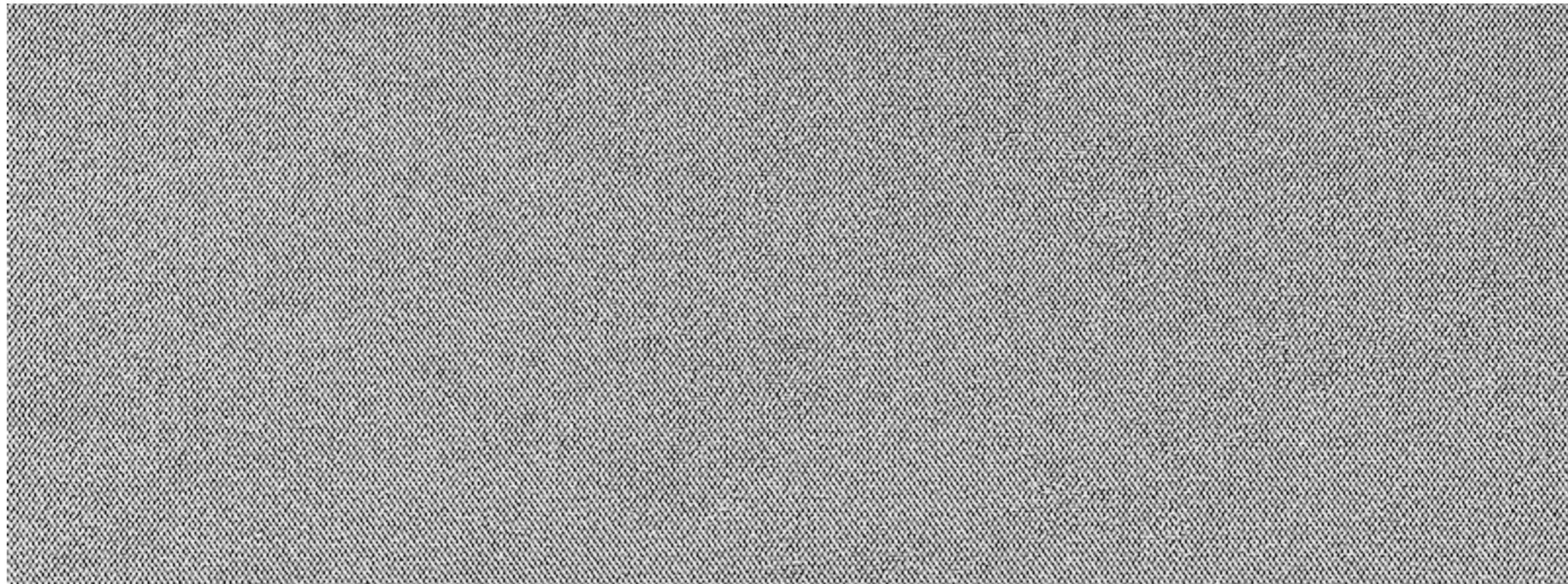
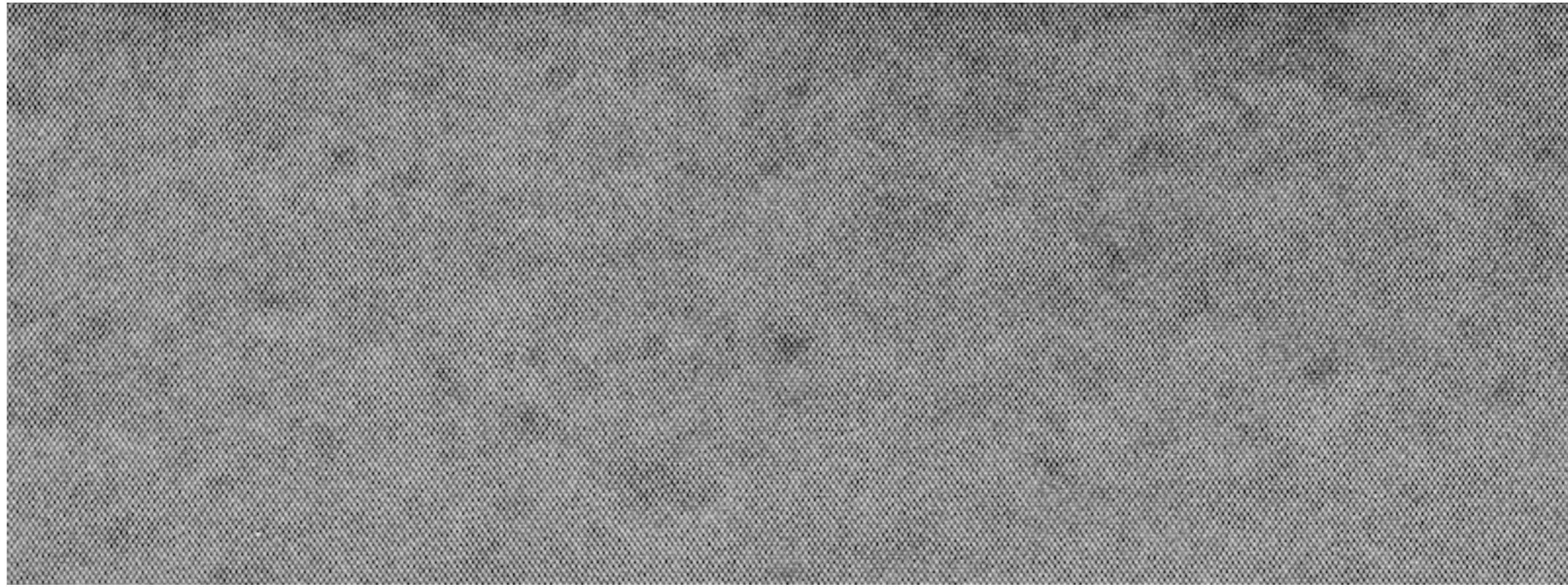


Sample2



Appropriate pre-conditioning

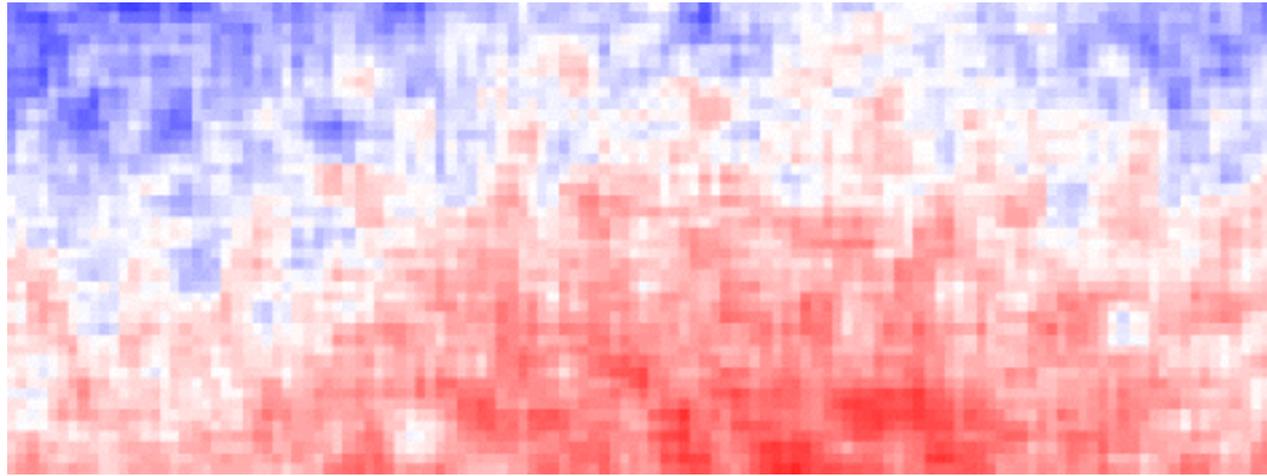
Si substrate



without pre-conditioning

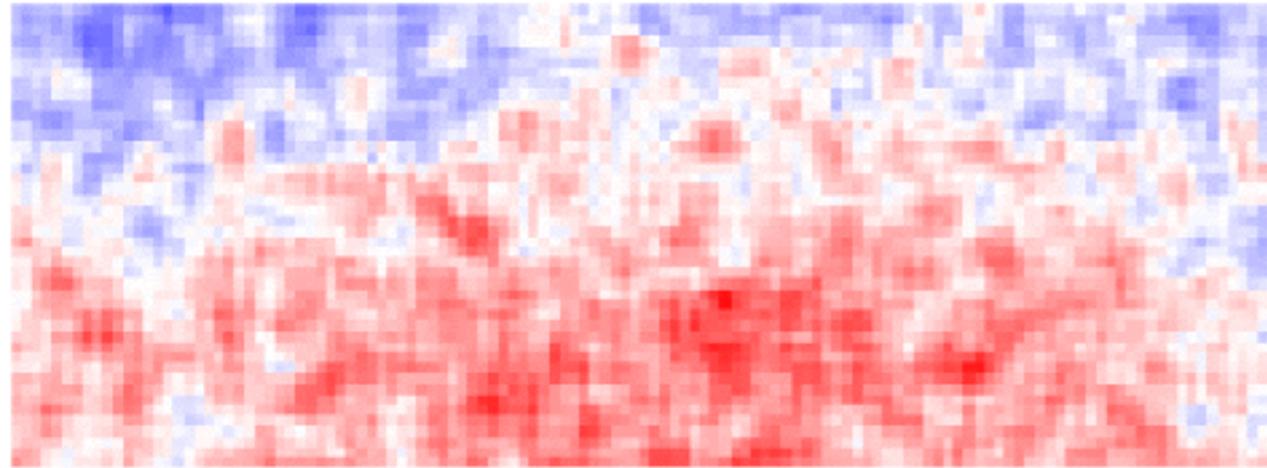
Binarized PD0 PC1

Sample1



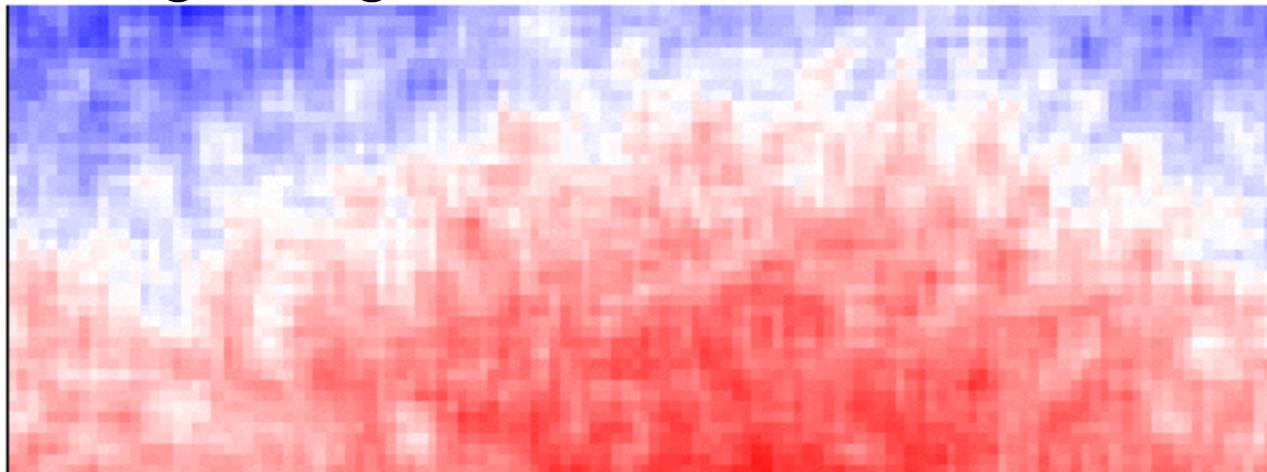
Binarized PD1 PC1

Sample1



Averaged Brightness

Sample1

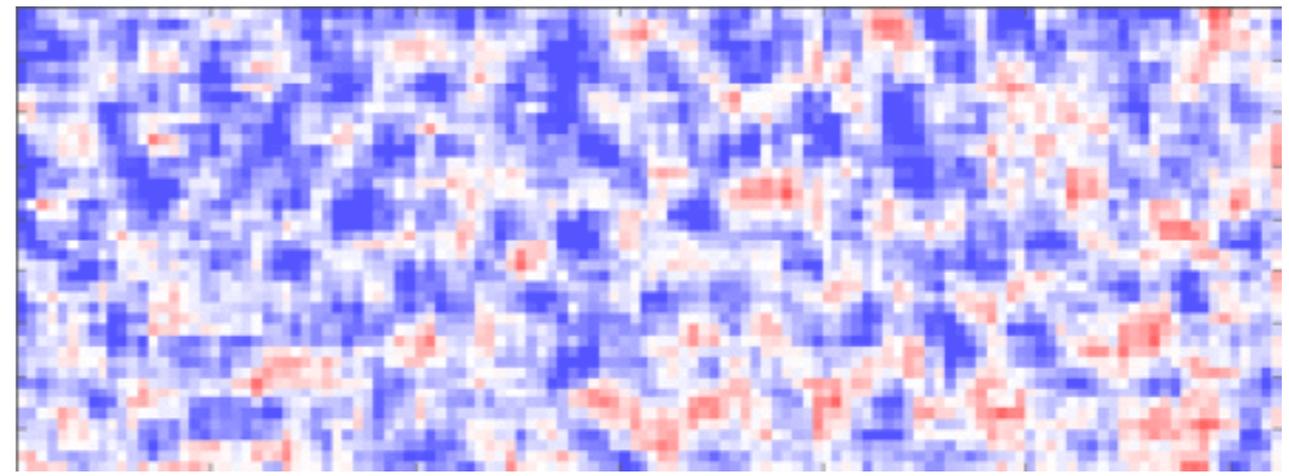


輝度情報が前面に出る (欲しい情報ではない)

with pre-conditioning

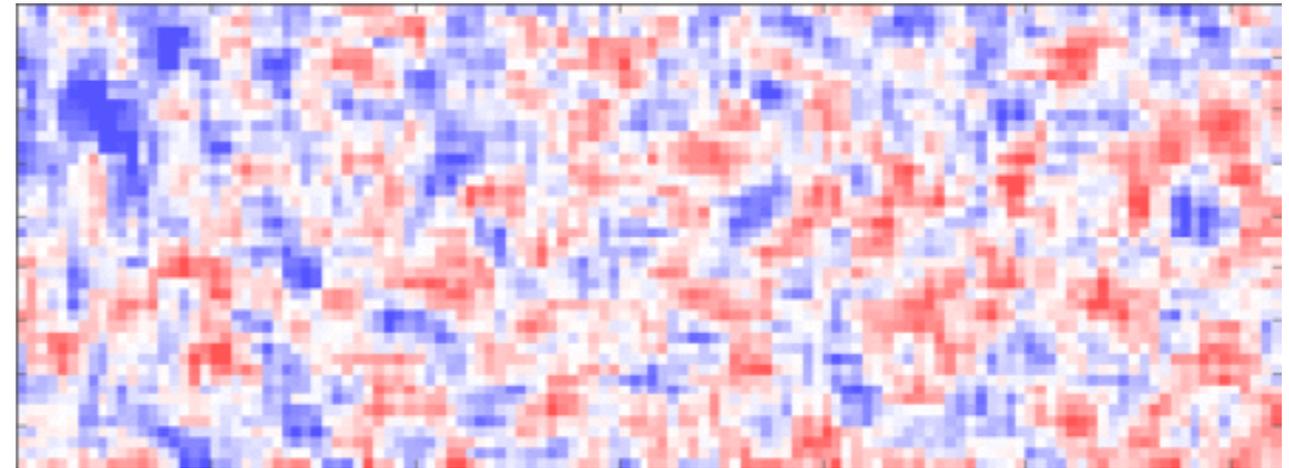
Binarized PD0 PC1

Sample1



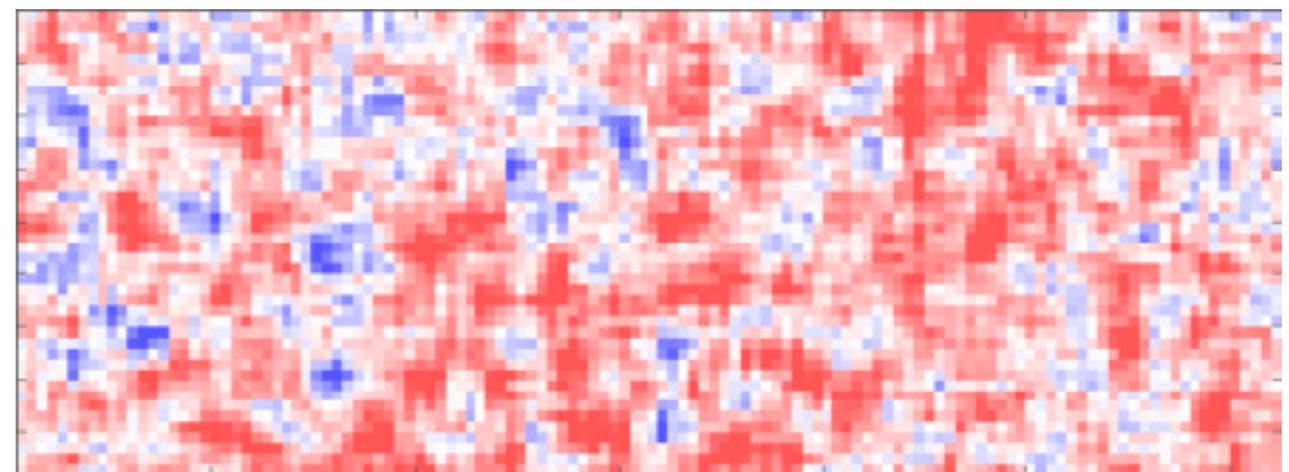
Binarized PD0 PC1

Sample2



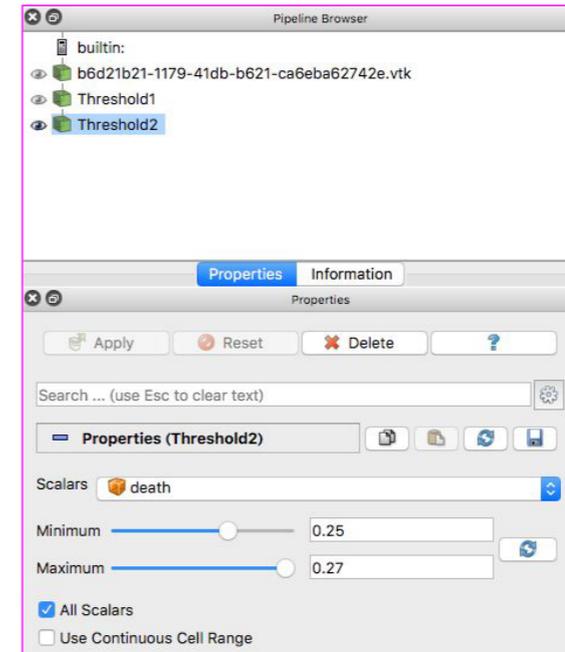
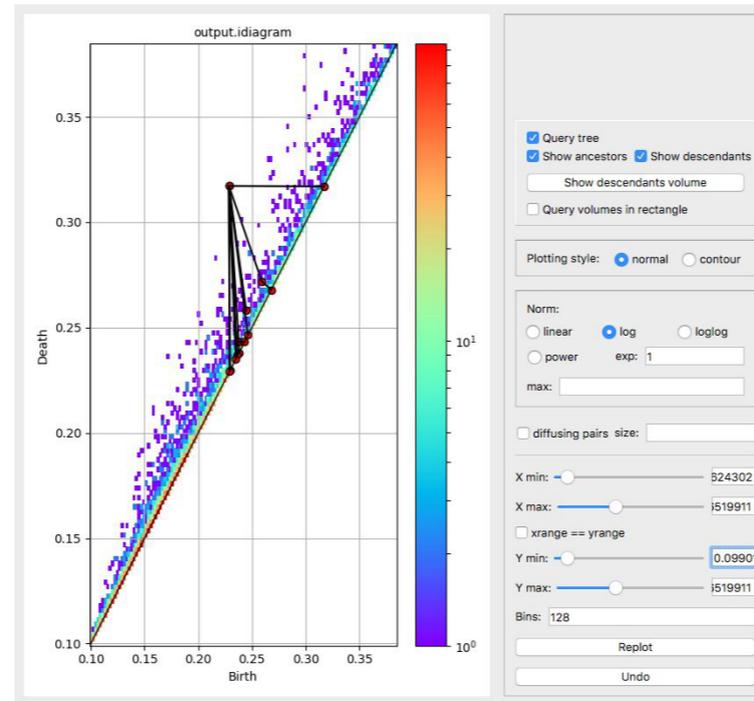
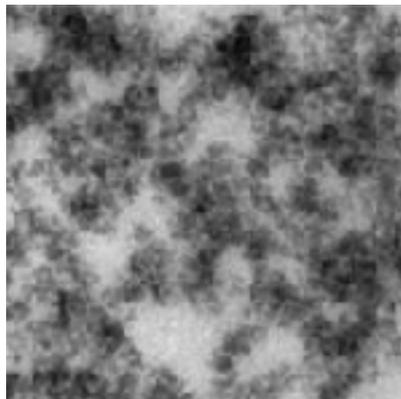
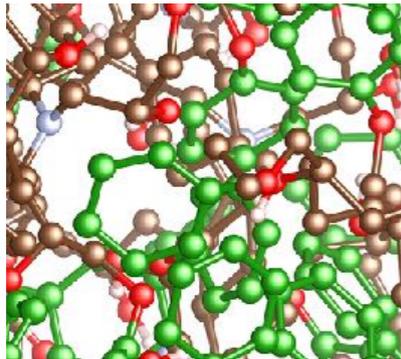
Binarized PD0 PC1

Sample3



「形」の情報に基づく分類

HomCloud



- 原子配置や画像データ (2D,3D) を入力
- パーシステント図の計算 (順解析)
- (b,d)点に対応する構造を入力データにマップ (逆解析)
- Python による実装
- GPL v3 の下での公開

Search now "HomCloud AIMR" !

HomCloud コミュニティの立ち上げへの要望

開発中心のフェーズから応用展開のフェーズへ

→ 共同研究の内容の深化

→ プロジェクトを通じた「社会実装」

一方、「使ってみただけれど…」の声も多数

- 普及と啓蒙（理解の向上、誤解の解消）
- 適用事例の集積と共有
- 「足りないもの」を見つける（学術側・産業側の両面で）
- HomCloudの継続的な開発を支援
- 窓口を明確化

参加に関心のある方（企業、研究者個人）は赤木までご連絡ください

→ akagi@wpi-aimr.tohoku.ac.jp

ひとまず、皆様のご支援に感謝！