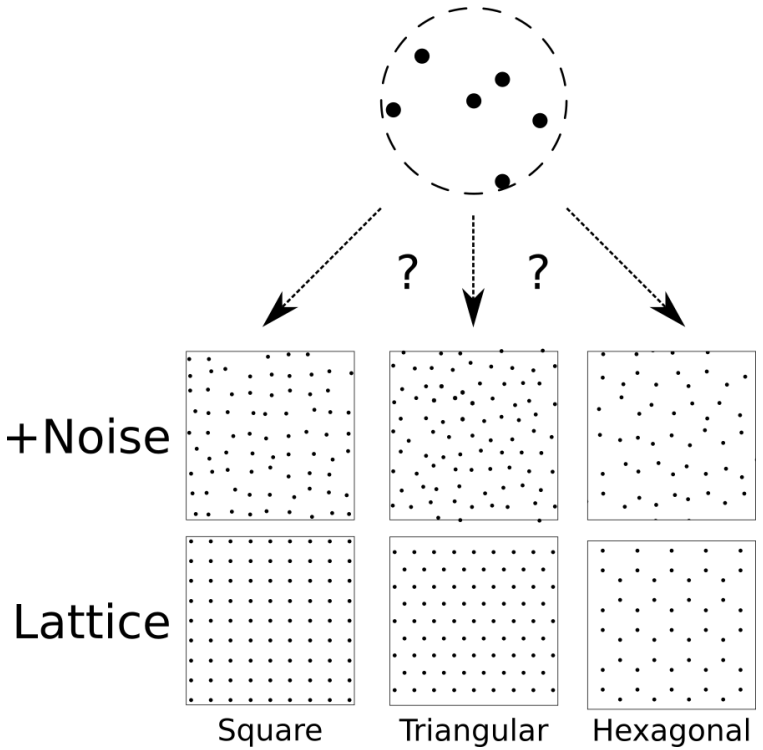
Local Feature Classification using the Euclidean Wasserstein Metric

Benjamin Schweinhart

joint work with Jeremy Mason

July 12, 2018

Main Question



What reference best matches a local atomic environment?

Input: a local atomic environment, a list of references, the temperature

Output: the most likely match

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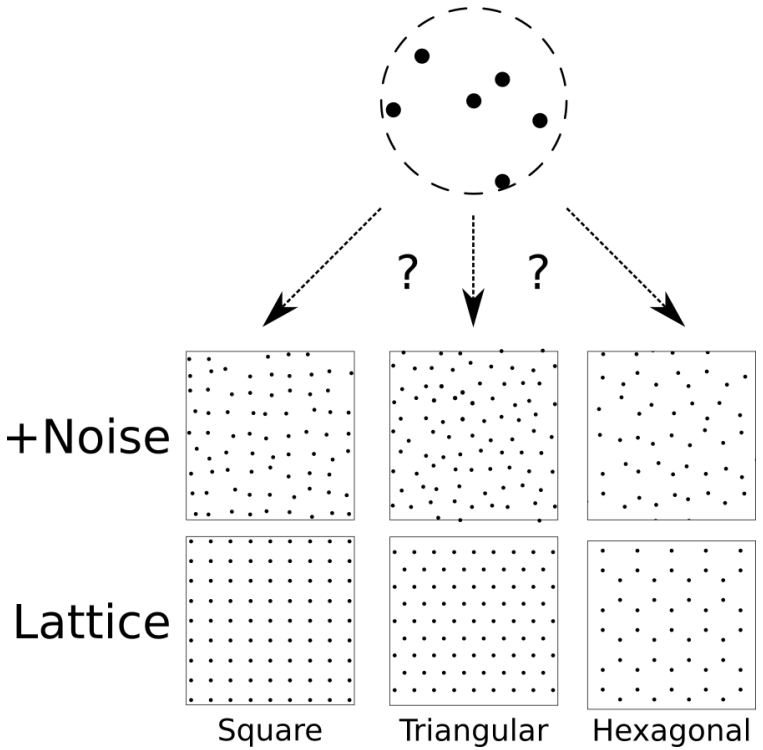

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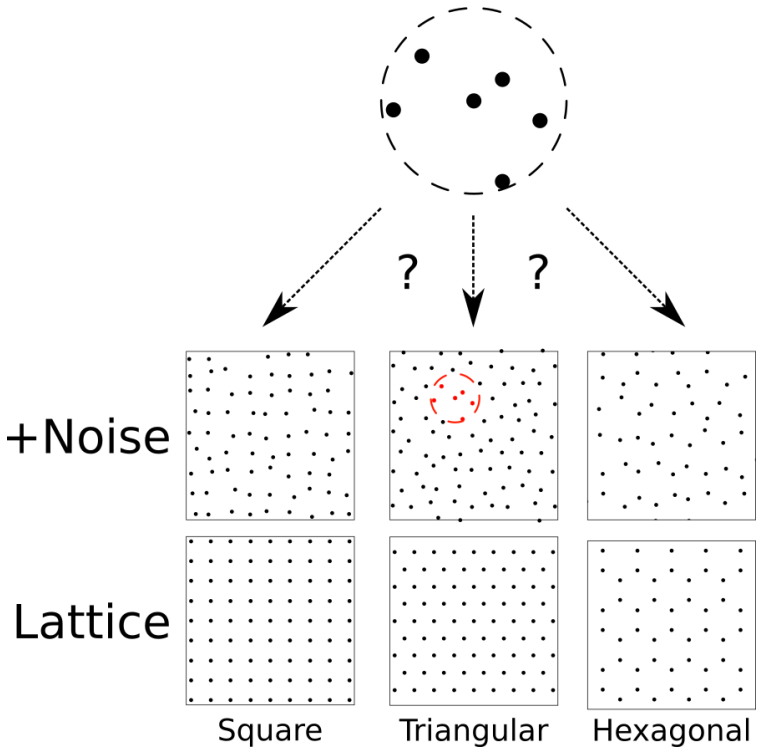

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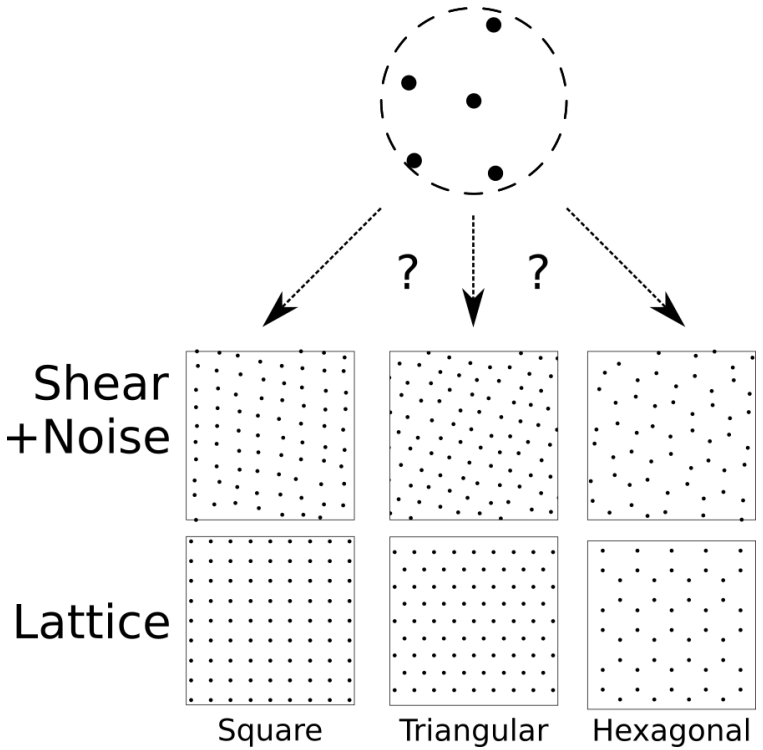

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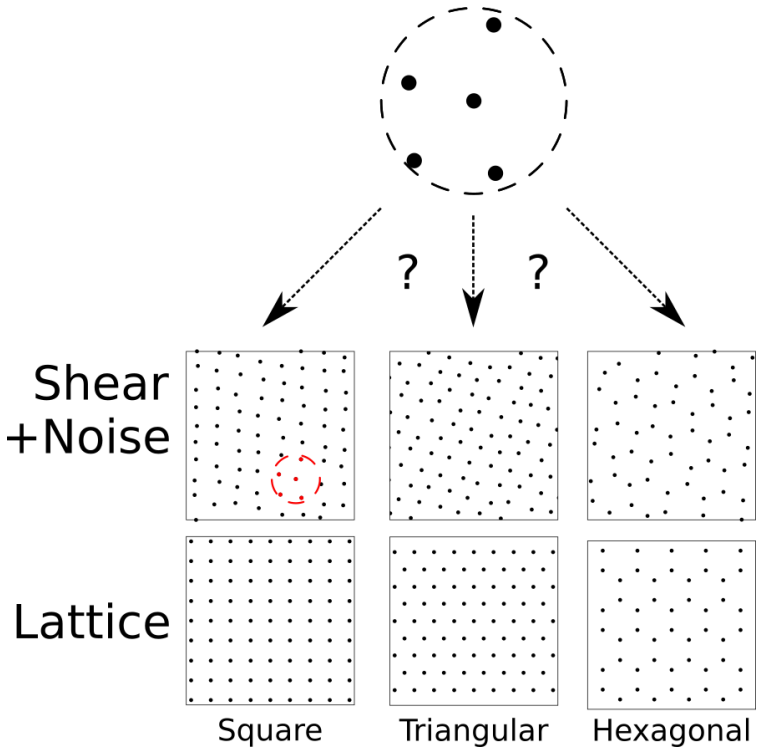

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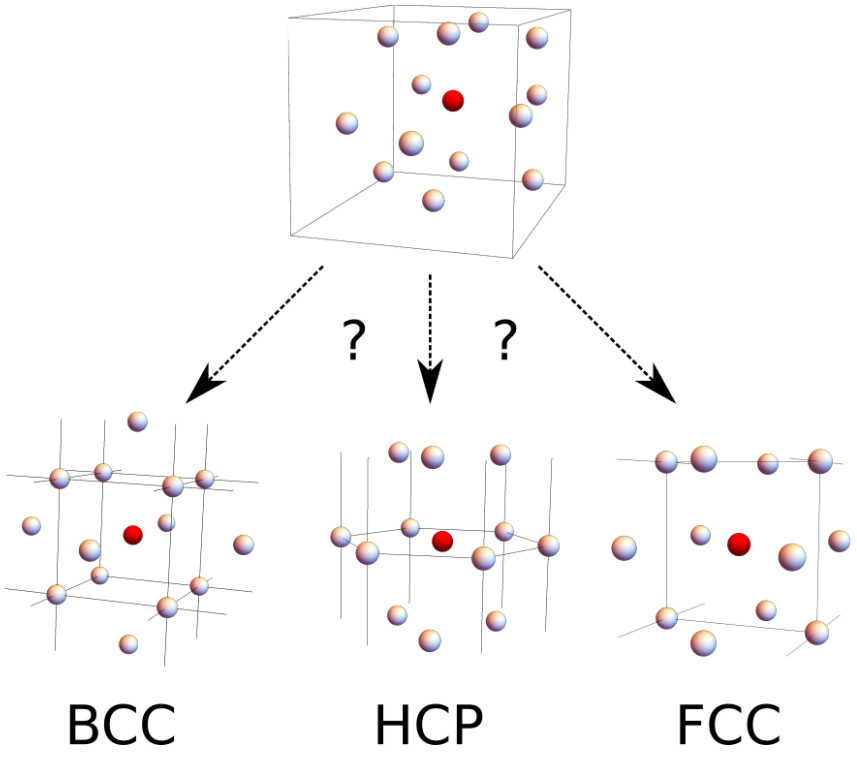

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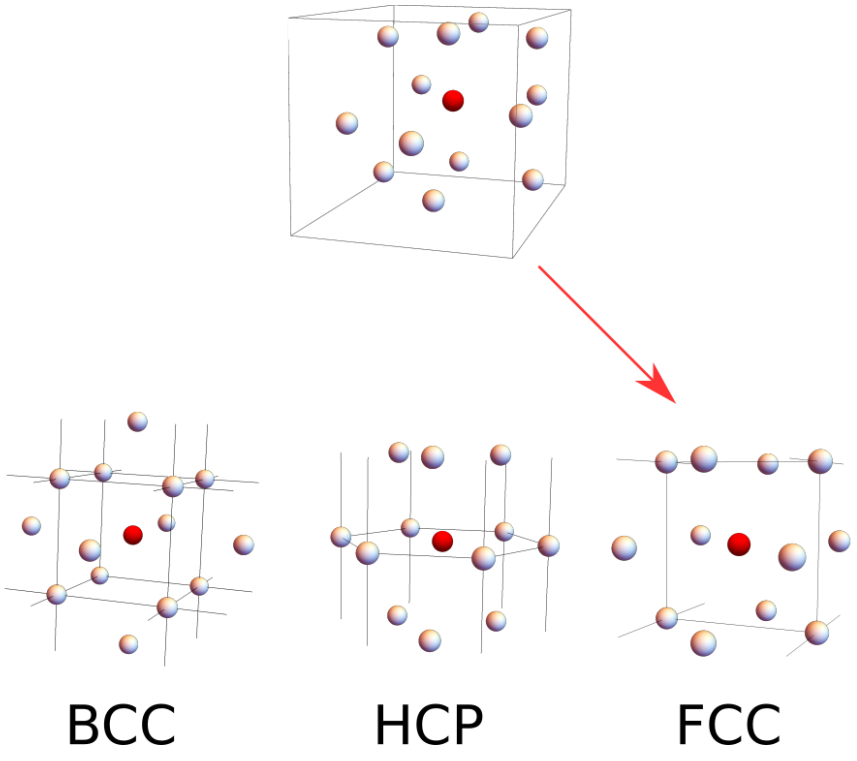

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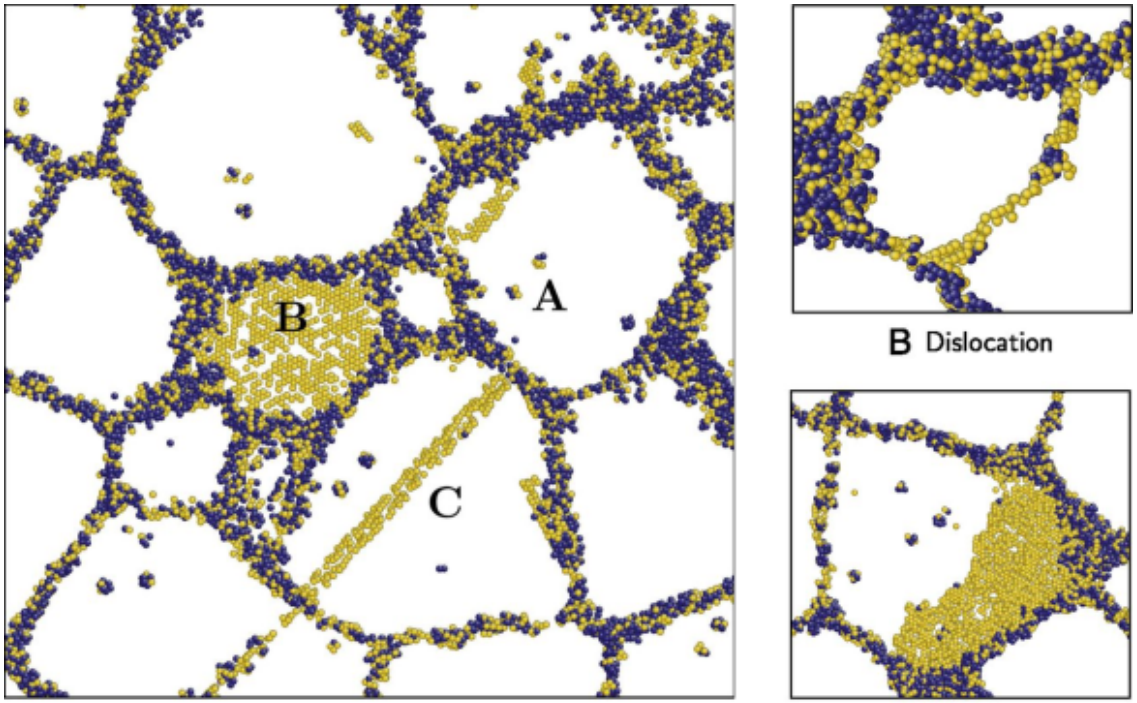
Application: Identifying Defects in a Polycrystal



A Polycrystal cross-section

B Dislocation

C Stacking fault

Many existing methods: Common Neighbor Analysis, Neighborhood Distance Analysis, Centrosymmetry, Voronoi Topology, Polyhedral Template Matching, . . .

Lazar et al, 2015

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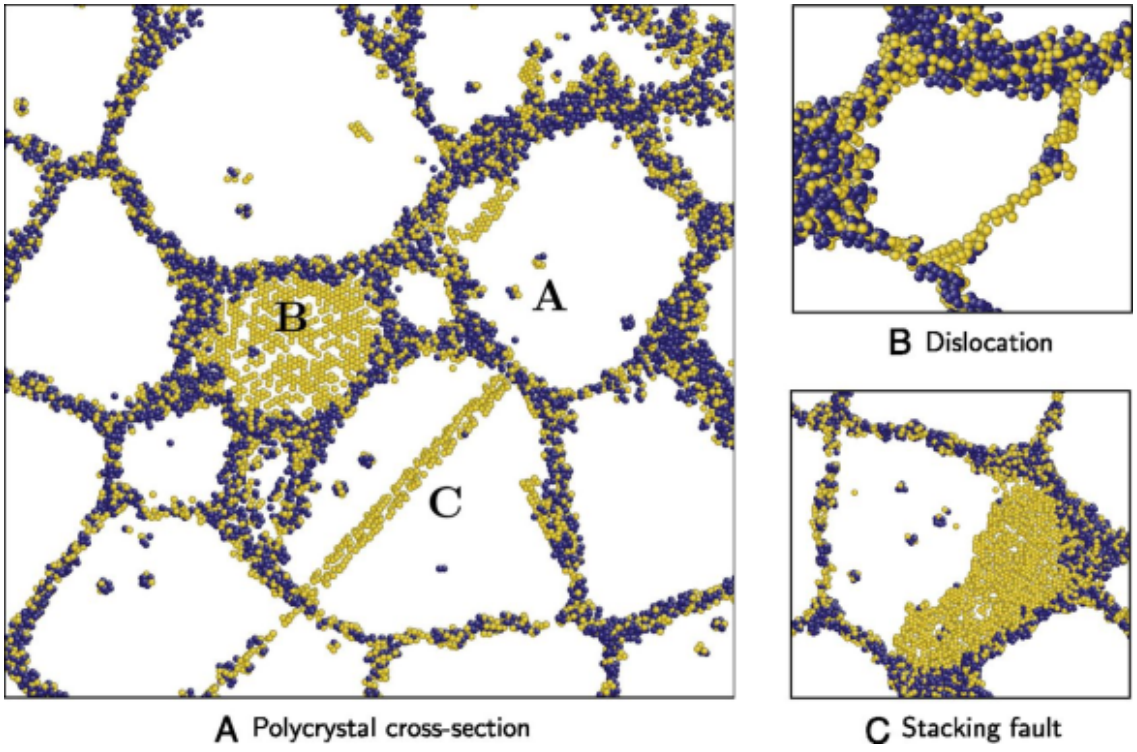

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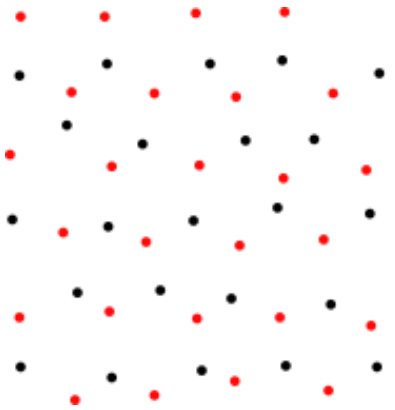
Definitions and Notation



- An **atomic configuration** is a point cloud in $\mathbb{R}^m$, labeled by atomic species. Our methods work for multiple species, but today we assume one.
- A **local atomic environment** is a point cloud in the ball of radius r, B_r, usually centered at an atom.
- For an atomic configuration X and $y \in \mathbb{R}^m$, let $\varphi_r(y; X)$ be the local atomic environment of radius r centered at y :

$$\varphi_r(y; X) = X \cap B_r(y)$$

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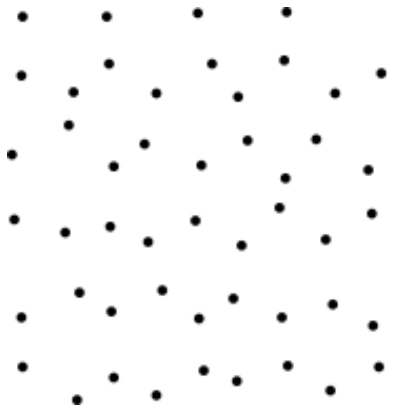

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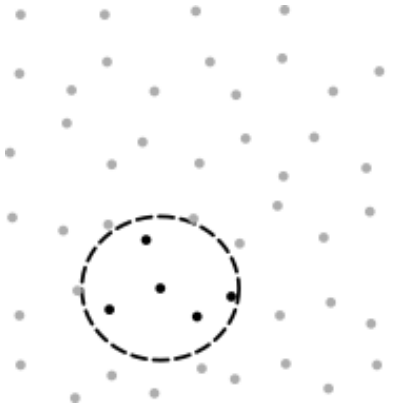

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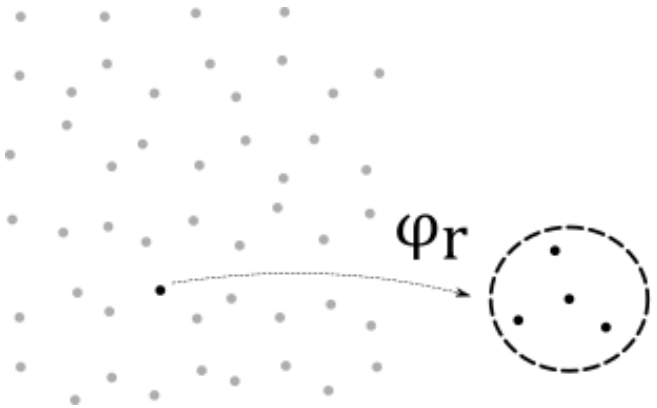

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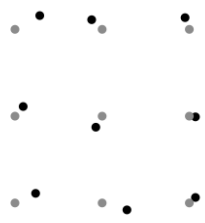
A Metric on Local Atomic Environments



Goal: define a metric d on local atomic environments. It should be continuous with respect to the atomic positions including atoms moving on and off the boundary of B_r. That is,

$$d\Big(\varphi_r(x;X),\varphi_r(y;Y)\Big)$$

should be continuous in x, y, r, and the positions of all atoms.

Most current methods rely on the choice of the "closest N points" to a root atom — not continuous in this sense!

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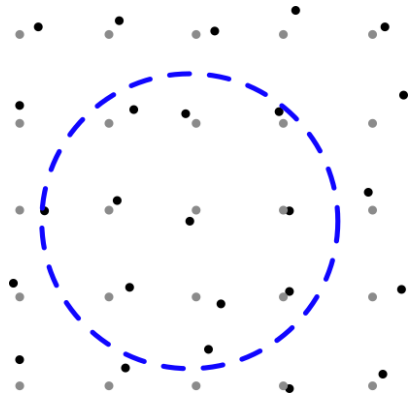

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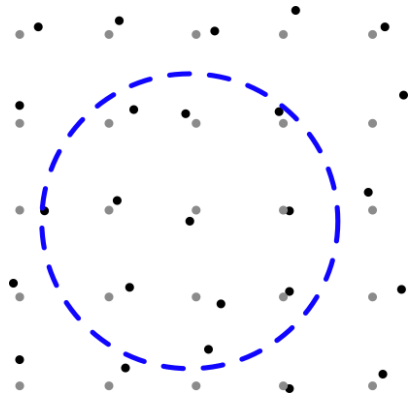

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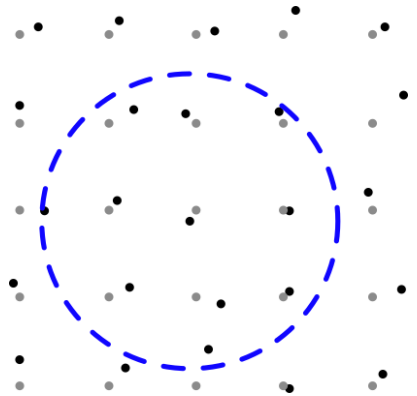

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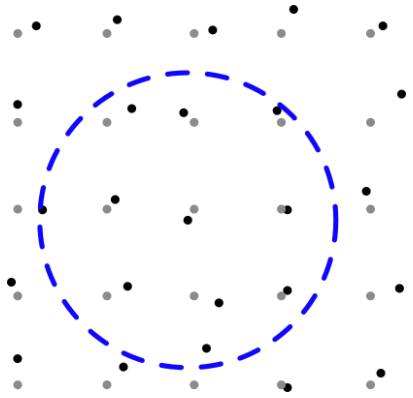

The metric should be invariant to Euclidean isometries. If X_r and Y_r are local atomic environments then

$$d(X_r, Y_r) = d\Big(X_r, \rho(Y_r)\Big)$$

for all $\rho \in \mathrm{SO}(m)$.

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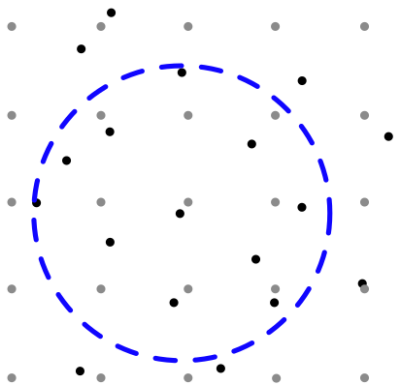

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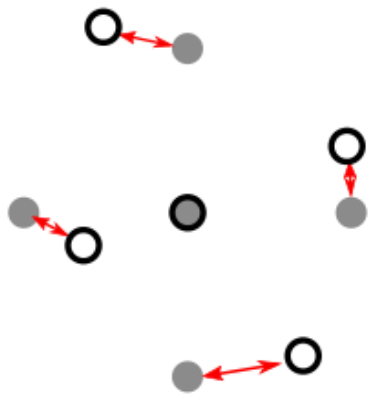
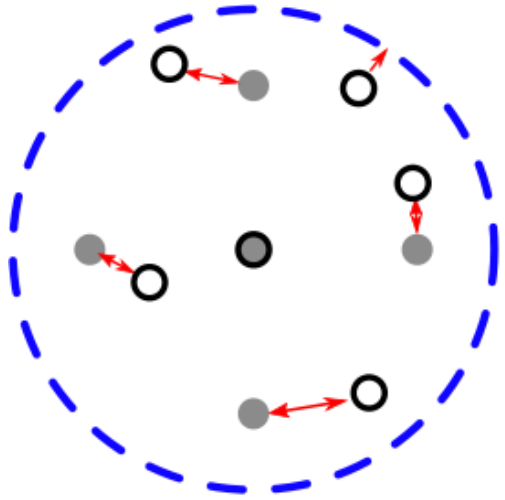


$$d_W(X, Y) = \min_{\eta: X \to Y} \left(\sum_{x \in X} d\Big(x, \eta(x)\Big)^2 \right)^{1/2}$$

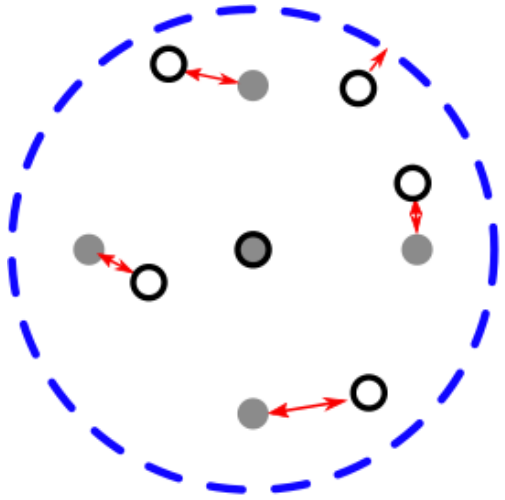
The minimum is taken over all matchings η from X to Y.

The Local 2-Wasserstein Metric



$$d_{LW}(X,Y) = \min_{\substack{X' \subseteq X, Y' \subseteq Y \\ |X'|=|Y'| \\ \eta: X' \to Y'}} \left(d_W(X',Y')^2 + \sum_{x \in X \setminus X'} d(x, \partial B_r)^2 + \sum_{y \in Y \setminus Y'} d(y, \partial B_r)^2 \right)^{1/2}$$

The Euclidean Wasserstein Metric



$$d_{EW}(X, Y) = \min_{\rho \in SO(m)} d_{LW}\Big(X, \rho(Y)\Big)$$

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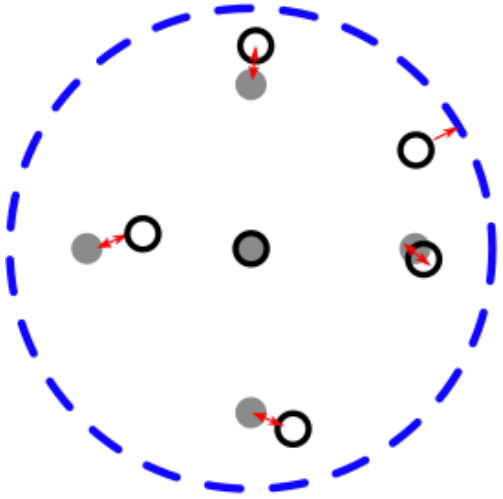

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Computation

- We compute the Euclidean Wassserstein Metric by a branch-and-bound algorithm on SO(3), taking advantage of the symmetries of the reference conditions.
- We compute the Local Wasserstein Metric using the Hungarian algorithm.
- Speed (using heuristics): $\approx .16$ seconds per local environment per thread for an *FCC* reference with 19 atoms, ≈ 1.3 seconds per local environment per thread for an *FCC* reference with 55 atoms.

Li and Hartley, 2007

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Proposed Test

- Data: a local atomic environment X centered at an atom x, reference atomic configurations $R_1, \ldots, R_k$, a temperature T, and a radius r.
- For each R_i, let R_i' be the random configuration:

$$R_i' = R_i + \text{thermal noise}$$

  If $y \in R_i$, let y' be the corresponding atom in R_i'.
- For each reference R_i, let $y \in R_i$ and compute

$$p_i = \mathbb{P}\left(d_{EW}\Big(X, \varphi_r(y\ Y)\Big) < d_{EW}\Big(\varphi_r(y'; Y'), \varphi_r(y; Y)\Big) \right)$$

- Classify X as type R_j if $p_i = \max_j p_j$.

Assume all atoms in the reference are identical, for clarity

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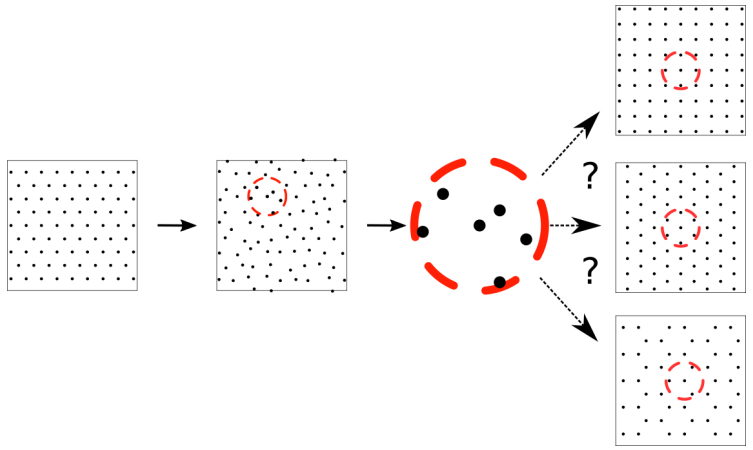

- References: FCC, BCC, HCP lattices with unit bond length.
- Thermal noise: add Gaussian displacements to each atom with standard deviation σ.
- For each reference R and $\sigma \in \mathbb{R}^+$, compute the probability that a local environment in R' is classified correctly.
- Compare accuracy with methods implemented in OVITO.

Stukowski, 2010

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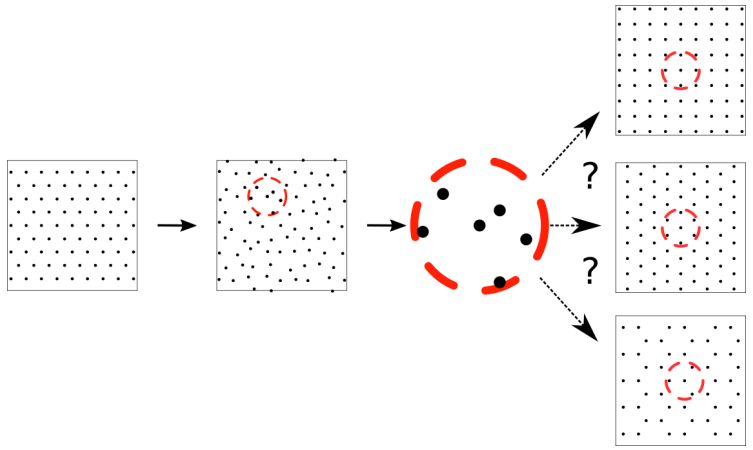

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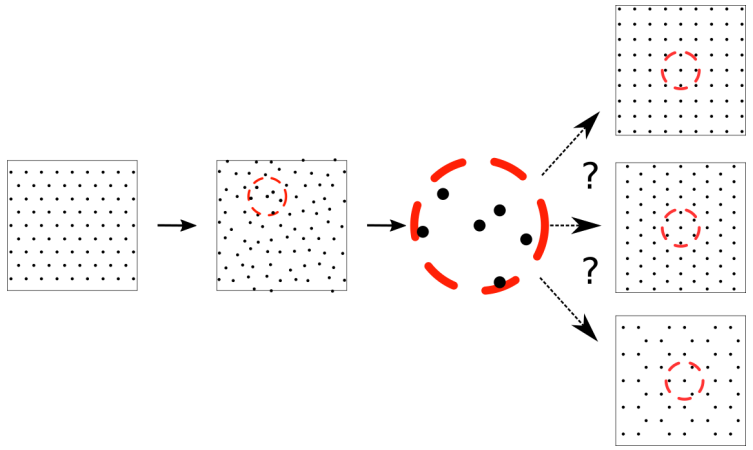

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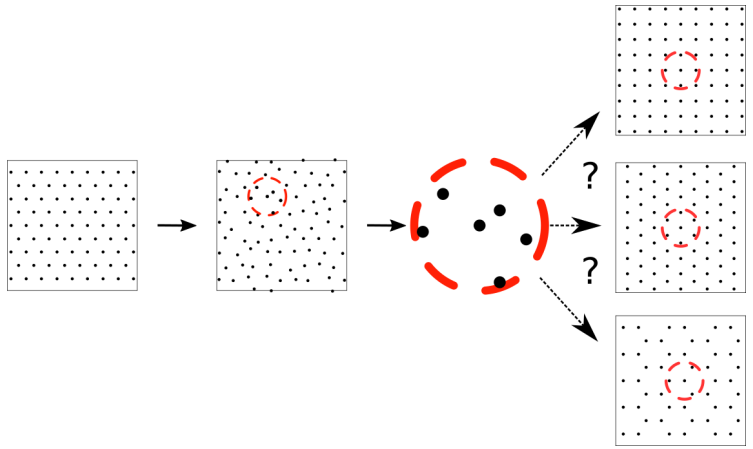

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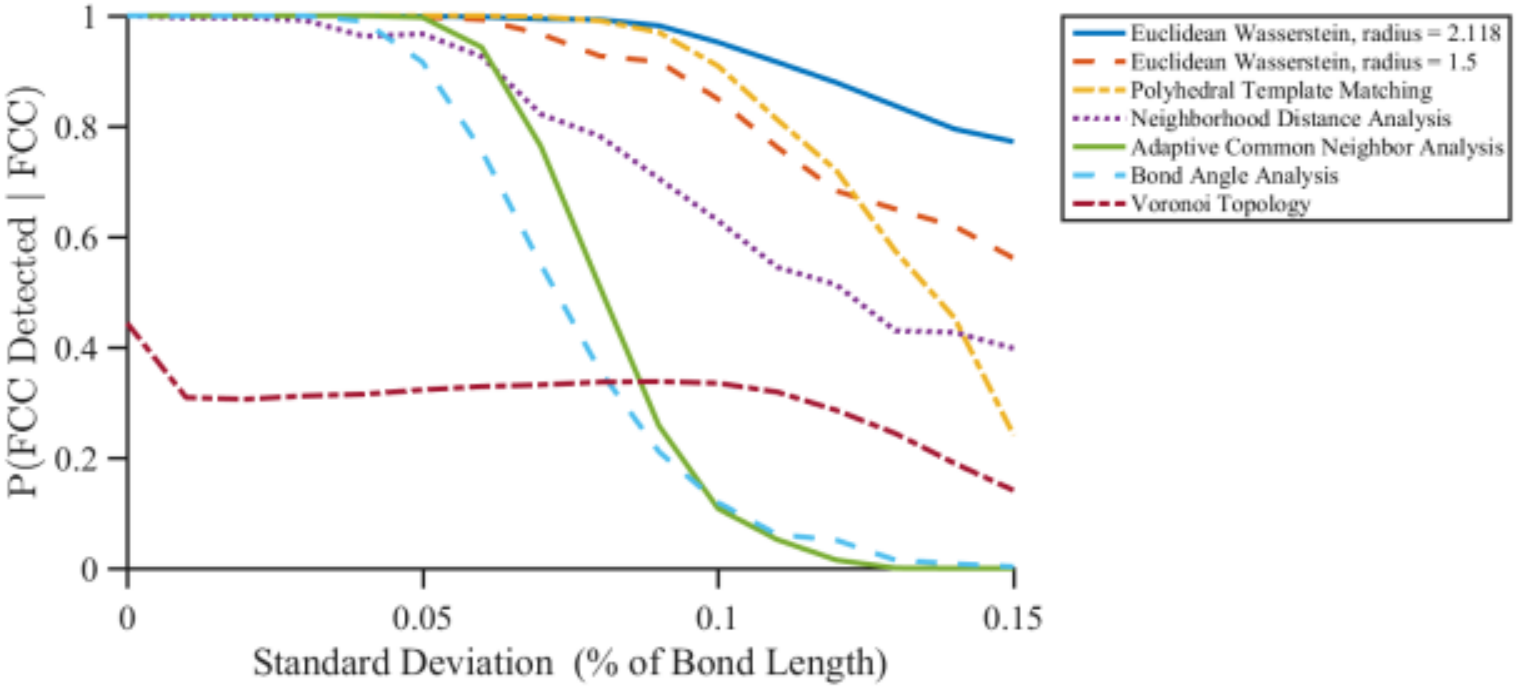

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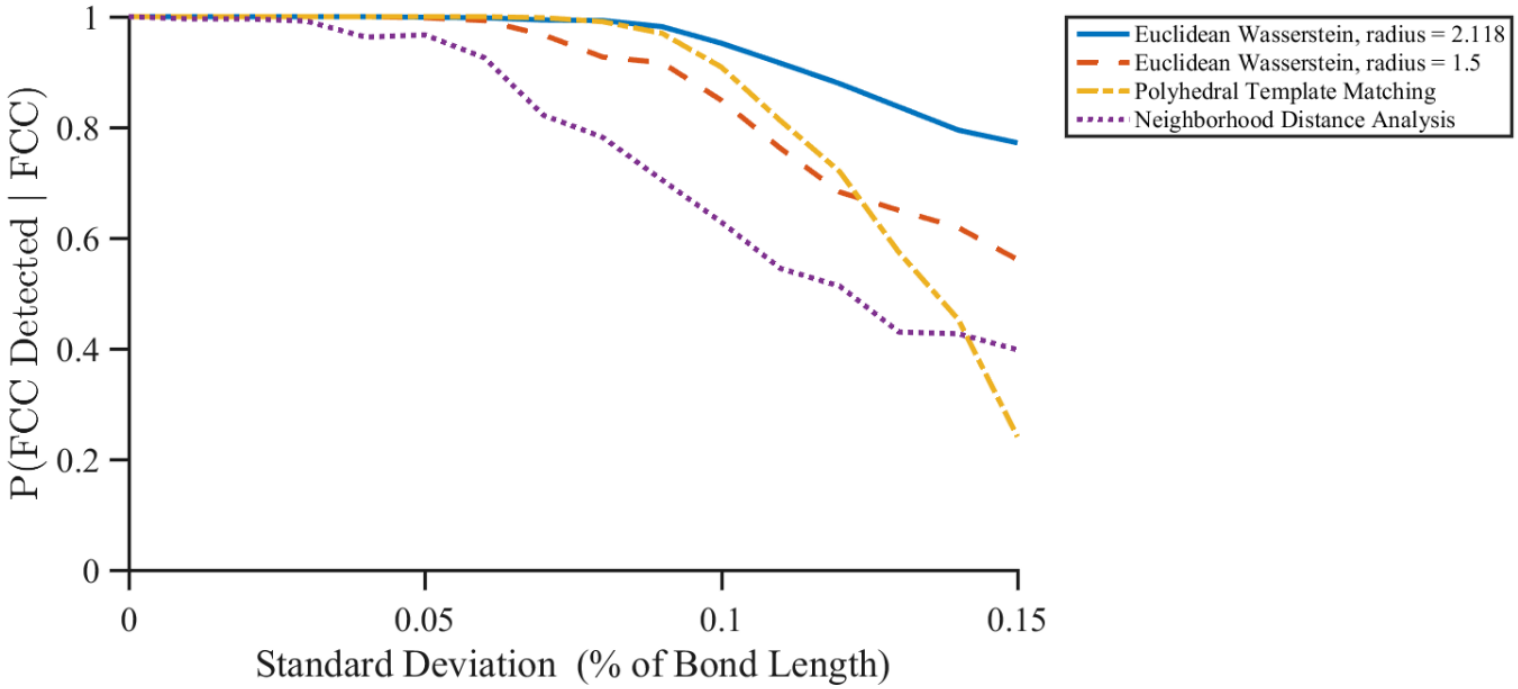
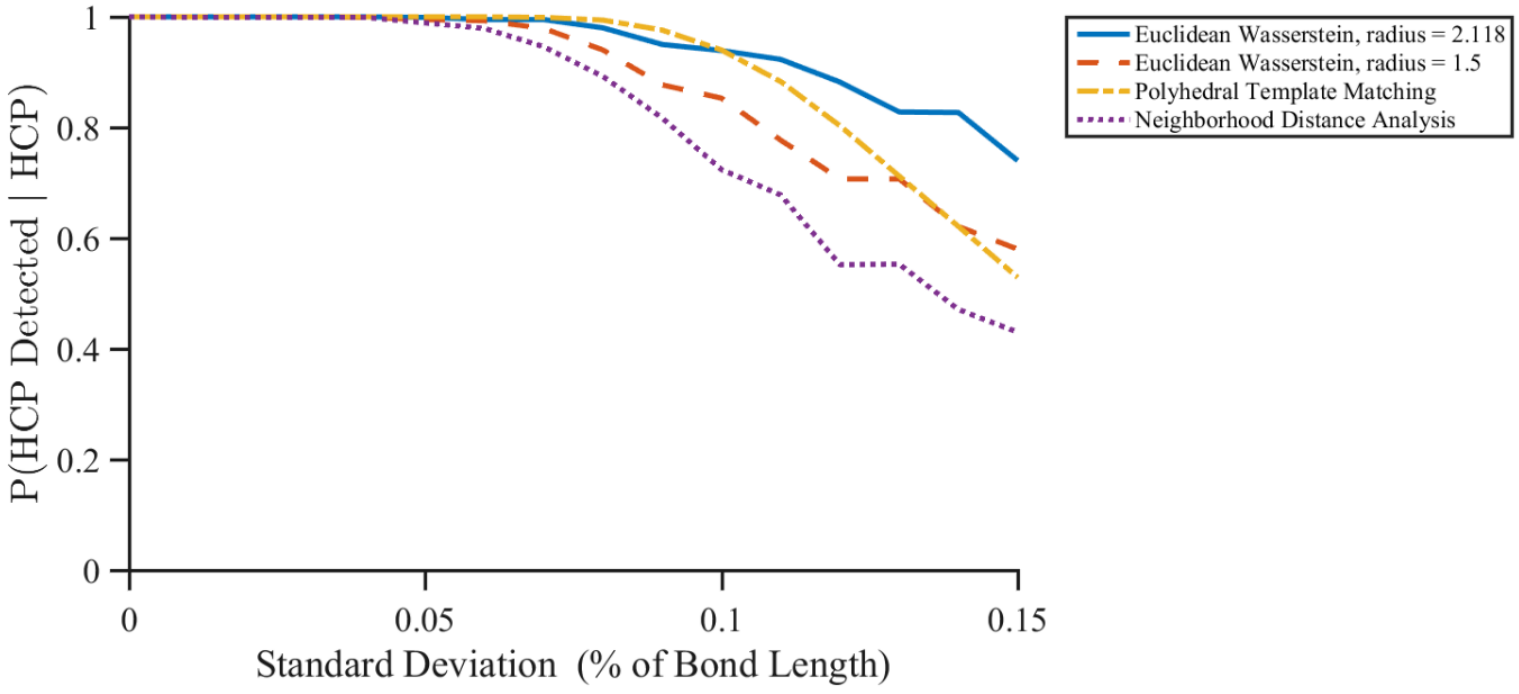
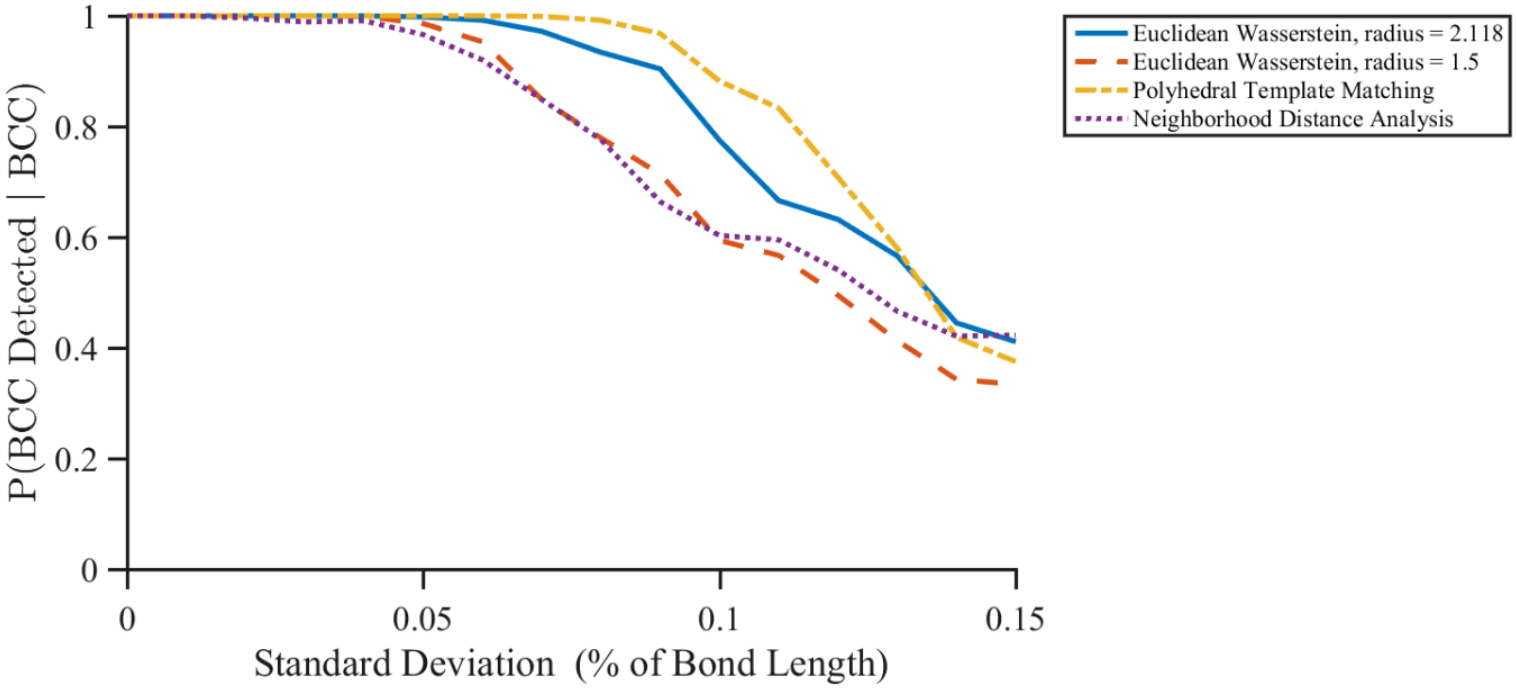


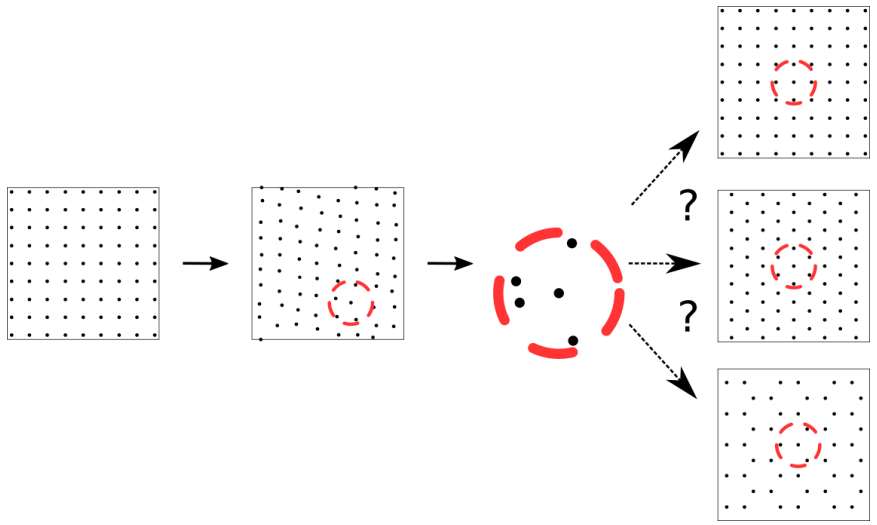
Performance Comparison: HCP



Performance Comparison: BCC



Shear Data

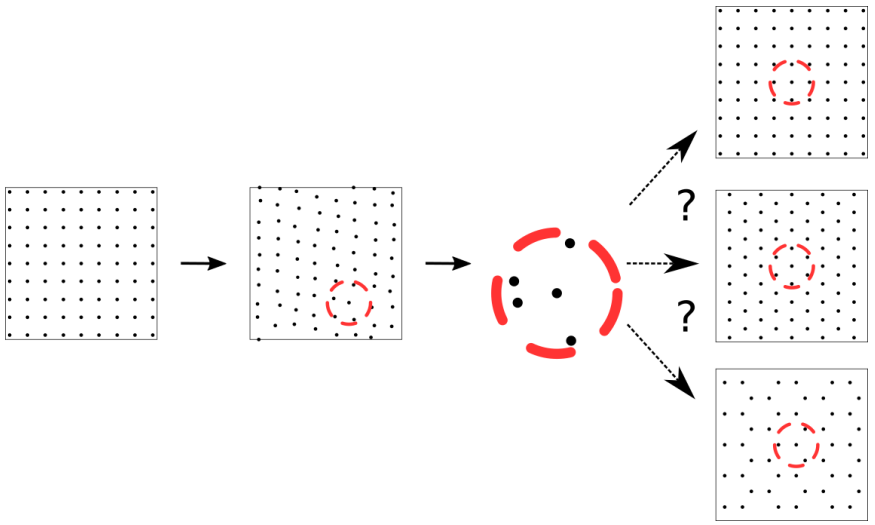


Different test for atomic environments with large non-thermal strains: Classify X as type R_i if

$$d_{EW}(X, R_i) = \min_j d_{EW}(X, R_j)$$

Synthetic Data: shear reference R_i in a random directly by a factor λ, add Gaussian noise, estimate probability of correct classification.

Shear Data



Different test for atomic environments with large non-thermal strains: Classify X as type R_i if

$$d_{EW}(X, R_i) = \min_j d_{EW}(X, R_j)$$

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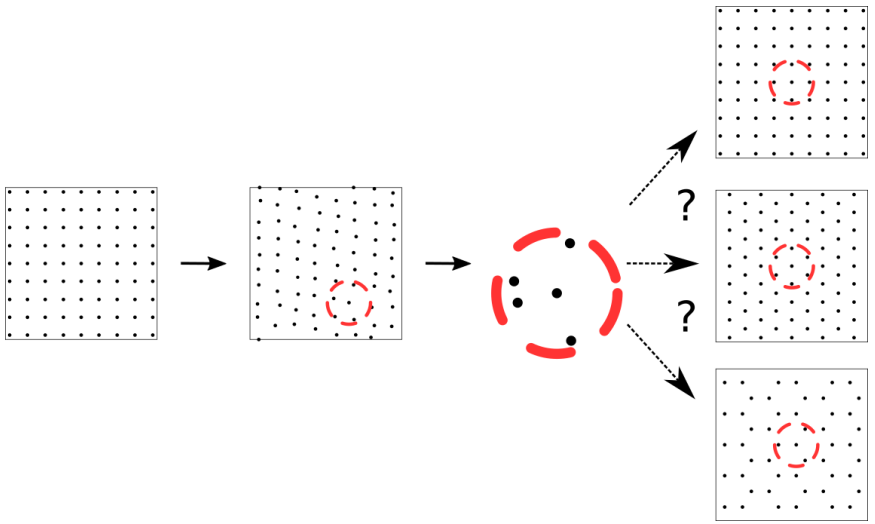

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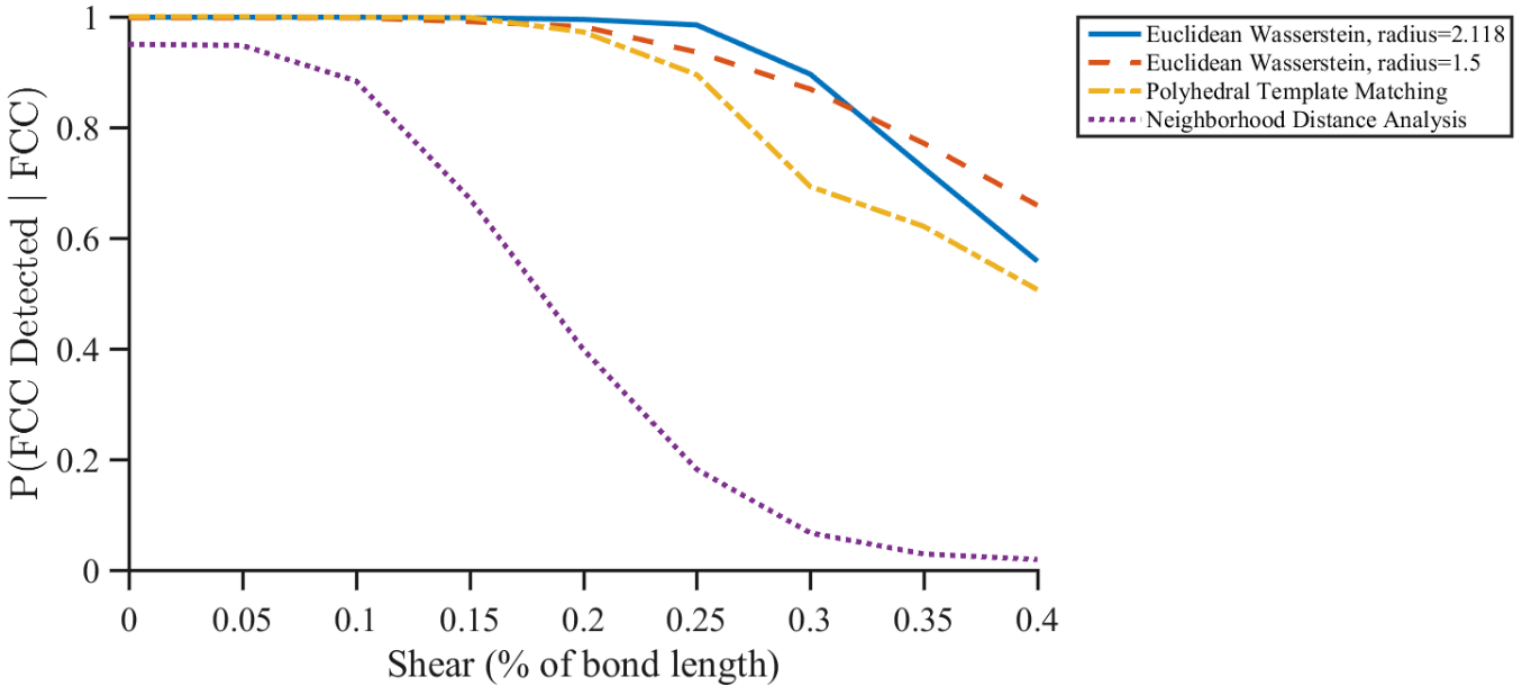
Shear Performance Comparison: FCC



Conclusion

- We propose using the (local) Euclidean Wasserstein metric for local atomic environment classification.
- The metric performs better than existing methods for distinguishing HCP and FCC environments at high temperatures.
- Proposed application: studying the phase transition from graphite to diamond

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