

Poster

Richard Feynman's visual hint gave birth to a new area of continuous crystallography

O. Anosova¹, V. Kurlin¹¹Materials Innovation Factory and Computer Science Department, University of Liverpool, Liverpool, L69 3BX, UK
vitaliy.kurlin@liverpool.ac.uk

For hundreds of years, crystals were studied almost exclusively by discrete tools such as symmetry groups. The classification of 230 space groups into 230 types was a great achievement at the end of the 19th century. These 230 classes were sufficient when hundreds of known crystals could be visually compared by experts until discontinuities were reported in 1965 [1]. In 2024, the Cambridge Structural Database (CSD) and others contain all together more than 2 million experimental structures, while simulated crystals emerge even in greater numbers. This scale requires a much finer (stronger) classification of all known periodic crystals into more than 230 classes.

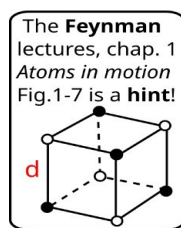
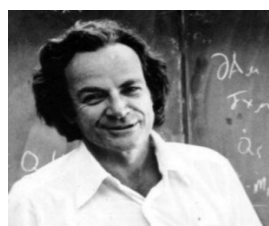
The questions ‘*What is a crystal?*’ and ‘*Same or different?*’ [2] need rigorous answers independent of symmetries or manual parameters. Since crystal structures are determined in a rigid form, their strongest equivalence in practice is rigid motion, which is a composition of translations and rotations. Under fixed ambient conditions, if we rigidly move a crystal, its structure should remain the same, though a standard representation in a Crystallographic Information File can easily change, e.g. if we shift all atoms within a fixed unit cell.

Hence there is no practical sense to distinguish crystals that can be ideally matched by rigid motion. But we need to distinguish crystals that cannot be ideally matched (are not rigidly equivalent). Indeed, if we call ‘the same’ any crystals whose all atoms can be matched up to a small perturbation, sufficiently many perturbations can geometrically deform any crystal to any other (of the same composition if we keep atomic types). This **continuum fallacy** (a version of the **sorites paradox**) is resolved by the following **new definition** [3]:

A **crystal structure** is an *equivalence class* of all periodic crystals that can be rigidly matched by rigid motion in 3-dimensional space.

Such a (say, *rigid*) *class* contains infinitely many crystals represented by infinitely many different CIFs, all encoding ‘the same’ periodic arrangement of atoms. Any slight perturbation of a single atom produces a crystal in a different rigid class, so there are infinitely many rigid classes, some of which can be very close (due to noise or atomic displacements) while others are very distant from each other.

A classification under isometry is only slightly weaker than under rigid motion because mirror images can be distinguished by a sign of orientation. We developed a **DNA-style invariant** (descriptor) that is preserved under isometry and continuously changes under any perturbation [4,5]. This *Pointwise Distance Distribution* PDD(S;k) is a matrix whose each row for any atom in an asymmetric unit of a periodic crystal S contains distances from the fixed atom to its k-nearest neighbors in increasing order (without keeping any indices or types of unordered atoms). Within 1 hour on a modest desktop computer, PDD(100;k) distinguished all real periodic crystals in the CSD and justified the **Crystal Isometry Principle** saying that all these periodic crystals live at unique locations in a common continuous space.

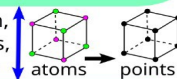


●	○	d (Å)
Na	Cl	2.82
K	Cl	3.14
Ag	Cl	2.77
Mg	O	2.10
Pb	S	2.98
Pb	Se	3.07
Pb	Te	3.17

Crystal Isometry Principle : chemistry → geometry

all real periodic crystals of atoms with chemical elements

- **injective modulo isometry** and rigid motion,
- **different crystals map to different structures**,
- **geometry suffices to reconstruct chemistry**



periodic structures of atomic centers without atomic types

isometry classes of other point sets outside the crystal space

Figure 1. Feynman's lecture 1 included the table showing that 7 cubic crystals differ by their smallest interatomic distance. Much stronger distance-based invariant PDD distinguished all periodic crystals in the CSD, which justified the Crystal Isometry Principle.

Now **continuous crystallography** studies all periodic crystals independent of symmetry and composition on the same continuous map.

[1] Lawton, S., Jacobson, R. The reduced cell and its crystallographic applications. Tech. Rep., Ames Lab., Iowa State University, 1965.

[2] Sacchi et al. Same or different - that is the question: identification of crystal forms from crystal data. *CrystEngComm*. v.22, p.7170-7185, 2020.

[3] Anosova, O., Kurlin, V., Senechal, M. [The importance of definitions in crystallography](#). *IUCrJ*, v.11 (4), p. 453-463, 2024.

[4] Widdowson, D., et al. Average Minimum Distances of periodic point sets. *MATCH Comm. Math. Comp. Chem*, v.87 (3), p.529-559, 2022.

[5] Widdowson, D., Kurlin, V. Resolving the data ambiguity for periodic crystals. *Adv. Neural Inform. Proc. Systems*, v.35, p.24625-24638, 2022.