Topological and combinatorial methods in crystallography

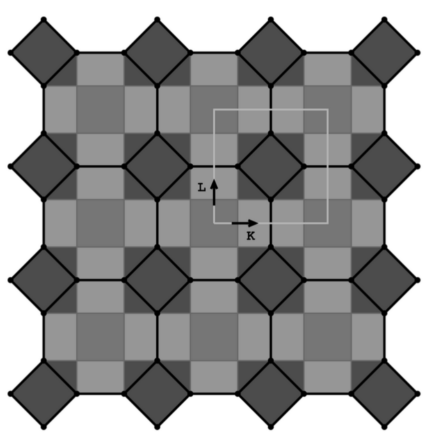
Bartosz Naskręcki;[1] Zbigniew Dauter;[2] Mariusz Jaskólski[3]; Jakub Malinowski[1]

[1] Faculty of Mathematics and Computer Science, A. Mickiewicz University in Poznań, Poland
[2] Macromolecular Crystallography Laboratory,
NCI, Argonne National Laboratory, Argonne, USA.
[3] Department of Crystallography, Faculty of Chemistry, A. Mickiewicz University in Poznań, Poland; Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, Poland

Abstract

Crystallography is a science of determining the arrangement of atoms in crystalline solids. From the mathematical point of view it is a study of tessellations of the Euclidean spaces. In our joint work [1], [2], [3] we have developed some connections between quantitative features of periodic space tessellations and topological invariants of flat manifolds. Following the original work of Coxeter we have constructed and studied certain "growth" functions for any given periodic tessellation. Seeing such a tessellation as a CW-complex gives a way to find features of the growth functions which uniquely identify the space group or even tessellation itself only from the numerical invariants. In the ongoing project we investigate relative growth functions which are restricted by either topological paths of rigid frames. This allows one to include defects of the lattice structure or even use some machine learning techniques to recognize the crystallographic group type from the numerical invariants.

Figure/Table



Growth polynomials diagram of the 884 tessellation

References

[1] The Euler characteristic as a basis for teaching topology concepts to crystallographers,
with Zbigniew Dauter and Mariusz Jaskólski, Journal of Applied Crystallography, (2022), Vol. 55, 154-167. (open access)

[2] A topological proof of the modified Euler characteristic based on the orbifold concept, with Zbigniew Dauter and Mariusz Jaskólski, Acta Crystallographica Section
A: Foundations and Advances (2021), Vol.7, No. 4, 317-326. (open access)

[3] Arithmetic proof of the multiplicity-weighted Euler characteristic for symmetrically
arranged space-filling polyhedra, with Zbigniew Dauter and Mariusz Jaskólski,
Acta Crystallographica Section A: Foundations and Advances (2021), Vol.7, No. 2, 126-129. (open access)