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Generative Symmetry in Crystal Modelling

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1. Introduction

Symmetry is ubiquitous in the materials world. Materials with higher symmetry are naturally more preferable, not just for their aesthetic appeal but primarily because their stability and functional applications originate from the symmetry. Understanding material symmetry and exploring its influence on properties is crucial for designing new materials. Among all materials classes, crystalline materials represent a particularly rich domain for symmetry exploration, as crystal can be described by a established framework (The 230 space groups). Recently developed generative models for crystal structures, including Wycryst [1], WyFormer [2] and SymmCD [3], incorporate symmetry as a key consideration in the generation process. These models share a common approach: encoding lattice symmetry and local atomic Wyckoff positions with the expectation that models gain insights from this discretized representation. However, such representations do not explicitly incorporate symmetry operations into the model architecture, serving instead as label-based guidance.

Representing symmetry through symmetry operations rather than simple labels constitutes a natural and principled evolution, as symmetry operations are the fundamental mathematical units describing crystallography. This approach offers two main advantages that address the limitations of existing methods. First, this representation allows composition, inversion, and closure verification of symmetry operations within the model. Unlike label-based approaches where space group information remains static, it allows models to learn the algebraic structure of symmetry groups and become genuinely space group-aware. Second, symmetry operation-based representation inherently encodes the hierarchical relationships between crystal symmetry groups, which naturally form group-subgroup hierarchies. Each subgroup contains only a subset of symmetry operations of its original space group. By adding or removing specific symmetry operations, our model can simulate group-subgroup transitions by design, which are frequently observed in finite-temperature phase changes.

Building on these insights, we introduce a symmetry operation based generative framework that, for the first time, treats symmetry as an emergent, learnable attribute rather than a static, prescribed constraint. This approach eliminates the need to condition on specific space groups during generation, as space groups emerge naturally as consequences of the symmetry operation sets, allowing the model to flexibly explore symmetry-reduced derivative structures, increasing the probability of discovering more stable, better functional materials. By navigating the hierarchical space of symmetry operations, researchers can systematically explore how symmetry reduction or enhancement affects desired material properties, opening new avenues for discovering materials with tailored functionalities.

2. Methodology

We propose a symmetry operation-based generative framework for crystalline materials, in which space group symmetry is explicitly represented as a learnable set of symmetry operations rather than predefined categorical labels. Each crystal is described by a set of atomic species, and a variable-sized set of symmetry operations parameterized as affine transformations in three-dimensional Euclidean space.

An SE(3)-equivariant neural network first predicts the set of symmetry operations, ensuring geometric consistency under rotations and translations. Only after the symmetry operations are determined, the network generates lattice vectors and atomic coordinates, such that the resulting crystal structure is fully compatible with the predicted symmetry. The full crystal is constructed by applying the symmetry operations to the atomic species within the generated lattice, allowing symmetry to emerge naturally from the learned operation set without conditioning on a specific space group (Figure 1).

To enforce valid crystallographic symmetry, we introduce group-consistency regularization terms that promote closure, inverse consistency, and identity preservation within the generated operation sets, as well as lattice–symmetry compatibility constraints. These encourage the model to learn the algebraic structure of symmetry groups while producing physically realizable lattice parameters and atom placements.

Furthermore, this representation naturally supports group–subgroup transitions by adding or removing symmetry operations and adjusting lattice degrees of freedom, enabling systematic exploration of symmetry reduction and enhancement pathways. This design allows the generation of symmetry-reduced derivative structures commonly associated with finite-temperature phase transitions while maintaining crystallographic validity.

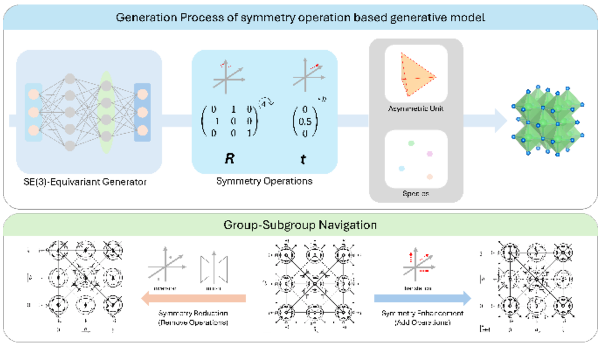

Fig. 1: Symmetry operation based generative framework

3. Related work

WyCryst [1] introduces the concept of "Wyckoff genes" to encode stoichiometry, space group, and site occupancy, delegating full structure reconstruction and relaxation to external tools such as PyXtal [4]. WyFormer [2] builds on this idea with a permutation-invariant autoregressive Transformer that generates Wyckoff site tokens conditioned on the space group, while still relying on external crystallographic and atomistic solvers to obtain atomic coordinates. WyckoffDiff [5] further extends the template-based paradigm by adopting a symmetry-aware diffusion process over discrete Wyckoff assignments, explicitly distinguishing symmetry-constrained and unconstrained sites. In contrast, DiffCSP++ [6] directly generates lattices, atomic coordinates, and species via a symmetry-aware diffusion framework, enforcing space group consistency through Wyckoff projection constraints. SymmCD [3] systematically encodes site symmetries and symmetry elements using structured binary representations and performs joint continuous–discrete diffusion to generate asymmetric-unit-based crystals. SGEquiDiff [7] combines discrete autoregressive sampling of lattice and Wyckoff attributes with a space-group-equivariant diffusion process over coordinates, ensuring atoms evolve strictly on Wyckoff manifolds. Despite these differences, all models adopt a common "space group first" strategy, in which symmetry-related sampling and generation are explicitly conditioned on a predefined space group.

4. Main Contributions

The main contributions of our work are:

(1). We introduce a novel symmetry-operation-based representation for crystal generative design, treating symmetry as an emergent, learnable property rather than a fixed space group.

(2). Our approach enables group–subgroup navigation, allowing the generation of symmetry-reduced derivative structures relevant to phase transitions and materials discovery.

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References

[1] R. Zhu, W. Nong, S. Yamazaki, and K. Hippalgaonkar, "WyCryst: Wyckoff inorganic crystal generator framework," *Matter*, vol. 7, no. 10, pp. 3469–3488, Oct. 2024, doi: 10.1016/j.matt.2024.05.042.

[2] N. Kazeev *et al.*, "Wyckoff Transformer: Generation of Symmetric Crystals," presented at the AI for Accelerated Materials Design - NeurIPS 2024, Nov. 2024. Accessed: May 13, 2025. [Online]. Available: https://openreview.net/forum?id=Jcy1bPOqrY

[3] D. Levy *et al.*, "SymmCD: Symmetry-Preserving Crystal Generation with Diffusion Models," Apr. 17, 2025, *arXiv*: arXiv:2502.03638. doi: 10.48550/arXiv.2502.03638.

[4] S. Fredericks, K. Parrish, D. Sayre, and Q. Zhu, "PyXtal: A Python library for crystal structure generation and symmetry analysis," *Computer Physics Communications*, vol. 261, p. 107810, Apr. 2021, doi: 10.1016/j.cpc.2020.107810.

[5] F. E. Kelvinius, O. B. Andersson, A. S. Parackal, D. Qian, R. Armiento, and F. Lindsten, "WyckoffDiff -- A Generative Diffusion Model for Crystal Symmetry," Apr. 30, 2025, *arXiv*: arXiv:2502.06485. doi: 10.48550/arXiv.2502.06485.

[6] R. Jiao, W. Huang, Y. Liu, D. Zhao, and Y. Liu, "Space Group Constrained Crystal Generation," in *The Twelfth International Conference on Learning Representations*, 2024. [Online]. Available: https://openreview.net/forum?id=jkvZ7v4OmP

[7] R. Chang *et al.*, "Space Group Equivariant Crystal Diffusion," Sep. 19, 2025, *arXiv*: arXiv:2505.10994. doi: 10.48550/arXiv.2505.10994.