Neural Structure Fields with Application to Crystal Structure Autoencoders

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Neural Structure Fields (NeSF): Neural Field-based crystal structure decoder

Representing crystal structures of materials to facilitate determining them via neural networks is crucial for enabling machine-learning applications involving crystal structure estimation. Here we propose **Neural Structure Fields (NeSF)** as an accurate and practical approach for representing crystal structures using neural networks. NeSF considers a **crystal structure as a continuous field** rather than as a *discrete set of atoms*. NeSF overcomes the tradeoff between spatial resolution and computational complexity. **NeSF can represent any crystal structure**.

- We developed **neural field-based (voxel-free) crystal decoder**
- Crystal structure can be written by proposed *vector fields representations*: **Structure Fields**
- Neural Field technique to model a structure field by a simple neural network: **NeSF**
- We also develop an algorithm that *reconstructs atom positions and species* from NeSF (or Structure Fields)

Voxel-based vs Continuous Representation

continuous field representation for crystal structure

Our idea of representing crystal structures as continuous vector fields has been partially and implicitly explored using voxelization in recent MI study [1], but without explicit consideration as discretized vector fields. The discretization of 3D data considerably suffers from the tradeoff between spatial resolution and computational complexity. The proposed NeSF is inspired by the concepts of Neural Field [2, 3, 4, 5]. Theoretically, the NeSF can achieve infinitely high spatial resolution with compact (memory- and parameter-efficient) neural networks in place of costly 3D CNNs. There is essentially no tradeoff between the spatial resolution and required memory.

Voxel-based representation

- Limited resolution (practically 32x32x32 in practice [1])
- Have tradeoff between resolution and computational costs (both time and memory)
- Many parameters (often causes overfittings)

Continuous (Neural Field-based) representation

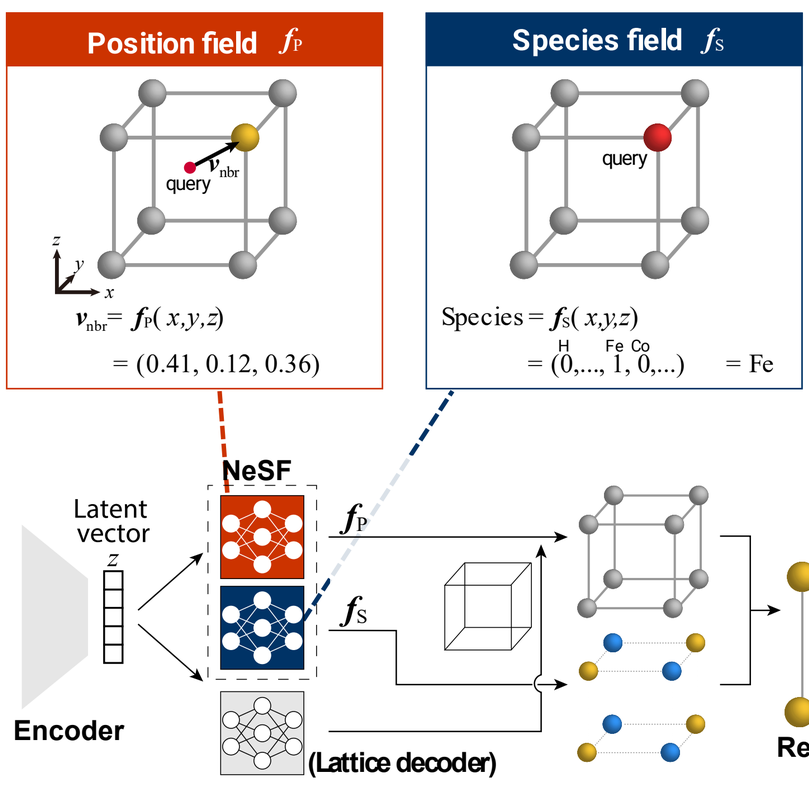
- Can represents infinitely high resolution
- Have no tradeoff between resolution and computational costs
- Less parameters

Neural Structure Field (NeSF)

Structure Field = Position Field + Species Field
NeSF: Modeling Structure Field using Neural Field technique

- **Position Field: a vector pointing to the nearest atom from a query point.**
- **Species Field: a one-hot vector of the nearest atom species**

We approximate the Structure Field by using neural networks via Neural Field technique. We also combine **PointNet-based simple encoder** to the NeSF decoder, which give an autoencoder for crystal structures.



Neural Field technique

Implicitly represents "field" by using a neural network

Neural Field is a technique that represents a (vector) field by using simple neural networks [2, 3, 4, 5]. The key idea of neural field is that the field is implicitly described point-by-point. When a query point is given, the network returns the value of the query point.

$$\boldsymbol{y} = f(\boldsymbol{x}, \boldsymbol{z})$$

Vector value corresponding to
- latent vector $\boldsymbol{z}$
- query point $\boldsymbol{x}$

Query point

Latent vector (given field-by-field)

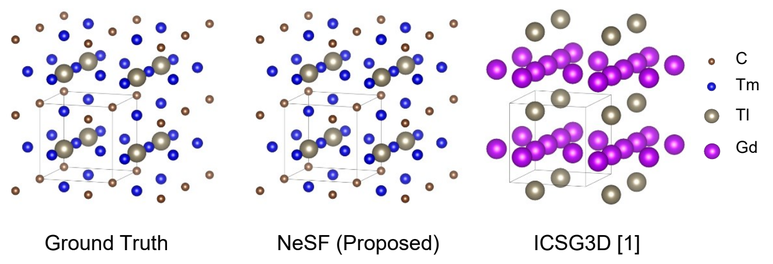
Modeled by neural network

Experimental Results

We compared proposed method with the ICSG3D as a autoencoder. On the ICSG3D using dataset (AB, ABX_2, and ABX_3 entries on the Material Project) the proposed method achieves high accuracy to reconstruct for the test entries.

Reconstruction Results in Test Dataset

Method	NeSF (Proposed)	ICSG3D [1]
Error in Number of Atoms [%]	0.53 ± 0.25	2.67 ± 0.84
Position Error (Actual) [Å]	0.0308 ± 0.0112	0.0877 ± 0.0306
Position Error (Detected) [Å]	0.359 ± 0.0226	0.1057 ± 0.0284
Species Error (Actual) [%]	4.31 ± 0.39	64.39 ± 1.91
Species Error (Detected) [%]	4.36 ± 0.39	65.05 ± 1.85



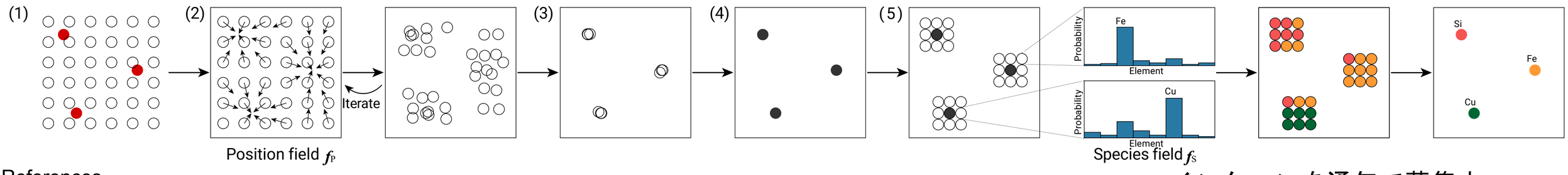
Ground Truth NeSF (Proposed) ICSG3D [1]

Example of Reconstruction Result in Test Dataset: mp-22556 (Tm3TlC)

Reconstruction Algorithm

Method to convert a crystal structure from a NeSF representation

1. **Initialize particles**: Regularly spread initial query points at 3D grid points within a bounding box (common to each dataset)
2. **Move particles**: Update the position of each query points using the position field. (Iterate this process)
3. **Score particles**: Score each query points and filter outliers by using estimated residual distance to the atom positions.
4. **Detect atoms**: Apply a simple clustering algorithm to detect each atomic position.
5. **Estimate species**: to estimate the atomic species by using Species Field at each atomic position.



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