AMDEN: Amorphous Materials DEnoising Network

Generation of Amorphous Materials with Tailored Properties

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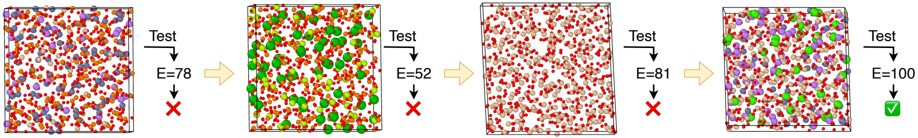
Discovering Amorphous Materials with Desired Properties

Trial-and-error

Screen through the design space until samples with desired properties are found.

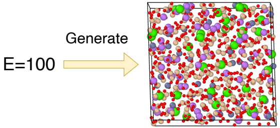


- Techniques like high-throughput screening, computer simulation, machine learning-based property prediction can be used to speed up the process
- Inevitably, a large number of material samples need to be created/generated, leading to **high manpower, material, and time costs**

Discovering Amorphous Materials with Desired Properties

Inverse Design

Begin with desired properties and determine the atomic configurations to achieve them.



- Far fewer material samples need to be screened, saving costs
- Has the potential to significantly speed up the discovery of novel amorphous materials

How do we achieve inverse design of amorphous materials?

Generative Modeling with Diffusion Models

A family of machine learning frameworks that **generate data from random noise by denoising the data step-by-step.**

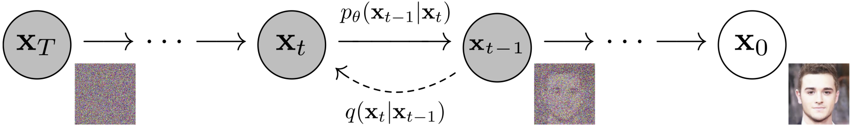


Figure 1: Image generation process of diffusion models[1]

- Huge success and widely adopted in image and video generation
- Inspired lots of efforts in inverse design of crystalline materials and molecules[2], but its adaptation in amorphous materials are understudied

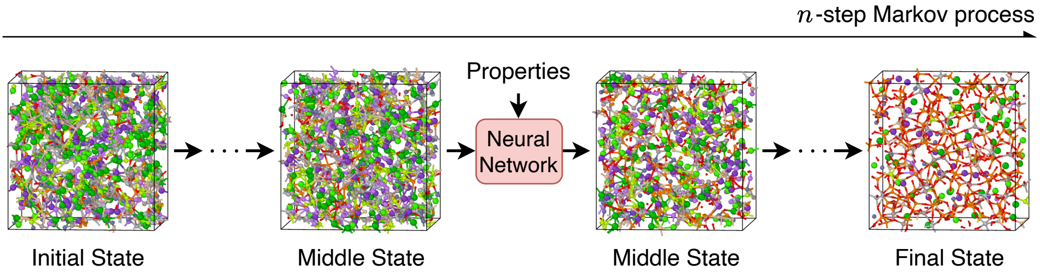
[1] Ho, Jonathan and Jain, Ajay and Abbeel, Pieter. "Denoising Diffusion Probabilistic Models." NeurIPS (2020).

[2] Zeni, Claudio, et al. "A generative model for inorganic materials design." Nature (2025).

Generative Modeling of Amorphous Materials

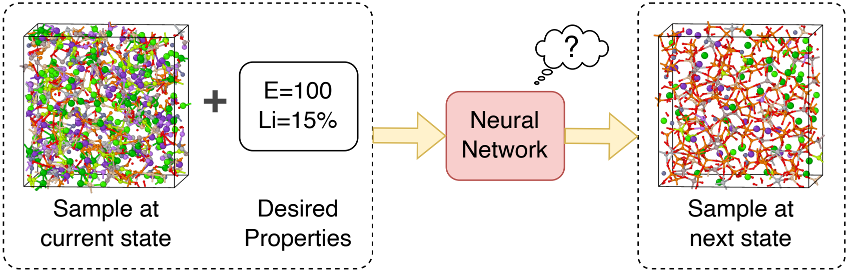
Start from an initial state of the sample, adjust its atomic positions and elements step-by-step towards the final state.

- Similar to a simulation pipeline but the atoms are not driven by energy and force
- Instead, a *neural network* predicts the movements of atoms at each step conditioned on the desired properties



Neural Network for Generative Modeling

- Input: Current state of an amorphous material sample at each step, and the desired properties
- Output: State of the sample at the next step

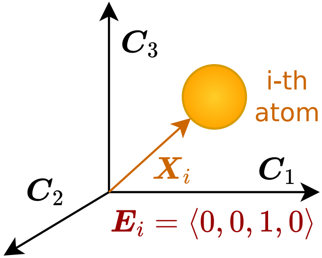


Representation of Amorphous Material Samples

Representing one amorphous material sample as a tuple $x = (\boldsymbol{C}, \boldsymbol{X}, \boldsymbol{E})$.

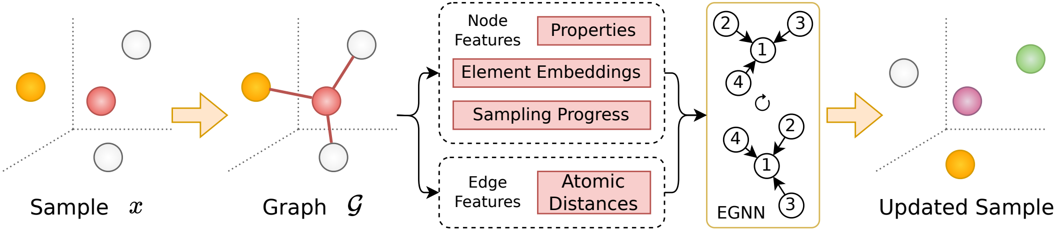
- $\boldsymbol{C} \in \mathbb{R}^{3\times 3}$ are the lattice vectors
- $\boldsymbol{X} \in \mathbb{R}^{N\times 3}$ are the atomic positions
- $\boldsymbol{E} \in \mathbb{R}^{N\times d}$ are the element one-hot embeddings

And its properties as a vector $\boldsymbol{y}$ where each value is a scalar property.



Equivariant Neural Network Architecture

Update the positions and elements of atoms while preserving the geometric equivariance of amorphous material samples.

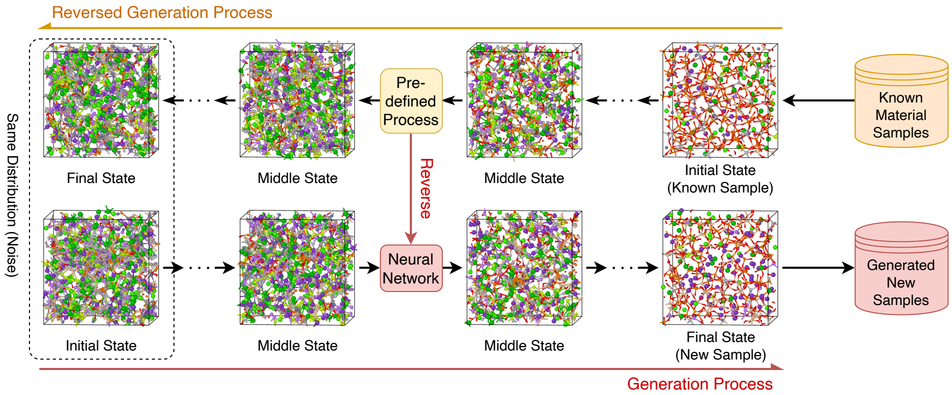


- A graph structure of each sample where node and edge features are invariant to permutation and translation
- EGNN[3] backbone whose update to each sample is invariant

[3] Satorras, Victor Garcia, Emiel Hoogeboom, and Max Welling. "E (n) equivariant graph neural networks." ICLR (2021).

Reversible Generation Process

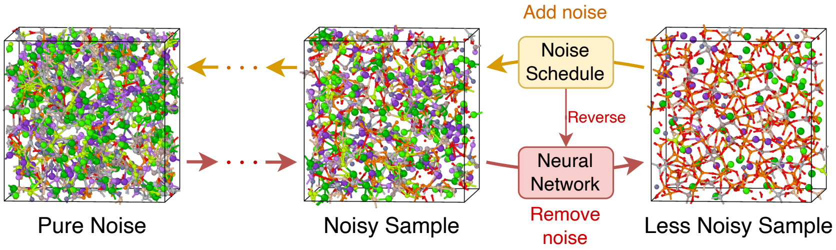
We cannot train a neural network with the generation process alone.



A reversed generation process providing ground truth for training.

Denoising Generation Process

- The reversed generation process gradually adds Gaussian noise to the sample until pure noise at the initial state
- The neural network learns to remove the noise added in each step
- The generation process can start from an initial state of pure Gaussian noise



Density Control in the Generation Process

Importance of density control

- Density in amorphous materials is a key parameter that affects numerous properties
- Being able to control the density during generation is essential for generating materials with certain property targets

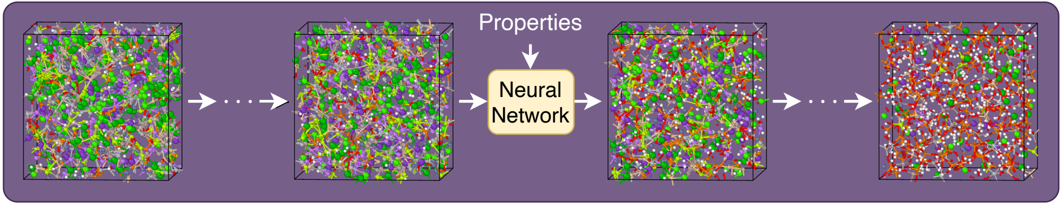
Limitation of diffusion models

- Diffusion models manipulate data by adding/removing noise from data — changing the position and element of each atom
- **Adding or removing atoms from the system will be technically challenging for diffusion models**

Density Control via Ghost Atoms

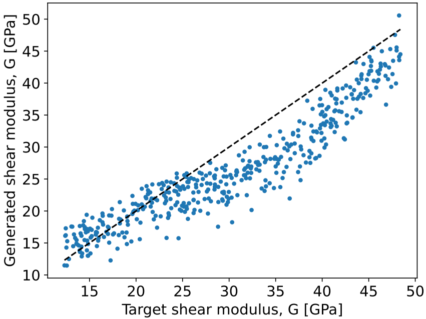
Framing the density control problem as changing elements of atoms.

- Ghost atoms are added to each material sample so that the density (number of atoms per unit volume) of all samples reaches one target maximum value
- Ghost atoms are treated as normal atoms by the model but assigned a special element class and removed in the final generated samples
- The model can control the density during generation by increasing/decreasing the proportion of atoms with the special element type

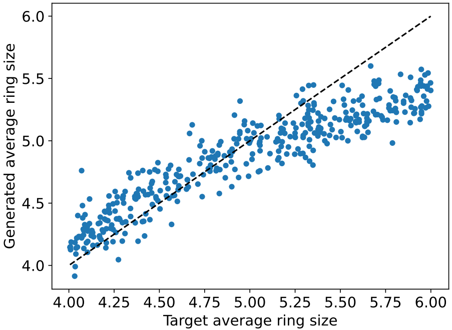


Generation of Amorphous Silica

With desired **shear modulus** and **average ring size** that are dependent on the samples' structures and densities.



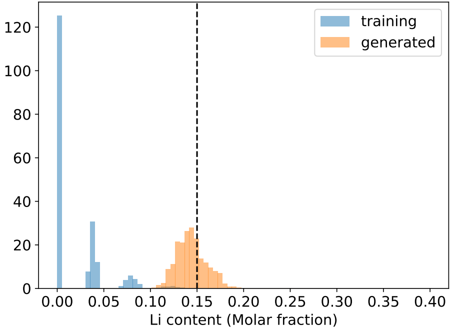
(a) Accuracy of shear modulus of generated samples



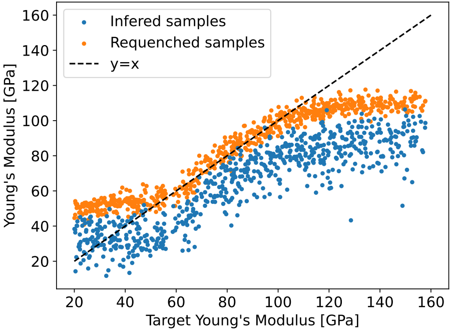
(b) Accuracy of average ring size of generated samples

Generation of Multi-element Glass

With desired **Young's modulus** and **Lithium ratio** that are largely dependent on samples' compositions.



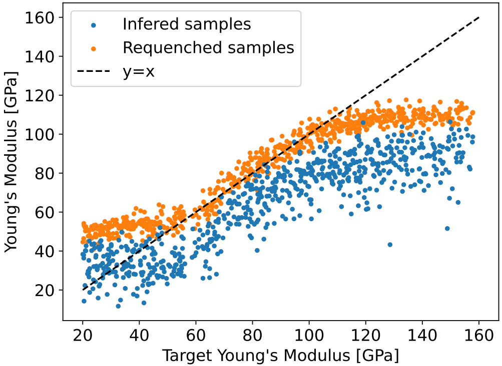
(a) Distribution of Lithium ratio of training data and generated samples (with target being 0.15)



(b) Accuracy of Young's modulus of generated samples

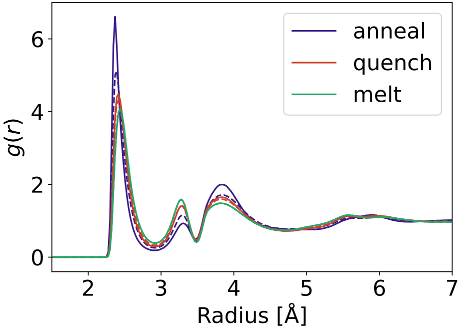
Generation of Multi-element Glass

- The flattening at both ends is primarily the result of extrapolation
- The Young's modulus of generated samples tend to be smaller than targets
- Requenched samples that are simulated with the compositions of generated samples align better with targets
- **The model is able to generate compositionally accurate samples but falls short in generating structures accurately**

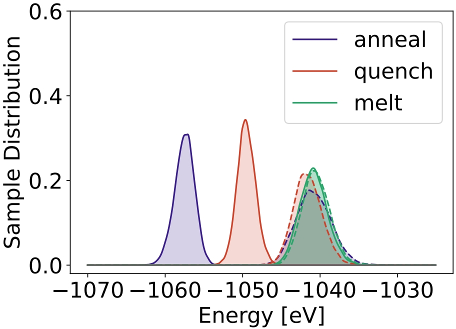


Generation of Amorphous Silicon

Trained with a-Si simulated with different thermal histories and perform generation.



(a) RDF of training (solid) vs. generated (dashed) samples



(b) Potential energy distribution of training vs. generated samples

This further demonstrates that **the model is unable to generate low-energy structures derived from relaxation processes.**

Limitations

Generation of samples with relaxed structures

Unable to generate amorphous materials with relaxed structures accurately, an inherent limitation of diffusion models.

Real-world synthesis of generated samples

New synthesis techniques are needed to fully take advantage of the generated atomic configurations.

Further discussion and solutions: stay tuned for the next presentation!

Thank you!

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