Distance between histograms

Bhattacharya Distance and Chi square distance

Purpose and why is it more robust than fingerprinting and previous scoring method

- Track the crystallization and amorphization of an interface.
- Independent of any reference structure.
- The fingerprinting compares the distance between the reference structure, but for a dynamically evolving system, where the conditions like temperature and pressure does not fit with the reference structure, the distance is not a perfect measure.
- The previous scoring method similarly makes comparison with the order parameters(Q4 and Q6) of a perfectly crystalline system which is equilibrated at different pressure-temperature condition.

Steps

1. First, we need to determine the q-sigma, which is the spread of the summation of order parameters(Q4+Q6) and there are 2 ways to determine that:

(a) While equilibrating a system, calculate the q parameters of randomly selected 5-10 atoms which belongs to the crystalline group. Then determine the q-sigma based on the calculated Q4+Q6.

(b) Calculate the q parameters of randomly selected 5-10 atoms which belongs to the crystalline group while simulating a dynamically evolving system. Then determine the q-sigma. [Determination of q-sigma script is attached.]

2. Initial histogram, final histogram and average of all the histograms of the time evolving [Q4+Q6] of the system is calculated.

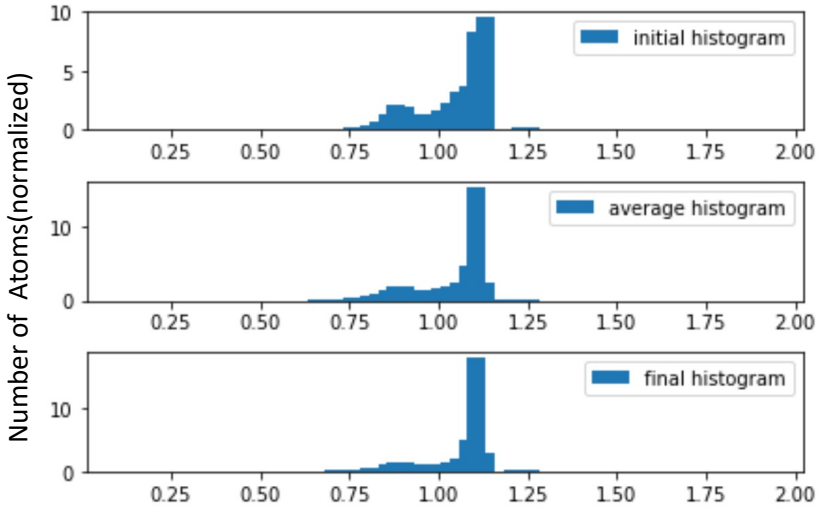
3. The shape of final histogram and time averaged histogram is compared as a checkpoint.

4. If the shape is similar, calculate the distance between the initial and time averaged histogram by Bhattacharya Distance and Chi square distance.

5. To trace crystallization, the bhattacharya distance with multiplied with a +ve index and to trace amorphization, it is multiplied with a –ve index. [Script attached]

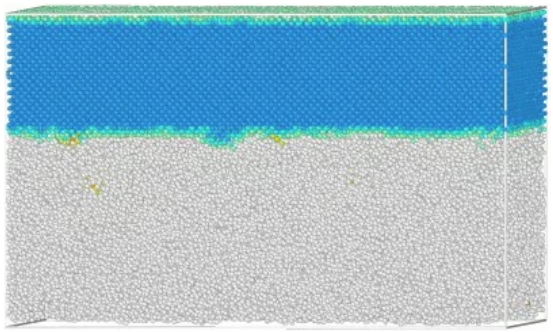
How Does it Work?

Determining Stability



2GPa,900K,0.1m/s

Q_4+Q_6



OVITO

% Change in Amorphous = 18.5% or 18.5% amorphous is crystallizing

The Q parameter is calculated while equilibrating a structure. This is the initial structure distribution. σQ is calculated from the initial equilibration which gives the max distance from the mean of the distribution which can be considered as crystal.
Q_4+Q_6 parameter of the initial structure as a distribution($Q_{initial}$) rather than an average over absolute number.

While incorporating any perturbation, the Q parameters are collected throughout the simulation time, and these are averaged over all the atoms and for all timesteps(Q_{avg})

The change in the maximum peak+ σQ of the average distribution from the initial gives us the change in orientation for all the atoms. The change can either be calculated by χ^2 or Bhattacharya Distance.

We can track the amorphization and crystallization by taking the summation of the change in maximum peak of the distribution of the initial and final histograms. If the summation is +ve, then it is crystallizing, -ve is amorphizing and equal is stable.

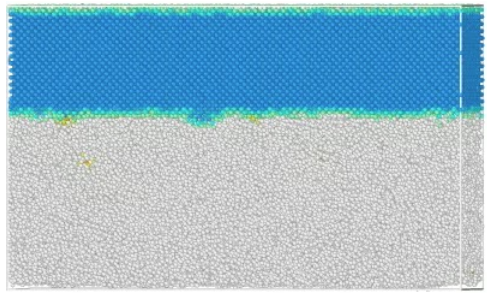
Crystallizing, Bhattacharya Distance(ϵ {-1,+1}) = 0.22002078501697508

Crystallizing, χ^2 (ϵ {-i,+i}) = 13.576591353200037

22% Of the structure is crystalizing

Examples

12GPa,900K,0.1m/s

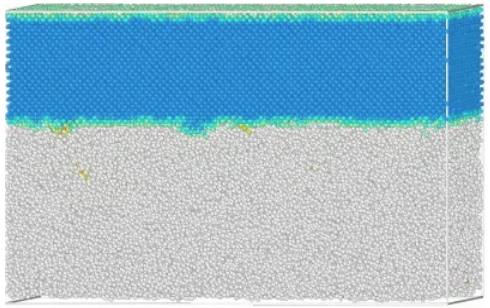


Amorphizing,
Bhattacharya Distance = - 0.14450725205468384

Amorphizing, χ^2= -3.1202222549260967

OVITO
% Change in Amorphous = 0.6% or
0.6% crystalline is amorphizing
Fixed amorphous =14.9%
Effective Crystallization %= 15.5%

5GPa,1200K,0.1m/s

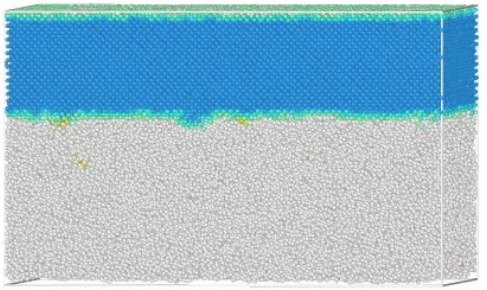


Crystallizing,
Bhattacharya Distance = 0.3042980601326322

Crystallizing, χ^2= 51.12525510654333

OVITO
% Change in Amorphous = 45.5% or
45.5% amorphous is crystallizing
Fixed amorphous =14.9%
Effective Crystallization %= 30.6%

14.5GPa,1300K,0m/s



Amorphizing,
Bhattacharya Distance = - 0.48248173833438857

Amorphizing, χ^2= -91.23072475087022

OVITO
% Change in Amorphous = 39.6% or
100% amorphous is crystallizing
Fixed amorphous =14.9%
Effective Amorphizing %= = 54.5%

Pros

1. Robust method of identifying the ordering stability of any system, regardless of the interface.
2. No reference file comparison. So, Comparing non-periodic complex system with a periodic perfect lattice is avoided.
3. The tolerance of 0.01 is manually adjusted for the previous scoring systems. Here it is avoided.

Cons

The only case where this identification will not work is when the crystalline percentage is same over time, but the amorphous orientation is completely changed or increases considerably.