Using a Self Organising Map for Clustering of Atomistic Samples

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Introduction

Testing

BCC Fe Bulk With a Void:

As a simple test, a 25×10^4 atoms BCC Fe bulk with a void was analysed. The sample was created and relaxed with LAMMPS. Since the sample has no defects, the goal was to use the SOM to identify the void in the center of the simulation box. This was achieved using parameters $\sigma = 1$, $\eta = 0.5$ and $f = 1$, clustering the atoms into 3 groups and using the centro-symmetry parameter and the coordination (both calculated with LAMMPS) as features.
The results are shown in Fig. 1 and Fig. 3, although the algorithm classified the atoms into 3 groups, no atom was assigned to group 1. For the previously specified parameters, the SOM didn't produce useful results when clustering the atoms into only 2 groups.

HEA Nano-foam Under Compression:

Fig. 5 shows the result of applying the SOM to a compressed HEA nano-foam sample, with the goal of classifying the atoms into 2 groups. The network was trained using parameters $\sigma = 1$, $\eta = 0.5$ and $f = 1$. The features used in this occasion were:

- Centro-symmetry parameter
- Coordination, via Coordination Analysis with cutoff radius $r_c = 6$
- Atomic volume, via Voronoi Analysis

On the other hand, Fig. 6 shows the same sample, with the atoms classified by structure type (FCC, HCP, BCC and Other) using the PTM algorithm. It can be observed that the yellow atoms in Fig. 5 correspond to the HCP, BCC and Other atoms in Fig. 6. While the atoms in the remaining group of the SOM classification correspond to the FCC atoms of the sample. In this sense, the SOM is correctly identifying the atoms associated with defects and/or that belong to the surface of the sample.

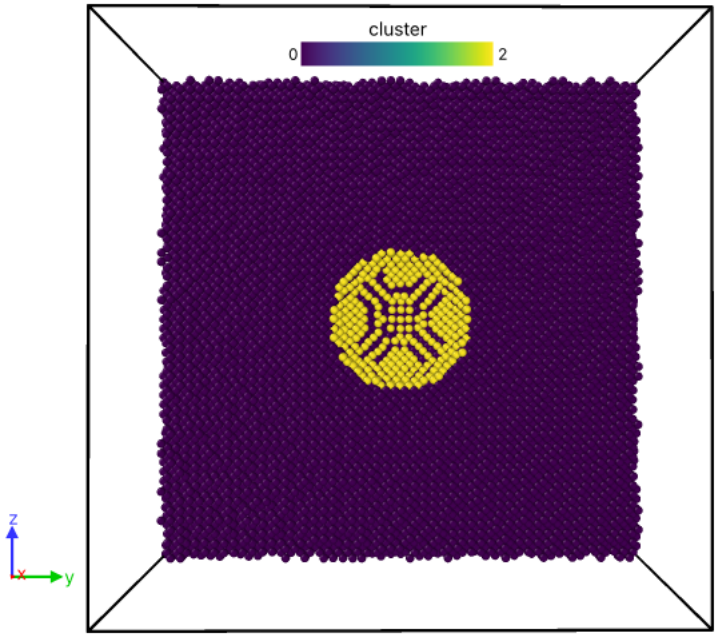

Figure 1: BCC Fe bulk with void. The atoms have been clustered into 3 groups using parameters $\sigma = 1$, $\eta = 0.5$ and $f = 1$. The centro-symmetry and coordination (via Coordination Analysis with $r_c = 6$) were used as features. A slice of the sample, with groups 0 (purple) and 2 (yellow), is shown.

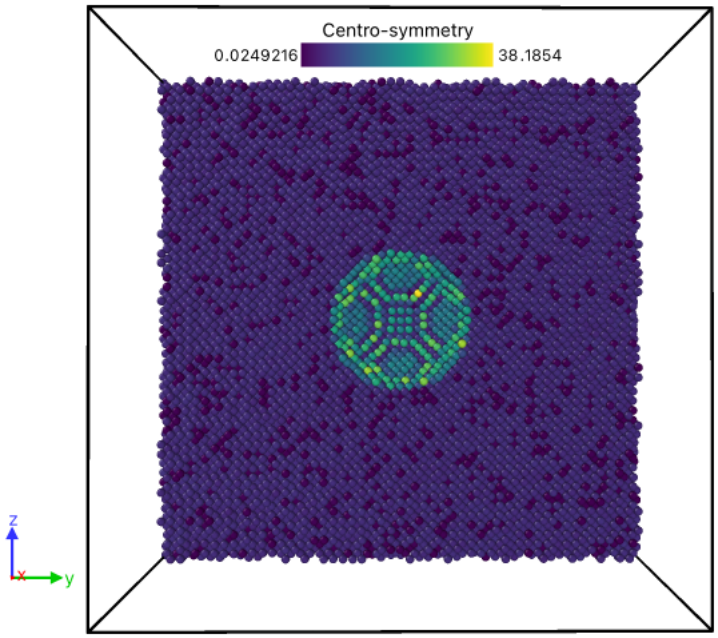

Figure 2: BCC Fe bulk with void. The atoms have been clustered using the centro-symmetry parameter (as calculated by LAMMPS). A slice of the sample is shown.

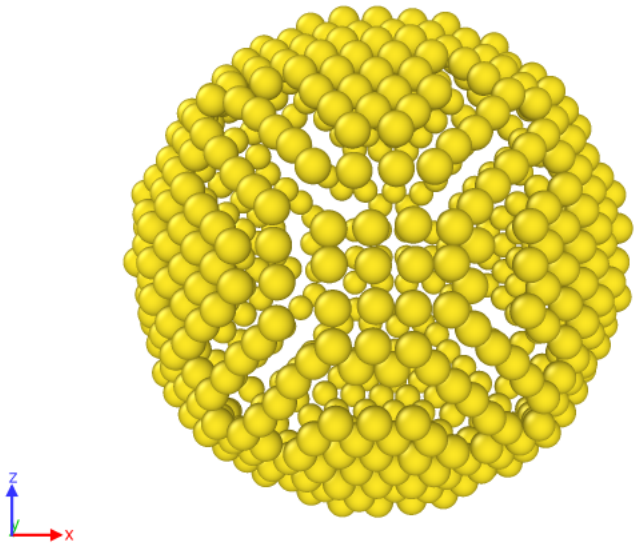

Figure 3: Void of the BCC Fe bulk sample. The atoms belonging to group 2, as classified by the SOM, are shown. The centro-symmetry and coordination (via Coordination Analysis with $r_c = 6$) were used as features.

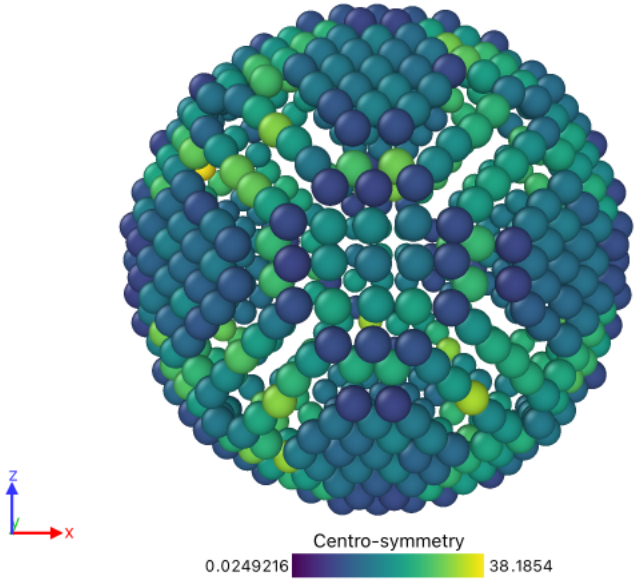

Figure 4: Void of the BCC Fe bulk sample. The atoms have been clustered using the centro-symmetry parameter (as calculated by LAMMPS).

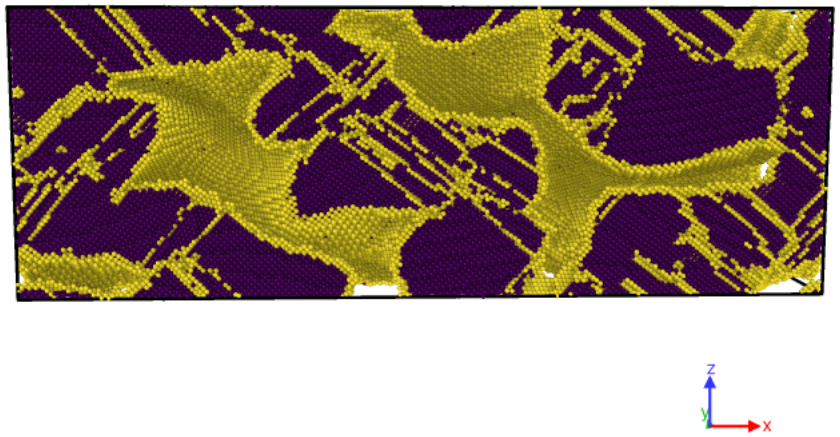

Figure 5: HEA Nano-foam under compression. The atoms have been clustered into 2 groups using parameters $\sigma = 1$, $\eta = 0.5$ and $f = 1$. The centro-symmetry, coordination (via Coordination Analysis with $r_c = 6$) and atomic volume (via Voronoi Analysis) were used as features.

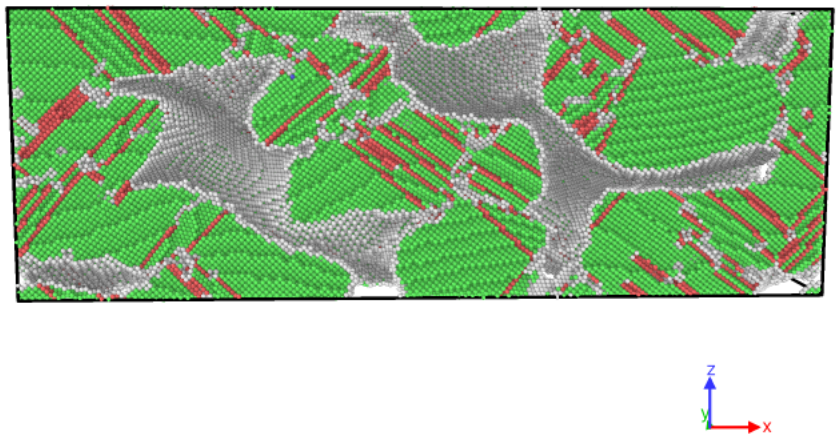

Figure 6: HEA Nano-foam under compression. The atoms have been clustered using the PTM algorithm into 4 categories: FCC (green), HCP (red), BCC (purple) and Other (white).