Unsupervised learning for structure detection in plastically deformed crystals

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Molecular Dynamics (MD) is a powerful method allowing to simulate different materials at the particle scale such as colloidal systems, glassy materials or metallic nanocrystals. To help in interpreting the simulations results, being able to determine the local structure at the particle-scale is essential. To do so, several approaches were developed, mainly relying on local order parameters to describe the surrounding environment of each particle (number of neighbors, angles formed with the neighbors, …) to detect underlying substructures in the simulated atomistic sample. Among these methods, we can cite the Bond Orientational Order (BOO) parameter, the Common Neighbors Analysis (CNA), or the Bond-Angle Distribution (BAD). Such methods were applied with success to study several phenomena such as crystal nucleation, melting or plasticity. However, they are mostly relying on hand chosen criteria and thus only works for already known structures.

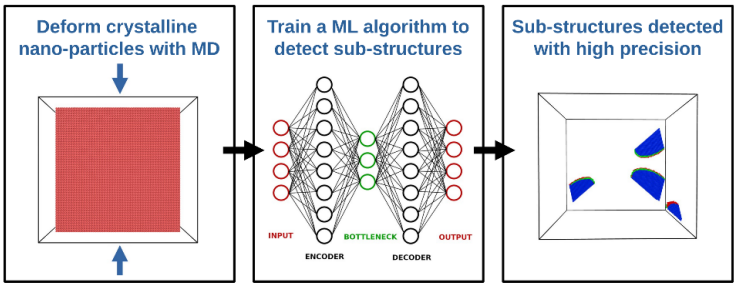

Figure 1: Graphical abstract of the unsupervised learning approach to detect sub-structures within a nano-crystal plastically deformed in MD.

In this study, we present a method, inspired by a paper from Boattini et al. [1], to automatically study and detect the different substructures appearing at the atomistic scale within a crystal under plastic deformation. This approach relies on the BAD parameters designed for single crystals to describe the environment around each atom. Our method, shown on Fig. 1, consists on (i) deforming a nanocrystal with MD simulation, (ii) training a Machine Learning (ML) model by: (1) extracting the most pertinent BAD parameters using an autoencoder neural networks before (2) applying two clustering models: K-means and DBSCAN to detect the different sub-structures in the system without a-priori knowledge of the existing structures. And finally, (iii) applying the pre-trained model to the other simulation steps to detect the location of the substructures. This method has the advantage of being computationally fast and easy to implement.

By applying our method on a Nickel FCC nanocrystal plastically deformed under uniaxial compression, we were able to detect more sub-structures associated with plasticity and with a higher degree of precision than traditional hand-made criteria. This study was published on [2].

[1] E. Boattini, M. Dijkstra, L. Filion. The Journal of Chemical Physics, 151 (15), 154901, 2019.
[2] A. Barbot, R. Gatti. Computational Materials Science, 230, 112459, 2023.