Magnetic crystal reconstruction and optimisation using Graph Neural Networks

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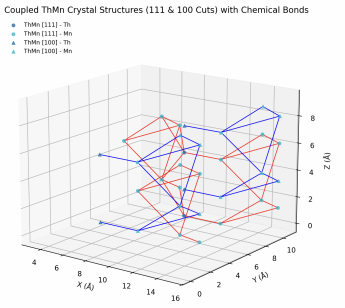
Magnetic crystals are described by complex electronic and spin interactions that govern magnetization dynamics, magnetic anisotropy, and phase transitions. These properties play an essential role in high-frequency and magnonic applications, especially in emerging technologies such as 6G communication systems. However, accurate prediction of their macroscopic magnetic behavior is challenging because of multiphase interactions, complex crystal symmetry, and differences in the boundaries of traditional computational methods.

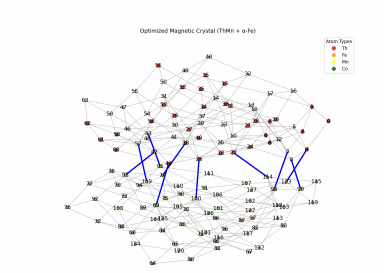
In the first step, we focus on single magnetic crystals, using graph theory to create graph representations of hence crystals where nodes represent the atoms and the edges the magnetic or chemical relations. Both of these extract local (node-level) and global (graph-level) structural features, which serve as input for an active teaching model that refines the predictions of magnetically prominent properties and topological features such as magnetization, Curie temperature, average degree, average shortest path length, clustering coefficient, maximum cluster size, and PageRank centrality. The number of data points increases the efficiency of the model by prioritizing data points with higher connectivity based on the graph model, reducing computational time and costs.

In the second phase, we extend this approach to polycrystals, characterized by complex atomic arrangements and long-range interactions. This involves the construction of larger and more complex systems (mixed interfaces and compositions) and the extraction of higher-order structural characteristics that capture the complexity of these systems. We employ machine learning techniques (such as XGboost for feature-based learning and Graph Neural Networks (GNNs)) to model dependencies between atomic interactions and magnetic properties with the aim to identify and reconstruct these supercell structures. The graphic analysis reveals that directional cutting changes local magnetic connectivity, leading to measurable changes in magnetization and anisotropic properties. In particular, the grouping coefficient and maximum cluster size display strong correlations with post-cut temperature variations. In detail, we investigate the impact of different cutting planes ([100], [110], [111], etc.) on magnetic connectivity and anisotropy, providing a comprehensive understanding of structural modifi-

cations in 1-12 type materials. This approach enhances predictive accuracy but also offers deeper insights into how graph topology governs macroscopic magnetic behavior, deepening our understanding of structure-property relationships.



(a) $ThMn$ Crystal interface (1,1,1) to (1,1,0)



(b) Crystal interface $ThMn$ to $\alpha - Fe$

In figure a, this is a $ThMn$ super-cell crystal with a (1,1,1) to a (1,1,0) interface. Figure b is the interface of a super-cell $ThMn$ and $\alpha - Fe$ structure. It is composed of multiple nodes, which are the atoms, and the black lines represent the topological connections between atoms. The blue lines are the connection between these two different crystals at the interface. The entire graph forms a complex topological network. The graph analysis reveals that structural modifications induce significant changes in local magnetic connectivity. Based on the calculation from *igraph* we can get its Topological characteristics (e.g *degree_avg, avg_path_length, clustering_coeff, pagerank_avgpagerank_avg* and *max_clique_size*). This is just one of the possibilities.
Notably, clustering coefficients, maximum cluster size, and connectivity metrics strongly correlate with post-cut magnetic variations, emphasizing the role of interfacial atomic bonding. The combined analysis of unit-cell and super-cell structures provides insights into the fundamental structure-property relationships, which offer a computationally efficient alternative to density functional theory (DFT) simulations. Compared with previous methods, this is more like a distillation-style ML method. The aim is to simplify the data used for training, use more targeted methods to derive an accurate result and simplify the branches during the training, and cut off unnecessary possibilities in a targeted manner, so that the noise of the answer can be reduced. In short, this is an artificial Mixture of Experts (MOE) machine learning technology. The purpose is to derive an accurate and faster analysis of complex systems with smaller data sets.