Graph theoretic modelling of Rare Earth Transition Material Properties

Gino Hrkac[1], Prathyush P Menon[1], Hao Zhang[1]

[1] *Department of Engineering, University of Exeter, Exeter, UK.*

Data science and optimization with machine learning have become an integral part of material and mathematical sciences. Automated optimization (Machine learning) methods are ever increasingly applied in all steps of materials development; searching for bespoke material and property prediction using inverse material design in parallel to material analysis. Thus accelerating the digital twin simulations as well as automated experimental data analysis and experimental planning [1].

In this paper we present a small data based graphical connectivity represented framework, although general in its methodolgy we aim to apply it to the design of hybrid multi-layer composite magnetic materials. We start from a magentic phase diagram of at least 3 elements and use graph theory to predict the probabikity of crystal phase formation based on element ratio and molecular potentials. Our simple graph theoretical edge model (GEO) will be implemeted and solved using Graph neural networks, which can be interpreted as the generalization of convolutional neural networks to irregular-shaped graph structures. The graphical representation of element dependencies sets it apart from general used machine learning methods, e.g., convolutional neural networks.

GEO Model: We consider network representation of n materials indexed from 1 to n that can interact with each other. It is possible to encapsulate the structural, configurational and functional relations of the materials in the form of graphs. Interactions among the materials is represented by a simple undirected weighted graph $\mathcal{G} := (\mathcal{V}, \mathcal{E})$ where $\mathcal{V} = \{1, 2, \ldots, n\}$ is the set of vertices representing the elements and $\mathcal{E} = \{e_{ij},\ i = 1, \ldots, n-1,\ j = 1, \ldots, n,\ i < j\}$ is the set of interactions between agents with the weight function

$$w : \mathcal{R}^p \times \mathcal{R}^p \to \mathcal{R}^+$$

where $\mathcal{R}^p$ represents a real space characterised by p functional properties of the material. The weight is assigned to each edge e_{ij} a function of the edge formed between two edges is determined by a function of the potential field function which in turn depends on the percentage combination of the materials. In our problem setting, we will analyse the connectivity of each graphs using the principle of randomisation and classify them and obtain a distribution yielding maximum connectivity.

Once the distribution functions are obtained they are feed into a Graph neural network with varying vertices numbers. Solving these for maximum connectivity will allow to map the distribution of maximum connectivity on possible crystal phases in a magentic phase diagram.

In short, we will apply graph neural networks (GNNs) to predict the relations of node, edge and higher order graphs in conjecture with crystal phase formation; a graph-level prediction model.

References

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