Computational Design of Materials via Neural Networks

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The phase diagram is a type of chart used to show the conditions at which thermodynamically distinct phases occur and coexist at equilibrium. In the case of alloys, these phases include the liquid stage and the different solid crystal structures that the alloy can be found depending on the temperature and percentage mixture of each metal. Determining a phase diagram is done experimentally, which is extremely expensive in terms of time and resources. We propose using a machine learning model to obtain phase diagrams of alloys. We use convolutional neural networks (CNN) since they are space invariant. The alloy of Copper (Cu) and Silver (Ag) were used to train the CNN model, since the Cu-Ag phase diagram is readily available, serving as a comparison for the CNN's predictions. Molecular dynamic simulations of the alloys in different conditions were used to generate the data in the form of cartesian coordinates of the atoms and the total potential energy of the system. The cartesian coordinates were transformed to a set of symmetry function values which served as an input for the model. The CNN model is trained on the symmetry function values as input and predicts the potential energy of the system. From the potential energy of an alloy at different conditions, a phase diagram can be derived.