Identify Phases in Materials – Human or Robot?

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Discovery of new materials is time consuming – typically 20 years. It is even more difficult identify a material if it is multi-component. High throughput (HiTp) experimentation, which is designed to run experiments or characterization in a parallel manner, could accelerate the process by 100-1000 times. The new challenge originated from HiTp experimentation is how to analyze the large data sets in a more efficient way and visualize them.

In the poster, the Co-Fe-Zr ternary system which contains potential metallic glass formers is included as an example (Figure 1 shows the prediction on the glass formation of Co-Fe-Zr). The methods involving human domain knowledge, robots, and the combination of the two, are used to identify the phases in the Co-Fe-Zr ternary. The results between different methods are compared and discussed.

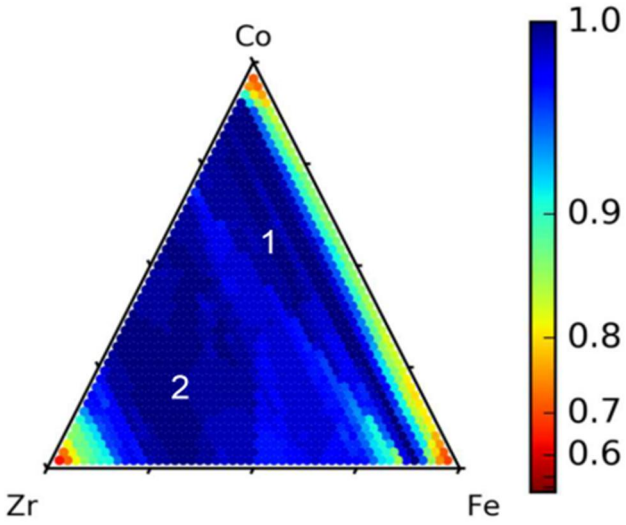

Figure 1. Glass formation predicted by the supervised machine learning tools. The alloys in the blue region are more likely to form metallic glasses.