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Experimental Verificagtion of Bulk Metallic Glass Prediction from Machine Learning

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Unlike crystalline alloys that have a regular atomic arrangement, atoms are randomly arranged in the novel bulk metallic glasses (BMGs). From a practical standpoint, BMGs are much stronger than ordinary metal alloys, and are thus potentially important materials for commercial and military applications. Why some alloys form these glasses, however, is incompletely understood. Chris Wolverton uses machine learning to predict certain compositions of elements that will form BMGs. Among others, Wolverton's code predicts glass formation in (i)$Zr_{58}Ni_{26}Ir_{16}$, (ii)$Hf_{66}Fe_{32}Co_2$, (iii)$Hf_{58}Fe_{42}$, (iv)$Zr_{40}Cu_{44}Cr_{16}$, and (v)$Zr_{50}Fe_{46}Cr_4$ alloys. The subscripts indicate the atomic percentages of the elements in the alloy. Our goal is to determine experimentally whether the aforementioned alloys will form BMGs.

One gram alloys of each composition were first prepared. The masses of elemental materials needed (determined from equation 1) were measured using an analytic balance and mixed together.

Equation 1: $m^* \frac{Xs*\mu s}{\sum_i Xi*\mu i}$, where X is the atomic percentage of the element s, μ is the atomic mass of the element s, and m is the mass of the sample, which we take to be 1g.

This mixture was then melted using an electric arc-furnace to obtain spherical ingots. The ingot was arc-melted again and suction-cast into a copper mold to produce samples having a varying thickness along their length. X-ray diffraction and Differential Scanning Calorimetry (DSC) measurements were made to determine whether a BMG was formed as a function of the thickness.

The purpose of this experiment was to determine whether the aforementioned five alloys formed BMGs, which would show whether Wolverton's machine learning model is predictive. With the exception of $Zr_{40}Cu_{44}Cr_{16}$, the 4 other predictions did not form metallic glass. For $Zr_{40}Cu_{44}Cr_{16}$, our data indicate that it is only partially amorphous at a thickness of 20 microns.