Metallic Glass Discovery and Science Using Combined Forces of Combinatorial, High-Throughput, Data Science, and Artificial Intelligence Strategies

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Abstract

The multicomponent nature of bulk metallic glasses imposes a challenge for their discovery process. Rough estimations suggest that only a minute fraction of potential compositional space for bulk metallic glass formers has been explored thus far.

Here we introduce combinatorial strategies to fabricate libraries comprising of ~1000 different compositions. We use magnetron co-sputtering from three elemental targets that are oriented to create compositional gradients. The resulting composition library is explored for promising compositions. We use a massively parallel characterization method to determine the solidification temperatures, which we correlate with glass forming ability. Also in a massively parallel fashion, we determine the thermoplastic forming ability, which reflects in addition to the glass forming ability, the BMG’s ability for plastic-like processing. Both methods are effective in navigating through the vast composition space towards glass forming compositions. We will introduce novel methods to quantify glass forming ability and related properties. The vast amounts of data are stored, managed, and shared through an online web site, which will be introduced. Such data will then be used applying data science and artificial intelligence strategies to identify unknown glass formers, to suggest alloys which provide most information about the underlying phenomena or to reveal scaling of other characteristics such as mechanical properties, processibility or corrosion.

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