Linear Regression Analysis for the Prediction of Phase Formation of Ti-Fe Based MPEA Systems

Alex Hansen

PhD Candidate, Metallurgical and Materials Engineering

Colorado School of Mines

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Overview

One of the overarching goals of this NSF Career project is to study the use of novel MPEAs (multi-principal element alloys) to facilitate the joining (welding, brazing) of titanium alloys to stainless steel alloys. To contribute to this goal, this portion of the project has focused on finding alloys that can maintain an FCC and/or BCC structure in the presence of diluting elements from Ti64 and SS304; Ti64 is the most widely used titanium alloy, and SS304 is one of the most popular stainless steels. Possible MPEA compositions have been identified through thermodynamic modeling and manual filtering based on volume fraction and freezing range temperature requirements. Several welding trials have been conducted with different alloy systems to demonstrate the weldability of the modeled MPEAs and to measure real dilution content and phase volume fraction. This has led to a better understanding of the compositional requirements of the alloy.

It is known that from the Ti64 side, Al, V, and Ti will dilute up to roughly 5%, 3% and 70%, respectively, into the MPEA; on the stainless-steel side Fe, Ni, and Cr will dilute up to roughly 40%, 5%, and 10%, respectively. On each side, there is a compositional gradient, where the amount of each diluting element will decrease further away from the base material. Several alloying elements in other and our own work have been identified as FCC and BCC stabilizers in Fe and Ti systems, respectively; Cu and Mn for the FCC structure in Fe, and Mo and Nb for the BCC structure in Ti. Further, Ni is a known FCC stabilizer in steels, while Nitinol (Nickle-Titanium-alloy) is a well-known alloy with a BCC structure stable between 40-60% Ti with Ni.

A large data set was inputted to a high throughput thermodynamic simulation via MatLab, python, and ThermoCalc. This dataset represented the sequential changing of a 10-element alloy system (Al, Ti, V, Cr, Mn, Fe, Ni, Cu, Mo, Nb) from 0.0001 at % (to represent 0%) up to 50 at % (except for Ti up to 70 at %). From this data set thermal and phase information will be extracted. The intention is to determine the interaction between each alloying element and phase formation. The first iteration of this analysis has the composition of one element changing while the rest of the elements are equally, but inversely changed, i.e., if Ti is increased by 1.25 At%, each other

element in the system will be decreased by (1.25/9) at%. If this set proves to be useful in understanding the relationship between alloying elements and freezing range temperatures and phase fractions (phase fractions being the most critical of the outputs), then further data sets will be generated where pairs or trios of elements will be modified together, while the remaining elements are inversely changed.

The “stretch” goal is to be able to predict phase volume fraction of an alloy without thermodynamic modeling, however this is likely too lofty of a goal from such a small dataset, as the interactions between each element(s) are more complex than just the modification of one. However, if several of the elements can be “locked” as the base of the alloy, then perhaps the impact of the other elements can be predicted. This would help with narrowing down the compositional ranges for thermodynamic modeling exploration, expediting the identification of alloys for welding trials.

Related Work

There is no shortage of new MPEA research being conducted. Given the vastness of the field and the plethora of potential applications, this should not be surprising. Primarily, researchers focus on the development of an MPEA alloy, typically single or dual phase [1, 2], that excels in a specific area/property, e.g., thermal or electrical conductivity, high temperature performance, mechanical strength or ductility [3]. There have also been machine learning studies where researchers perform similar simulations as those conducted by this group to identify possible compositions with unique properties, and meta studies conducted on the capabilities of researched MPEAs where the performance of multiple (dozens) of alloys in a specific engineering space are analyzed [4].

Dissimilar joining research has been ongoing for decades for virtually every metal system that exists and even metal to ceramic systems. In the world of engineering and manufacturing, the joining of dissimilar systems is a critical barrier to design. In particular, titanium to stainless steel joining has had decades of research, still there are no reliable methods for joining these systems that is viable for manufacturing settings [5]. However, with the emergence and greater understanding of newer technologies such as additive manufacturing, advanced manufacturing processes (e.g., laser and e-beam welding), and MPEA’s method may be on the horizon [6].

There are studies similar, for instance the study of MPEA brazing fillers for Ni superalloy applications, that look at how MPEAs can handle dilution of base metal elements while maintaining a beneficial microstructure with good mechanical properties [7]. However, thus far there has not been a publication on combining all the above approaches to the application of joining titanium to stainless steel alloys. This is likely due to the extreme complexity of modeling and predicting the dilution of two different metals into the filler material.

References

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