A Machine Learning Approach to Predict Martensitic Transition Temperatures for Shape Memory Alloys

Shreyas Honrao (KRB Inc, NASA ARC), Othmane Benafan (NASA GRC), John Lawson (NASA ARC)

Shape memory alloys (SMAs) are a unique class of materials with several remarkable properties including shape recovery, superelasticity, etc. Especially important for many NASA applications is the ability to tune the martensitic phase transition temperature by varying the alloy composition. Nickel-titanium (NiTi) based alloys are the most widely studied of this class, with compositions involving ternary, quaternary, or higher additions being considered. Over the past several years, a significant database of SMA properties has been assembled by NASA researchers. Such a database is ideal for data science-based approaches including machine learning. We present results from a developed machine learning model capable of accurately predicting the transition temperature of SMAs across a wide range of compositions. Our model has the added benefit of interpretability and even provides confidence intervals for our predictions. This model will make rapid screening and design of new SMA materials possible. Predictions from the machine learning model can be validated by empirical and/or atomistic scale modeling.