

A Machine Learning Approach to Design Shape Memory Alloys for NASA Applications

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Shape memory alloys (SMAs) are a unique class of materials with several remarkable properties including shape recovery, superelasticity, etc. Nickel-titanium (NiTi) based alloys are the most widely studied of this class, with compositions including ternary, quaternary, or higher additions being considered. Especially important for many NASA applications is the ability to tune the martensitic phase transition temperature of NiTi alloys by varying the alloy composition and processing conditions. In addition, low hysteresis and an acceptable recoverable transformation strain are required. 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. We present results from our machine learning approach for designing new SMAs with target properties within our range of interest. Our developed models are capable of accurately predicting the transition temperature, hysteresis, and transformation strain of SMAs across a wide range of compositions. This approach has the potential to significantly accelerate the discovery and design of new SMA materials.