New shape memory alloy discovered through artificial intelligence framework
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Researchers from the Department of Materials Science and Engineering at Texas A&M University have used an Artificial Intelligence Materials Selection framework (AIMS) to discover a new shape memory alloy. The shape memory alloy showed the highest efficiency during operation achieved thus far for nickel-titanium-based materials. In addition, their data-driven framework offers proof of concept for future materials development.

This study was recently published in the Acta Materialia journal.

Shape memory alloys are utilized in various fields where compact, lightweight and solid-state actuations are needed, replacing hydraulic or pneumatic actuators because they can deform when cold and then return to their original shape when heated. This unique property is critical for applications, such as airplane wings, jet engines and automotive components, that must withstand repeated, recoverable large-shape changes.

There have been many advancements in shape memory alloys since their beginnings in the mid-1960s, but at a cost. Understanding and discovering new shape memory alloys has required extensive research through experimentation and ad-hoc trial and error. Despite many that have been documented to help further shape memory alloy applications, new alloy discoveries have occurred in a decadal fashion. About every 10 years, a significant shape memory alloy composition or system has been discovered. Moreover, even with advances in shape memory alloys, they are hindered by their low energy efficiency, caused by incompatibilities in their microstructure during the large shape change. Further, they are notoriously difficult to design from scratch.

To address these shortcomings, Texas A&M researchers have combined experimental data to create an AIMS computational framework capable of determining optimal materials compositions and processing these materials, which led to the discovery of a new shape memory alloy composition.

"When designing materials, sometimes you have multiple objectives or constraints that conflict, which is very difficult to work around," said Dr. Ibrahim Karaman, Chevron Professor I and materials science and engineering department head. "Using our machine-learning framework, we can use experimental data to find hidden correlations between different materials' features to see if we can design new materials."
Doctoral student William Trehern operating a vacuum arc melter—a synthesis method commonly used to create high-purity alloys of various compositions. Trehern and his team used an Artificial Intelligence Materials Selection framework to discover a new shape memory alloy. Credit: Texas A&M Engineering

The shape memory alloy found during the study using AIMS was predicted and proven to achieve the narrowest hysteresis ever recorded. In other words, the material showed the lowest energy loss when converting thermal energy to mechanical work. The material showcased high efficiency when subject to thermal cycling due to its extremely small transformation temperature window. The material also exhibited excellent cyclic stability under repeated actuation.

A nickel-titanium-copper composition is typical for shape memory alloys. Nickel-titanium-copper alloys typically have titanium equal to 50% and form a single-phase material. Using machine learning, the researchers predicted a different composition with titanium equal to 47% and copper equal to 21%. While this composition is in the two-phase region and forms particles, they help enhance the material's properties, explained William Trehern, doctoral student and graduate research assistant in the materials science and engineering department, and the publication's first author.

In particular, this high-efficiency shape memory alloy lends itself to thermal energy harvesting, which requires materials that can capture waste energy produced by machines and put it to use, and thermal energy storage, which is used for cooling electronic devices.

More notably, the AIMS framework offers the opportunity to use machine-learning techniques in materials science. The researchers see potential to discover more shape memory alloy chemistries with desired characteristics for various other applications.

"It is a revelation to use machine learning to find connections that our brain or known physical principles may not be able to explain," said Karaman. "We can use data science and machine learning to accelerate the rate of materials discovery. I also believe that we can potentially discover new physics or mechanisms behind materials behavior that we did not know before if we pay attention to the connections machine learning can find."

Other contributors include Dr. Raymundo Arróyave and Dr. Kadri Can Atli, professors in the materials science and engineering department, and materials science and engineering undergraduate student Risheil Ortiz-Ayala.

"While machine learning is now widely used in materials science, most approaches to date focus on predicting the properties of a material without necessarily explaining how to process it to achieve target properties," said Arróyave. "Here, the framework looked not only at the chemical composition of candidate materials, but also the processing necessary to attain the properties of interest."


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