An alloy that retains its memory at high temperatures

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Alexander Paulsen (right) and Alberto Ferrari have brought theory and practice together. Credit: RUB, Marquard

Using computer simulation, Alberto Ferrari calculated a design proposal for a shape memory alloy that retains its efficiency for a long time even

at high temperatures. Alexander Paulsen manufactured it and experimentally confirmed the prediction. The alloy of titanium, tantalum and scandium is more than just a new high-temperature shape memory alloy. Rather, the research team from the Interdisciplinary Centre for Advanced Materials Simulation (Icams) and the Institute for Materials at Ruhr-Universität Bochum (RUB) has also demonstrated how theoretical predictions can be used to produce new materials more quickly. The group published its report in the journal *Physical Review Materials* from 21 October 2019. Their work was showcased as an Editor's suggestion.

Avoiding the unwanted phase

Shape memory alloys can re-establish their original shape after deformation when the temperature changes. This phenomenon is based on a transformation of the crystal lattice in which the atoms of the metals are arranged. Researchers refer to is as phase transformation. "In addition to the desired phases, there are also others that form permanently and considerably weaken or even completely destroy the shape memory effect," explains Dr. Jan Frenzel from the Institute for Materials. The so-called omega phase occurs at a specific temperature, depending on the composition of the material. To date, many shape memory alloys for the high temperature range would withstand only a few deformations before they became unusable once the omega phase set in.

Promising shape memory alloys for high temperature applications are based on a mixture of titanium and tantalum. By changing the proportions of these metals in the alloy, researchers can determine the temperature at which the omega phase occurs. "However, while we can move this temperature upward, the temperature of the desired phase transformation is unfortunately lowered in the process," says Jan Frenzel.

Admixture alters properties

The RUB researchers attempted to understand the mechanisms of the onset of the omega phase in detail, in order to find ways to improve the performance of shape memory alloys for the high-temperature range. To this end, Alberto Ferrari, Ph.D. researcher at Icams, calculated the stability of the respective phases as a function of temperature for different compositions of titanium and tantalum. "He was able to use it to confirm the results of experiments," points out Dr. Jutta Rogal from Icams.

In the next step, Alberto Ferrari simulated small amounts of third elements being added to the shape memory alloy of titanium and tantalum. He selected the candidates according to specific criteria, for example they should be as non-toxic as possible. It emerged that an admixture of a few percent of scandium would have to result in the alloy functioning for a long time even at high temperatures. "Even though scandium belongs to the rare earths and is, consequently, expensive, we only need very little of it, which is why it's worth using anyway," explains Jan Frenzel.

Prediction is accurate

Alexander Paulsen then produced the alloy calculated by Alberto Ferrari at the Institute for Materials and tested its properties in an experiment: the results confirmed the calculations. A microscopic examination of the samples later proved that even after many deformations no omega phase was found in the crystal lattice of the alloy. "We have thus expanded our basic knowledge of titanium-based shape memory alloys and developed possible new high-temperature shape memory alloys," says Jan Frenzel. "Moreover, it's great that the computer simulation predictions are so accurate." Since the production of such alloys is very complex, the

implementation of computer-aided design proposals for new materials promises much faster success.

More information: Alberto Ferrari et al, Discovery of ω -free high-temperature Ti-Ta- X shape memory alloys from first-principles calculations, *Physical Review Materials* (2019). DOI: 10.1103/PhysRevMaterials.3.103605

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