Researchers uncover kinky metal alloy that won't crack at extreme temperatures at the atomic level

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A map of the crystal structure of the alloy made with electron backscatter diffraction in a scanning electron microscope. Each color represents a section of the crystal where the repeating structure changes its 3D orientation. Credit: Berkeley Lab

A metal alloy composed of niobium, tantalum, titanium, and hafnium has shocked materials scientists with its impressive strength and toughness at both extremely hot and cold temperatures, a combination of properties that seemed so far to be nearly impossible to achieve.

In this context, strength is defined as how much force a material can withstand before it is permanently deformed from its original shape, and toughness is its resistance to fracturing (cracking). The alloy's resilience to bending and fracture across an enormous range of conditions could open the door for a novel class of materials for next-generation engines that can operate at higher efficiencies.

The team, led by Robert Ritchie at Lawrence Berkeley National Laboratory (Berkeley Lab) and UC Berkeley, in collaboration with the groups led by professors Diran Apelian at UC Irvine and Enrique Lavernia at Texas A&M University, discovered the alloy's surprising properties and then figured out how they arise from interactions in the atomic structure. Their work is described in a study that was published in *Science*.

"The efficiency of converting heat to electricity or thrust is determined by the temperature at which fuel is burned—the hotter, the better. However, the operating temperature is limited by the structural materials which must withstand it," said first author David Cook, a Ph.D. student in Ritchie's lab. "We have exhausted the ability to optimize further the materials we currently use at high temperatures, and there's a big need for novel metallic materials. That's what this alloy shows promise in."

The alloy in this study is from a new class of metals known as refractory high or medium entropy alloys (RHEAs/RMEAs). Most of the metals we see in commercial or industrial applications are alloys made of one main metal mixed with small quantities of other elements, but RHEAs and RMEAs are made by mixing near-equal quantities of metallic elements with very high melting temperatures, which gives them unique properties that scientists are still unraveling.

Ritchie's group has been investigating these alloys for several years because of their potential for high-temperature applications.

"Our team has done previous work on RHEAs and RMEAs, and we have found that these materials are very strong but generally possess extremely low fracture toughness, which is why we were shocked when this alloy displayed exceptionally high toughness," said co-corresponding author Punit Kumar, a postdoctoral researcher in the group.

According to Cook, most RMEAs have a fracture toughness of less than 10 MPa√m, which makes them some of the most brittle metals on record. The best cryogenic steels, specially engineered to resist fracture, are about 20 times tougher than these materials. Yet the niobium, tantalum, titanium, and hafnium ($Nb_{45}Ta_{25}Ti_{15}Hf_{15}$) RMEA alloy was able to beat even the cryogenic steel, clocking in at over 25 times tougher than typical RMEAs at room temperature.

But engines don't operate at room temperature. The scientists evaluated strength and toughness at five temperatures total: -196°C (the temperature of liquid nitrogen), 25°C (room temperature), 800°C, 950°C, and 1200°C. The last temperature is about 1/5 the surface temperature of the sun.

The team found that the alloy had the highest strength in the cold and became slightly weaker as the temperature rose but still boasted impressive figures throughout the wide range. The fracture toughness, which is calculated from how much force it takes to propagate an existing crack in a material, was high at all temperatures.

Unraveling the atomic arrangements

Almost all metallic alloys are crystalline, meaning that the atoms inside the material are arranged in repeating units. However, no crystal is perfect; they all contain defects. The most prominent defect that moves is called the dislocation, which is an unfinished plane of atoms in the crystal. When force is applied to a metal, it causes many dislocations to move to accommodate the shape change.

For example, when you bend a paper clip that is made of aluminum, the movement of dislocations inside the paper clip accommodates the shape change. However, the movement of dislocations becomes more difficult at lower temperatures, and as a result, many materials become brittle at low temperatures because dislocations cannot move. This is why the steel hull of the Titanic fractured when it hit an iceberg.

Elements with high melting temperatures and their alloys take this to the extreme, with many remaining brittle up to even 800°C. However, this RMEA bucks the trend, withstanding snapping even at temperatures as low as liquid nitrogen (-196°C).

To understand what was happening inside the remarkable metal, co-investigator Andrew Minor and his team analyzed the stressed samples alongside unbent and uncracked control samples, using four-dimensional scanning transmission electron microscopy (4D-STEM) and scanning transmission electron microscopy (STEM) at the National Center for Electron Microscopy, part of Berkeley Lab's Molecular Foundry.

The electron microscopy data revealed that the alloy's unusual toughness comes from an unexpected side effect of a rare defect called a kink band. Kink bands form in a crystal when an applied force causes strips of the crystal to collapse on themselves and abruptly bend.

The direction in which the crystal bends in these strips increases the force that dislocations feel, causing them to move more easily. On the bulk level, this phenomenon causes the material to soften (meaning that less force has to be applied to the material as it is deformed).

The team knew from past research that kink bands formed easily in RMEAs but assumed that the softening effect would make the material less tough by making it easier for a crack to spread through the lattice. But in reality, this is not the case.

"We show, for the first time, that in the presence of a sharp crack between atoms, kink bands actually resist the propagation of a crack by distributing damage away from it, preventing fracture and leading to extraordinarily high fracture toughness," said Cook.

The $Nb_{45}Ta_{25}Ti_{15}Hf_{15}$ alloy will need to undergo a lot more fundamental research and engineering testing before anything like a jet plane turbine or SpaceX rocket nozzle is made from it, said Ritchie, because mechanical engineers rightfully require a deep understanding of how their materials perform before they use them in the real world. However, this study indicates that the metal has the potential to build the engines of the future.

More information: David H. Cook et al, Kink bands promote exceptional fracture resistance in a NbTaTiHf refractory medium-entropy alloy, *Science* (2024). DOI: 10.1126/science.adn2428

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