New advanced material shows extraordinary stability over wide temperature range

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Researchers from UNSW have found an extraordinary material that does not expand or contract over an extremely wide temperature range and may be one of the most stable materials known.

Using instruments at ANSTO's Australian Synchrotron and Australian Center for Neutron Scattering as well as other techniques, the team led by UNSW A/Prof Neeraj Sharma, an ARC Future Fellow, demonstrated that the zero thermal expansion material made of scandium, aluminum, tungsten and oxygen did not change in volume from 4 to 1400 Kelvin (-269 to 1126 °Celsius).

Their research, published in the *Chemistry of Materials*, confirmed the structural stability of $Sc_{1.5}A_{l0.5}W_{3}O_{12}$ with only minute changes to the bonds, position of oxygen atoms and rotations of the atom arrangements.

Materials with zero expansion are used in high-precision mechanical instruments, control mechanisms, aerospace components and medical implants, for environments in which stability at varying temperatures is critical.

Because of the relatively simple synthesis of the materials and the good availability of alumina and tungsten oxide, large-scale manufacture is a possibility.

"We were conducting experiments with these materials in association with our batteries-based research, for unrelated purposes, and fortuitously came across this singular property of this particular composition," said Sharma.

Comprehensive neutron scattering measurements were conducted at the Australian Center for Neutron Scattering.

"Echidna is fantastic at determining structure, especially on the details of the lighter elements," said Senior Instrument Scientist Dr. Helen Maynard-Casely, who assisted with the measurements on the high-resolution powder diffractometer Echidna.

"Curiously, the experiments suggest these minute atomic displacements and adjustment appear to be undertaken cooperatively," she added.

"Movements and rotations of atoms and radii are quite ordinary, but this correlated behavior was quite unexpected," said Maynard-Casely.

The crystallographic data from the diffraction experiments reflects the combination of subtle but observable distortions of the polyhedral units, bond lengths, angles and oxygen atoms that allow the material to absorb temperature changes.

"Is it the bond lengths that are expanding? Is it the displacement of the oxygen atoms? Or, is the whole polyhedral rotating? We have three factors that are correlating.

"At this point, it is not clear if one or all of these contributing factors are responsible for the stability over a range of temperatures and we are investigating further to try and isolate the mechanism," said Sharma.

The researchers noted, however, that because this specific material composition demonstrated this property, factors other than atomic radii could be at play, such as more complex crystallographic or dynamic behavior.

Investigations of other forms of the material of interest were undertaken on the powder diffraction beamline at the Australian Synchrotron with the assistance of Senior Instrument Scientist, Dr. Helen Brand. Slightly different ratios of the elements did not show the zero thermal expansion.

The group is currently undertaking inelastic neutron scattering measurements at the Center for Accelerator Science on this composition.

More information: Junnan Liu et al, $Sc_{1.5}A_{l0.5}W_3O_{12}$ Exhibits Zero Thermal Expansion between 4 and 1400 K, *Chemistry of Materials* (2021). DOI: 10.1021/acs.chemmater.1c01007

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