Neutrons and X-rays reveal structure of high-temperature liquid metal oxides

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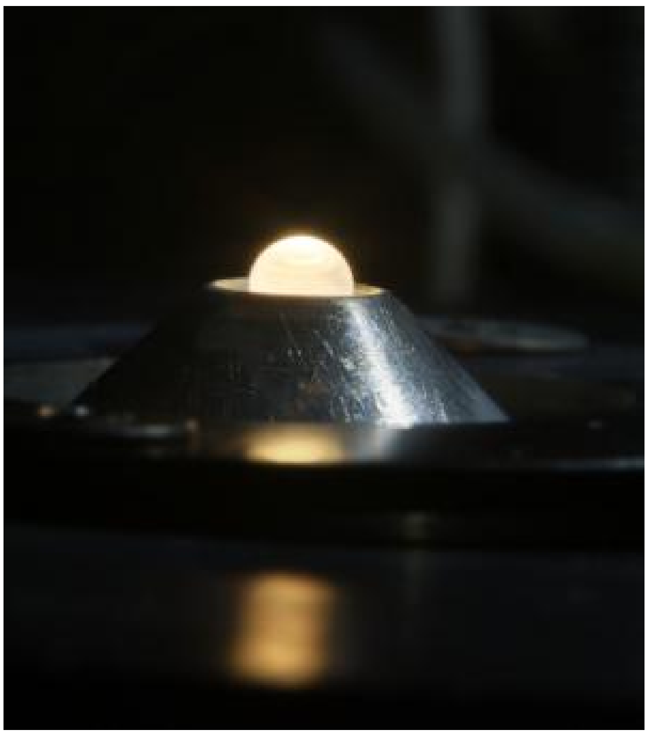

A metal oxide drop levitated in a flow of gas is being heated from above with a laser beam so that researchers can study the behavior of this class of ceramics under high temperatures.

(Phys.org) —By levitating a bead of ceramic oxide, heating it with a 400-watt carbon dioxide laser, then shooting the molten material with X-rays and neutrons, scientists with the Department of Energy's Oak Ridge and Argonne national laboratories have revealed unprecedented detail of the structure of high-temperature liquid oxides.

This class of ceramics is often used to resist high temperatures, but its behavior under extreme temperatures is also critical for understanding the evolution of planetary bodies, nuclear meltdown scenarios, and glass formation.

In a study published in *Physical Review Letters*, researchers from Stony Brook University joined forces with colleagues at Oak Ridge and Argonne scientific user facilities to study the structure and properties of high melting point non-glass forming oxide liquids, such as yttrium and holmium oxides.

The research team observed a general trend towards lower metal and oxygen coordination in a wide range of oxide melts, suggesting that this behavior is a widely occurring phenomenon. The structure of oxide melts determines most of their physical properties, which in turn are directly relevant to planetary research as well as glass making and crystal growth processes including laser garnets and display phosphors.

"In principle, with this knowledge we could make new families of materials by capturing unusual structural motifs present in the melt that don't occur in the crystal," said Chris Benmore, physicist at Argonne's Advanced Photon Source. "We want to find out how to stabilize that structure – maybe by adding components or through vitrifying the melt – and end up with same material, but with different properties."

By combining the analysis of separate X-ray and neutron diffraction experiments, the researchers made the first determination of the complete set of pair distribution functions for a high temperature oxide melt, which gives element-specific information on the probability of finding two atoms with a given separation distance. These separation probabilities provide specific information on local coordination and connectivity, such as between the metal and oxygen atoms, which helps scientists understand physical properties such as density, viscosity, and conductivity.

"Neutrons show us the oxygens in the material clearly, while X-rays reveal the cations [positively charged atoms]," said Benmore. "If you want to extract the detailed structure, you need both techniques."

Joerg Neuefeind, instrument scientist at Oak Ridge's Spallation Neutron Source, said, "There's no way with one experiment to get that information." Neuefeind explained that the experiment required not only collaboration among the two DOE labs, but also a unique sample environment to reach temperatures exceeding 3,000 degrees kelvin, or almost 5,000 degrees Fahrenheit.

For perspective, Neuefeind added, steel melts at approximately 2,600 degrees Fahrenheit, while 6,700 degrees Fahrenheit is the melting point of diamond and 10,300 degrees Fahrenheit is the surface temperature of the sun.

The sample environment where the liquid metal oxide was measured involves a levitation system and a laser. The levitation system is made of a special nozzle designed to produce a gas flow that can trap a small bead of material–about an eighth of an inch in diameter— "floating in air" above the nozzle. The levitation ensures the sample is not in contact with any solid surface that would melt, react with, and contaminate the sample at these temperatures, while a laser is used to heat the sample as it floats on the gas flow. Richard Weber, owner of Materials Development Inc. in Arlington Heights, Illinois, has collaborated with this research team for many years to develop the levitation system and optimize the method.

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