Atoms in advanced alloys find preferred neighbors when solidifying

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The transformation mechanism from molten liquid metal to a high-entropy alloy solid is unclear, as illustrated by the image where a cloud blocks the view of such a transformation process. In a recent study published in Nature Communications, a team of researchers' findings may clarify this process. Credit: Yang Yang/Ying Han

A discovery that uncovered the surprising way atoms arrange themselves and find their preferred neighbors in multi-principal element alloys (MPEA) could enable engineers to "tune" these unique and useful materials for enhanced performance in specific applications ranging from advanced power plants to aerospace technologies, according to the researchers who made the finding.

MPEAs represent a novel approach to alloy design, differing significantly from traditional alloys that typically have one or two principal elements. Instead, MPEAs consist of multiple principal elements in nearly equal atomic ratios.

This design strategy, first reported in 2004, has shown promise in creating a new class of materials with properties desirable for aerospace, automotive or similar industries, such as being very tough at extreme temperatures.

"Previously, alloys like steel were designed with one or two principal elements and trace elements to enhance performance," said Yang Yang, Penn State assistant professor of engineering science and mechanics and of nuclear engineering and co-corresponding author of the study published Aug. 1 in *Nature Communications*. "MPEAs use a different method, where all components are principal elements."

One of the major gaps in understanding MPEAs has been the formation and control of short-range order (SRO), which refers to a non-random arrangement of atoms over short distances—typically only a few atoms wide.

The researchers discovered that SRO is an inherent characteristic in MPEAs, forming during the solidification process when fabricating such materials, which involves the liquid components hardening. Instead of being completely random, like the locations of ingredients in vegetable soup, SRO features atoms clustering in a specific order. This clustering can affect MPEA properties, such as strength or conductivity.

"Such materials are targeted for structural applications where mechanical performance is crucial, like in nuclear reactors or aerospace components," said Yang, who also has an affiliation with the Materials Research Institute.

The researchers' findings challenge the previous notion that, if the cooling rate during solidification is rapid, elements in MPEAs randomly arrange themselves in the crystal lattice. It also challenges the idea that SRO primarily develops during annealing, a process where heating and gradual cooling enhance the material's microstructure to improve properties like strength, hardness and ductility, or the ability to be mechanically stressed without breaking.

The team used advanced additive manufacturing techniques and an improved semi-quantitative electron microscopy method to study SRO in cobalt/chromium/nickel-based MPEAs. Surprisingly, they said, they found that SRO forms during the solidification process, regardless of cooling rates or thermal treatments applied.

"We discovered that even at extremely high cooling rates, up to 100 billion degrees Celsius per second, SRO still forms," said Penghui Cao, assistant professor in mechanical and aerospace engineering and materials science and engineering at the University of California, Irvine and co-corresponding author of the study. "This was contrary to previous beliefs that SRO only developed during annealing."

This was confirmed through detailed computer simulations, which showed that atoms quickly organize themselves as the metal cools and solidifies.

This discovery has profound implications for material science and engineering, according to Yang. Understanding that SRO is inherent and forms during solidification means that traditional methods of thermal processing methods may not effectively control it.

"Our findings suggest that SRO is ubiquitous in MPEAs with a face-centered cubic structure—a type of crystal structure shaped like a cube with six atoms at each face—and cannot be avoided through typical cooling rates achievable in experiments," Yang said. "This realization can help resolve a long-standing debate in the field about the role of SRO in enhancing a material's mechanical strength."

The researchers also discovered that the pervasive nature of SRO enabled them to "tune" MPEAs for particular properties.

"Controlling the degree of SRO in MPEAs can possibly be achieved by mechanical deformation or radiation damage," Cao said. "This provides a new dimension to engineer the material's properties via tuning SRO-controlled mechanisms."

According to Yang, the study marks a significant step forward in the understanding of MPEAs and their inherent properties. By revealing that SRO is an inevitable characteristic formed during solidification, the research opens new possibilities for material design and engineering.

"Understanding how atoms find their neighbors, even at rapid cooling rates, helps us control the structure and enhance the performance of these innovative materials," Yang said. "This is still at the fundamental science stage, and I look forward to seeing how this develops."

More information: Ying Han et al, Ubiquitous short-range order in multi-principal element alloys, *Nature Communications* (2024). DOI: 10.1038/s41467-024-49606-1

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