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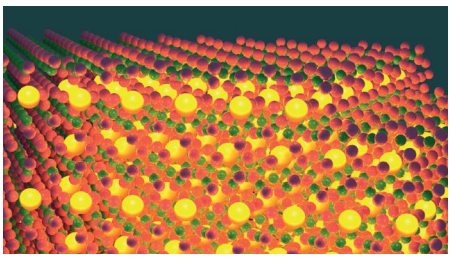
Gaining from mixing

Increasing chemical complexity expands the design space and drives the coupling of materials science and computational techniques.



Alloys are mixtures of metallic and other chemical elements. The addition of a different element, even in a very small amount, may give rise to drastic changes in properties. While alloying has long been pursued, increasing attention is being given to more complex combinations of different elements that increase the variety of microstructural features and hence facilitate the manipulation of properties. This month, we present a joint focus titled 'Complex element coupling' with *Nature Computational Science* that explores the opportunities of designing materials with increasing compositional complexity.

In alloy mixtures, precipitates form when the concentrations of certain elements exceed their solubility limit, impeding the movement of dislocations or defects; this is one of the main strengthening mechanisms of alloys. The precipitate size, density and coherency with the matrix all have an impact on the strengthening, and are determined by the fine-tuned compositions and processing conditions. Mismatched interfaces between the precipitates and the matrix are commonly used to trap defects. In an Article in this issue of *Nature Materials*, Jinlong Du and colleagues report a steel with fully coherent Ni(Al, Fe) superlattice nanoprecipitates to promote defect recombination. Owing to the minimal lattice mismatch with the matrix and a large compositional tolerance, as well as their supersaturated state, these intermetallic nanoprecipitates undergo a rapid and reversible disordering–ordering transition during irradiation, suppressing radiation-induced defects and leading to excellent radiation resistance. This strategy was also demonstrated with an Fe-based medium-entropy alloy containing three principal elements and similar superlattice nanoprecipitates. However, an in-depth understanding of how the chemical effects can be tuned to enhance nanoprecipitate formation and how the transient process restores structural ordering remain to be further explored, as pointed out by Yanwen Zhang in the accompanying News & Views article.

Effective strengthening requires a sufficient volume fraction of nanoprecipitates. Usually, highly soluble and fast-diffusing atoms can form high-density precipitates, but they may not be stable at high operating temperatures. Aluminium can only dissolve a few relatively fast diffusing elements in sufficient quantity, limiting the high-temperature applications of aluminium alloys. In another Article, Hang Xue and colleagues show that in a Sc-added Al–Cu–Mg–Ag alloy, the slow-diffusing Sc elements in the matrix move into the interstitial sites of the high-density Cu-rich nanoprecipitates through the coherent ledges on the interfaces, which increases the heat resistance of the precipitates and enables a high tensile strength at 400 °C and high creep resistance of the alloy. The authors show that the addition of other slow-diffusing elements, such as Zr, Mn or Ce, also produces highly stable nanoprecipitates in a similar way. As emphasized in a News & Views article by Amit Shyam and Sumit Bahl, this ledge-aided in situ transformation mechanism that integrates slow-diffusing and high-solubility solutes is expected to be applicable to other alloy systems such as Ni, Cu, Ti and steel for the design of nanoprecipitates with improved capabilities.

To achieve the designed properties, compositions and structures need to be controlled precisely, and this is particularly important for materials that involve the processing of various types of raw material. But unintentional impurities cannot always be avoided during fabrication. In a Q&A, Zhi-Wei Shan talks about the origin and non-negligible impact of trace impurities in structural metals and alloys, and provides suggestions for controlling their negative effects.

Besides bulk alloys that are of use for their mechanical properties, multi-element materials with reduced dimensions are of use for their rich physical properties in the diverse areas of magnetism, superconductivity, spintronics and excitonics. However, selective synthesis with on-demand composition and structure is challenging because of variable valence states, polymorphs and phases. In another Article, Jiadong Zhou and collaborators report the growth of 67 types of transition metal chalcogenide and transition metal phosphorus chalcogenide including alloys with a defined phase, controllable structure and tunable components, synthesized using a competitive-chemical-reaction-based growth mechanism. As pointed out in the accompanying News & Views article by Weiguang Yang and colleagues, this will spur scientists to create a full library of these material families for exploring novel phenomena, while applications would require further improvement for uniform growth over a large area.

The development of compositionally complex materials would rely heavily on the selection of elements, their concentrations and synthesis conditions. Such design involves high-dimensional phase diagrams as well as non-equilibrium processes, microstructures and properties, posing challenges for classic simulations. In this joint focus, *Nature Computational Science* has collected expert opinions on the progress of computational techniques in this field. The hybrid methods combining physics models and artificial intelligence are discussed in a Perspective by Dierk Raabe and colleagues[1], while computational approaches for quantifying and understanding microstructures and defects in chemically complex materials are highlighted in a Review by Alberto Ferrari and colleagues[2] and a Perspective by Xie Zhang and colleagues[3].

Coupling multiple types of element greatly expands the realm of materials properties, bringing complexity in design, characterization, understanding and processing. Thus, there is a need for computational tools and experiments to complement each other, stimulating interesting directions between disciplines.

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References

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