

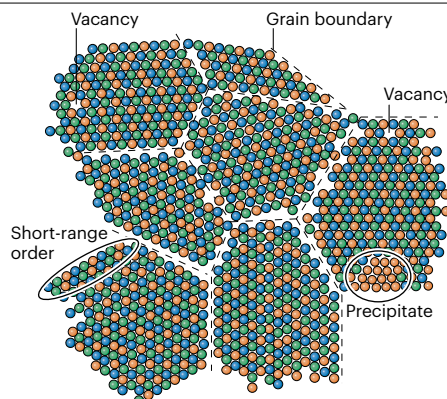
Order or disorder



In multi-principal-element alloys the local chemical order is of increasing research interest for understanding their structures and correlation with properties, requiring systematic exploration with definitive and quantitative characterizations.

Multi-principal-element alloys (MPEAs) with high configurational entropy, known as medium- or high-entropy alloys with three or more principal elements, have been drawing increasing attention due to their design flexibility in terms of composition and properties. They exhibit long-range structural order in the crystalline lattice but are chemically disordered, ideally with each site in the lattice occupied randomly by one of the principal elements. Similar to glasses that are amorphous but can have local structural order, MPEAs can possess local chemical order (LCO). LCO, including chemical short-range order (CSRO) that involves local ordering of elemental species over a few nearest-neighbour spacings, is widely suggested to be prevalent in MPEAs and linked to their mechanical properties^{1,2}; but much debate exists owing to the difficulties in characterizing and quantifying such a subtle and local feature as well as correlating it with materials behaviour³.

In MPEAs, complex interactions among constituent elements could result in various degrees of LCO. Non-imaging methods, such as X-ray-based techniques and neutron scattering, have been used to provide averaged information indicating the presence of CSRO⁴. As an imaging technique, transmission electron microscopy (TEM) is a powerful tool for characterizing atomic arrangements in local regions of a sample, and could be potentially used to reveal the structure of CSRO. Recently, in face-centred cubic (fcc) MPEAs, some features of diffuse intensities observed by TEM in reciprocal-space diffraction patterns with specific zone axes have been attributed to CSRO^{5,6}. However, it has been argued in the community that this alone, if not complemented by other local chemical information, might not be considered incontrovertible evidence of CSRO. In this issue of *Nature Materials*, Flynn



Structural disruption in high-entropy alloys. Figure adapted with permission from ref. 3, Springer Nature Ltd.

Walsh and colleagues discuss in a [Comment](#) the other possibilities that could lead to such superlattice reflections. In particular, they point out that additional expected reflections from CSRO are absent in the diffraction patterns, casting doubt on this interpretation of local chemical ordering. They propose that these diffuse superlattice intensities could alternatively be explained as reflections from symmetry-breaking effects, such as nanoscale stacking disorder in an fcc lattice. However, on the other hand, there are no stacking faults observed in the imaged regions; such imperfections are usually clearly visible by TEM. The authors suggest that the planar defects might be too small to be detected.

Walsh and colleagues do not intend to negate the existence of CSRO or the capability of TEM to characterize it, but suggest that further investigations are required to identify the special structural features in MPEAs and definitively detect CSRO by TEM. For example, the extent of ordering required to produce identifiable superlattice intensities, which might depend on the materials system and TEM specimen thickness, needs to be established.

Different forms of LCO are expected at different MPEA compositions. In an [Article](#) in this issue, Liang Wang and colleagues applied the same TEM technique to body-centred cubic (bcc) MPEAs. In their $\text{Ti}_{50}\text{Zr}_{18}\text{Nb}_{15}\text{V}_{12}\text{Al}_5$ bcc alloy, they observed diffuse reflections by TEM, but at locations indicating B2-like LCO,

a chemical order different from that of the equilibrium intermetallic precipitates at this alloy composition. Also different from the fcc case, bcc alloys are known not to develop stacking faults, eliminating their contribution to diffuse reflections observed here.

Regardless of the exact structures of the local entities, LCO and CSRO have been cited in many reports and widely suggested to have an impact on properties^{1,2}. A definitive characterization of these local features and quantitative correlation with properties may ultimately reveal some of the unknown deformation mechanisms for future materials designs.

The work by Wang and colleagues serves as an example of how to improve the mechanical properties by tuning the interplay of LCO with dislocations in MPEAs. They show that the B2-like LCO and lattice distortion induced by LCO destruction can affect the evolution of planar slip bands and achieve high tensile ductility at gigapascal yield strength. As expected, an increase in LCO enhances strength, but its positive effect on ductility is unexpected considering that LCO confines plastic strains into localized planar slip bands. The explanation offered is that along with the slip-induced destruction of the LCO inside the band, Zr and Al gradually separate such that the lattice distortion increases around each of these two species, eventually leading to strain hardening. This allows for the proliferation of second-generation planar slip bands, involving more slip systems and interband volume into plastic flow.

Despite the long history of research on alloys, there are still many unanswered questions related to their microstructure and mechanical behaviour. For MPEAs, an emerging material in recent years, efforts are still needed to reach a consensus even on the basic understanding of their representative structures. Future work should explore the ways in which these materials behave and can be tailored.

Published online: 31 July 2023

References

- Ding, J. et al. *Proc. Natl Acad. Sci. USA* **115**, 8919–8924 (2018).
- Li, Q. J., Sheng, H. & Ma, E. *Nat. Commun.* **10**, 3563 (2019).
- George, E. P., Raabe, D. & Ritchie, R. O. *Nat. Rev. Mater.* **4**, 515–534 (2019).
- Zhang, F. X. et al. *Phys. Rev. Lett.* **118**, 205501 (2017).
- Zhang, R. et al. *Nature* **581**, 283–287 (2020).
- Chen, X. et al. *Nature* **592**, 712–716 (2021).