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Introduction to structure–property relationships in alloys

Xiaoxiang Wu,^a Seok Su Sohn,^b Zhongji Sun^c and Qingqing Ding^d

Understanding the structure–property relationships in alloys plays a key role in developing high-performance alloys, either by alloy development or advanced fabrication techniques. This themed collection highlights the latest developments on the alloy theory and methods, alloy fabrication and properties–deformation mechanisms of alloys, which contributes a new perspective in alloy design and deformation mechanisms.

First, Chan *et al.* review the critical relationships between process, structure and properties in manufacturing neodymium permanent magnets, using state-of-art laser powder bed fusion (<https://doi.org/10.1039/D4MA00341A>). The review emphasizes how specific variations in LPBF processing can result in microstructures that either enhance or impair magnetic performance, providing valuable insights into the development of more efficient manufacturing strategies.

Feng *et al.* modify the chemistry and heat treatment of HAYNES 282 superalloy and investigate the corresponding effect on creep properties and associated

deformation mechanisms (<https://doi.org/10.1039/D4MA00334A>). The novel results contribute to a new perspective in the optimization of alloy composition and processing of the superalloy.

Based on machine-learning and multi-objective optimization, Yang *et al.* accelerated the design of L₁₂-strengthened single-crystal multi-component alloys (<https://doi.org/10.1039/D4MA00189C>). The tensile properties at high temperatures and creep properties of the designed alloys can be even better than some of the single-crystal superalloys. This alloy strategy can optimize multiple targets simultaneously and provide valuable guidance for the L₁₂-strengthened single-crystal alloys.

Davidson *et al.* delve into the effect of build orientation and heat treatment on the microstructure, mechanical and corrosion performance of super duplex stainless steels processed by laser powder bed fusion (<https://doi.org/10.1039/D4MA00448E>). This study offers a detailed and systematic investigation into the factors controlling the mechanical and corrosion properties of duplex stainless steels.

Ehsan *et al.* present another perspective of metallic alloys as thin film materials used as a catalyst for the hydrogen evolution reaction (<https://doi.org/10.1039/D4MA00410H>). This study presents a straightforward deposition technique to design robust and efficient thin film electrocatalysts and optimize electrochemically active sites to achieve

faster hydrogen evolution reaction rates with low overpotential.

Mnisi *et al.* employ first-principals theory calculations to study the stability and electronic properties of B2 structured X–Ru alloys for high-temperature applications (<https://doi.org/10.1039/D4MA00478G>). The calculations and analysis indicate that Sc–Ru, Ti–Ru, V–Ru, and Mn–Ru alloys are promising materials for high-temperature structural applications.

Zhou *et al.* explore the relationship between crystal orientation and the dwell fatigue cracks of a titanium alloy (<https://doi.org/10.1039/D4MA00230J>). The findings shed light on the quantitative analysis of crack nucleation and the prediction of fatigue performance.

Zhang *et al.* investigate the impact of elemental concentration in ternary CoNiFe medium entropy alloys, on lattice thermal conductivity and thermal expansion (<https://doi.org/10.1039/D4MA00167B>). Medium entropy alloys show great potential in the field of aerospace and nuclear energy. The study contributes to the understanding of the thermal behavior of MEAs and promotes the development of MEAs in the field of thermal science.

The final article by Noronha *et al.* shows promising results to fabricate AlSi10Mg lightweight multifunctional metamaterials using laser powder bed fusion and provides analysis of the failure modes with numerical simulations (<https://doi.org/10.1039/D3MA00813D>).

^a School of Iron and Steel, Soochow University, Suzhou, 215137, PR China.
E-mail: x.wu@suda.edu.cn

^b Department of Materials Science and Engineering Korea University, 02841 Seoul, Republic of Korea

^c Institute of Materials Research and Engineering (IMRE), Agency for Science, Technology and Research (A*STAR), Singapore, Republic of Singapore

^d School of Materials Science and Engineering, Zhejiang University, Hangzhou 310027, China



Conclusion

This themed collection covers a wide range of metallic properties in the field of mechanical properties and functional properties, and highlights novel alloy

design techniques and fabrication methods. We believe that these papers would benefit researchers in both industry and academia. We acknowledge the contributions from our colleagues worldwide to

this themed collection and hope that readers find the collection insightful and enlightening.

