ICSMA19 Metz, France, June 26 - July 1, 2022
International Conference on Strength of Materials

Novel Co-free multi principal element alloys (MPEAs) for nuclear applications: computational design and experimental evaluation

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Structural materials in nuclear environments support heavy mechanical loads associated to corrosive and irradiation damages. Needs for improved alloys are always present. This work presents a computational design approach of precipitation hardened Co-free MPEAs with different reinforcing phases, with a long-term objective of obtaining mechanical and stress corrosion resistance at least equal to the existing Ni-based superalloys (e.g.: 718 grade), along with a superior tolerance to irradiation damage. Predictive models that co-relate composition, structure and properties were developed, using both machine learning and CALPHAD (Thermo-Calc) approach. On this basis, multi-objective optimizations were set up on the Ni-Cr-Fe-Mn-Mo-Nb-W-Al-Ti system. Some alloys were selected from a set of Pareto-optimal compositions for fabrication and process optimization, as well as characterization of both microstructure (SEM, TEM, EDX) and mechanical properties (hardness, tensile test). The new alloys exhibit satisfactory microstructure and mechanical behavior, in good agreement with predictions.

Keywords: alloy design, high entropy alloys, MPEAs, mechanical behavior, nuclear industry