Design of a nickel-base superalloy using a neural network

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Abstract

A new computational tool has been developed to model, discover, and optimize new alloys that simultaneously satisfy up to eleven physical criteria. An artificial neural network is trained from pre-existing materials data that enables the prediction of individual material properties both as a function of composition and heat treatment routine, which allows it to optimize the material properties to search for the material with properties most likely to exceed a target criteria. We design a new polycrystalline nickel-base superalloy with the optimal combination of cost, density, γ' phase content and solvus, phase stability, fatigue life, yield stress, ultimate tensile strength, stress rupture, oxidation resistance, and tensile elongation. Experimental data demonstrates that the proposed alloy fulfills the computational predictions, possessing multiple physical properties, particularly oxidation resistance and yield stress, that exceed existing commercially available alloys.

Keywords: Neural network; materials design; nickel-base superalloy

Despite the central importance of materials in enabling new technologies, historically the only way to develop new materials has been through experiment driven trial and improvement [1]. This means that commercially available alloys are the result of many years of empirical development, and whilst they have good properties, they do not necessarily offer the right balance of properties needed for specific engineering applications. The capability to discover materials computationally has the potential to empower engineers to utilize materials optimized for their application [2]. The development of new algorithms