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Integrated CALPHAD-neural network method for design of low density Ni-base super-alloys

Mehdi Montakhabrazlighi, Mert Bacak and **Ercan Balikci**
Bogaziçi University, Türkiye

The Neural Network (NN) method is applied to alloy development of single crystal Ni-base super-alloys with low density and high rupture resistance. A set of 1200 datasets which include chemical composition of the alloys, applied stress and temperature as inputs and density and time to rupture as outputs is used for training and testing the network. The model capability is then improved by adding gamma-prime phase volume fraction data at desired temperatures which is obtained from modeling by CALPHAD method. The model is first trained by 80% of the data and the rest 20% is used to test it. Comparing the predicted values and the experimental ones showed that a well-trained network is capable of accurately predicting the density and time to rupture strength of the Ni-base super-alloys. Modeling result is used to determine the effect of alloying elements, stress, temperature and gamma-prime phase volume fraction on rupture strength of the Ni-base super-alloys. This approach is in line with the materials genome initiative and integrated computed materials engineering approaches promoted recently.

mehdimon@gmail.com

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