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Alloy Design of Single Crystal Ni-base Superalloys by Combined Method of Neural Network and CALPHAD

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Abstract : The neural network (NN) method is applied to alloy development of single crystal Ni-base Superalloys with low density and improved mechanical strength. A set of 1200 dataset which includes 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. Thermodynamic phase diagram modeling of the screened alloys is performed with Thermocalc software to model the equilibrium phases and also microsegregation in solidification processing. The model is first trained by 80% of the data and the 20% rest 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 superalloys. Modeling results is used to determine the effect of alloying elements, stress, temperature and gamma-prime phase volume fraction on rupture strength of the Ni-base superalloys. This approach is in line with the materials genome initiative and integrated computed materials engineering approaches promoted recently with the aim of reducing the cost and time for development of new alloys for critical aerospace components. This work has been funded by TUBITAK under grant number 112M783.

Keywords : neural network, rupture strength, superalloy, thermocalc
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