Elastic constants of austenitic stainless steel: Investigation by the first-principles calculations and the artificial neural network approach

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Abstract/Résumé : In this paper, two methods were applied to determine the different elastics constants of the face centered cubic austenitic stainless steel Fe0.62Cr0.185Ni0.185. Firstly, the quantum mechanical simulation was applied based on the first principles calculations within the generalized gradient approximation (GGA) by using the efficient strain-stress method. Secondly an artificial neural network (ANN) is used based on back propagation algorithm training. ANN model has been developed for the analysis and simulation of the correlation between the elastic properties and composition. In the training model three input layers each accept the weight percentage of the alloy component (Fe, Cr and Ni), while the three different elastics constants c(11), c(12) and c(44) were employed as outputs. Different models of ANN were developed to predict the elastic constants. The performance indices such as coefficient of determination, mean square error were used to control the performance of the prediction capacity of the models developed in this study. In addition to this, elastic constants obtained from ANN models were compared with those obtained from quantum mechanical simulation and with those reported in the literature. The prediction results obtained by the two methods seem to be satisfactory.

Keywords/Mots cléfs :

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