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# First Principle studies of Effect of Solute Segregation on Grain Boundary Strength in Nickel Based X-750 Alloy

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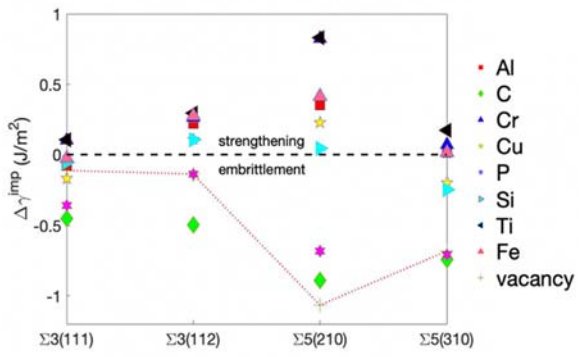
## Abstract

Thermal annealing or radiation induced segregation of solute and impurity elements to grain boundaries (GBs) in metallic alloys changes GB chemistry and thus may alter the GB cohesive strength. In this work, first principles based density functional theory calculations are conducted to study how the segregation of substitutional solute and impurity elements (Al, C, Cr, Cu, P, Si, Ti, Fe) influences the cohesive strength of $\Sigma3(111), \Sigma3(112), \Sigma5(210)$ and $\Sigma5(310)$ GBs in Ni-based X-750 alloys. It is found that C and P show strong embrittlement potencies while Ti and Cr can strengthen GBs. Other solute elements, including Si, have mixed but insignificant effects on GB strength. In terms of GB character effect, these solute and impurity elements affect the GB strength of the $\Sigma5(210)$ GB most and that of the $\Sigma3(111)$ least. Detailed analyses of solute-GB chemical interactions are conducted using electron localization function, charge density map, partial density of states, and Bader charge analysis. The results show that the bond type and charge transfer between solutes and Ni atoms at GBs play important roles on affecting the GB strength.




## Biography

*Ziqi Xiao is a graduate student in Dr.Xian-Ming Bai's group. He graduated from Wuhan University of Technology in China with a bachelor's degree in Materials Science and Engineering in 2015 and got a master's degree from University of Florida also in MSE. Now he is pursuing his Ph.D degree in Virginia Tech. He focusses on the segregation and corrosion behavior in nickel and iron based alloy by using the first principle simulation method*