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Molecular Dynamics Study of Alloying and Impurity Element Segregation Effects on Grain Boundary Cohesive Strength in α-Fe

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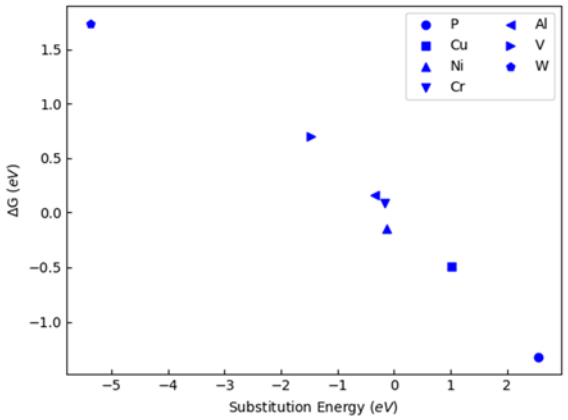
Abstract

Ferritic-Martensitic steels are important structural materials for many engineering applications. Their mechanical properties depend on the chemical composition of grain boundaries (GBs). The segregation of alloying elements or impurities at GBs can reduce or enhance the GB cohesive strength. It is, therefore, important to study the effect of different elements on the GB cohesive strength. In this work, we use molecular dynamics simulations to study the changes of GB cohesive strength due to the substitutional segregation of P, Al, V, W, Cu, Ni and Cr in the Σ5<013> GB. It is found that P, Cu and Ni have a detrimental effect on the GB cohesive strength while Al, Cr, V and W enhanced the GB cohesion. It is also found that the change in GB cohesive strength is correlated to the bulk substitution energy.



The change in grain boundary cohesive strength (ΔG) showed a linear correlation with the substitution energy of the impurity or alloying element in the α-Fe bulk

Biography

Axel Seoane completed his undergraduate studies in Physics at Brigham Young University-Idaho on spring 2017. He began his PhD studies here on fall 2017 and is expected to graduate on spring 2021. He is currently working in Dr. Bai's group on atomistic computational simulations of radiation induced segregation in FM steels.