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Molecular Dynamics Investigation of Nanostructure and Characterization of $Al_xCoCrFeNi$ High-Entropy Alloy

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Extended Abstract

High entropy alloys (HEAs) have gained significant attention for their remarkable mechanical properties [1]. Among these, alloys based on the $Al_xCoCrFeNi$ system are particularly noteworthy. Their high-temperature strength makes them ideal for demanding applications such as aerospace components, engine parts, turbine blades, etc. Understanding the atomic-scale mechanical behavior of these alloys is essential for their widespread engineering utilization.

Previous research suggests that increasing the aluminum content (x) in $Al_xCoCrFeNi$ alloys improves their strength but reduces plasticity, which may compromise ductility in practical applications [2]. Additionally, the solidified microstructure of these alloys transitions from columnar cellular to equiaxed dendritic grains when the aluminum molar ratio varies in the range of $0.9 \leq x \leq 1.5$. Interestingly, Fig. 1 from our study depicts the peak values of yield strength and Young's modulus when (x) is between 0.13 and 0.15, indicating that this composition may offer an optimal balance of mechanical properties. Furthermore, Monte Carlo simulations have been used to explore short-range ordering (SRO) as shown in Fig. 2 by minimizing potential energy, which has been overlooked in previous studies [3] of microstructural behavior.

This study aims to investigate the relationship between aluminum content and mechanical performance under varying deformation conditions using molecular dynamics simulations. By correlating aluminum composition with performance, this research seeks to design $Al_xCoCrFeNi$ HEAs with enhanced mechanical properties for specific high-temperature applications. The findings of this study are expected to provide valuable insights into the compositional and operational factors affecting the mechanical behavior of HEAs and contributing to the development of advanced materials that achieve both high strength and ductility for critical engineering applications.

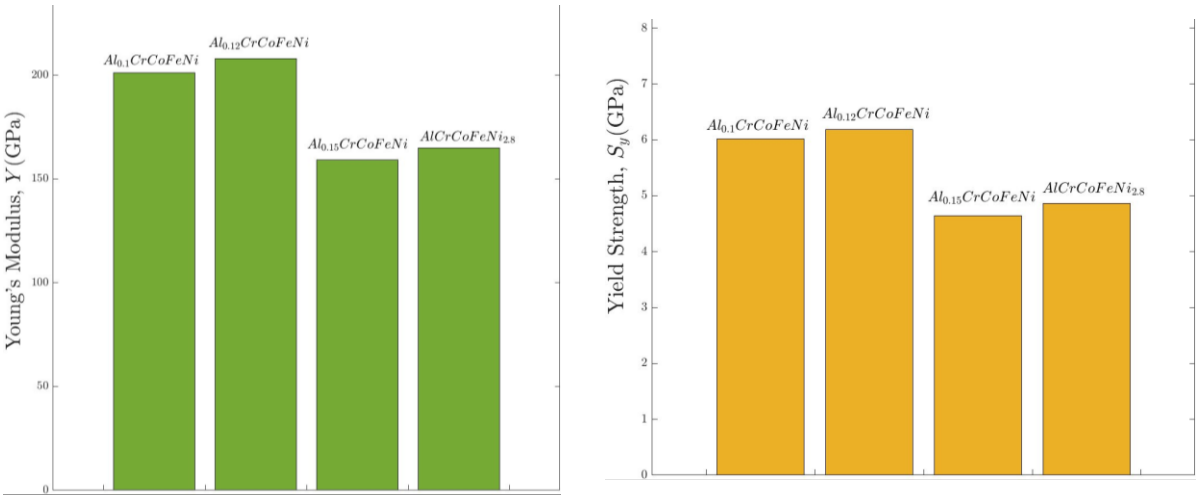
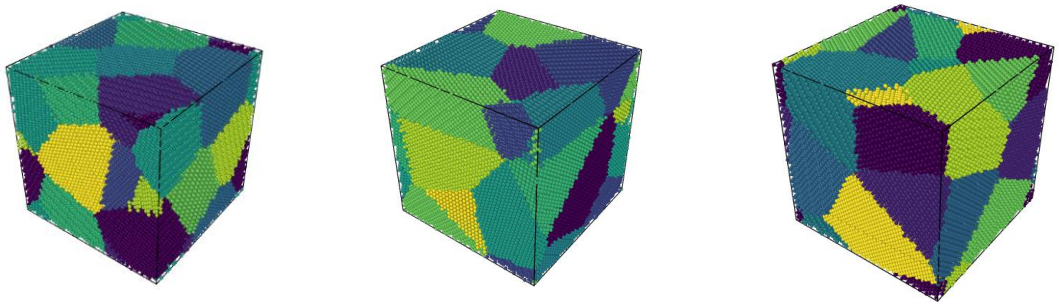


Figure 1: Variation of yield strength and young's modulus with Al concentration in $Al_xCoCrFeNi$ HEA.



(a) $Al_{0.13}CoCrFeNi$ **(b) $Al_{0.14}CoCrFeNi$** **(c) $Al_{0.15}CoCrFeNi$**

Figure 2: Different short range ordered compositions of the $Al_xCoCrFeNi$ HEA.

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