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Structure of the high-entropy alloy $Al_xCrFeCoNi$: fcc versus bcc

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ABSTRACT

The effect of Al on the crystal structures of the high-entropy alloy $Al_xCrFeCoNi$ is discussed using first-principles electronic structure calculations. When the atomic configuration is totally random, $Al_xCrFeCoNi$ has the fcc structure. However, the total energy difference between the fcc and bcc structures decreases as the Al concentration increases. In the calculations Cr and Fe stabilize the bcc structure and Ni and Co work as fcc stabilizer in the alloys, as is observed in experiments. Moreover, the interactions between Al and transition metal elements are strongly attractive. As a result, partially disordered structures such as $L1_2$, $D0_3$ and B2, where the Al atoms are ordered and the transition metal atoms are still random, are more stable than the totally disordered phases. Especially, the energy gain by the $D0_3$ structure is large and this leads to the transition from fcc to bcc for strongly increased Al concentration.

Keywords: Transition metal alloys and compounds; Crystal structure; Electronic properties; Magnetization; Computer simulations