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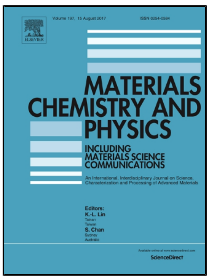

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Mechanical performance of $FeCrCoMnAl_x$ high-entropy alloys from first-principle

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Highlights

- Curie temperature predicted for the presence of ferromagnetism at room temperature.
- Single crystal and polycrystalline elastic moduli used to explore the Al effect.
- Ideal tensile strength of high-entropy alloys calculated from first principle.

Abstract

The elastic parameters and ideal tensile strength in the [001] direction for the body-centered cubic solid solution phase of $FeCrCoMnAl_x$ ($0.6 \leq x \leq 1.5$) high-entropy alloys are determined using first-principle alloy theory. Based on the estimated theoretical Curie temperatures, all alloys considered here are predicted to order ferromagnetically at room temperature. The mechanical behaviors are analyzed through the single crystal and polycrystalline elastic moduli, Pugh ratio, and Debye temperature by making use of a series of phenomenological models. High ideal tensile strength is found for the equi-atomic FeCrCoMnAl system, and the intrinsic strength increases with decreasing Al content.

Keywords: High-entropy alloys; Mechanical performance; First-principle calculations.

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