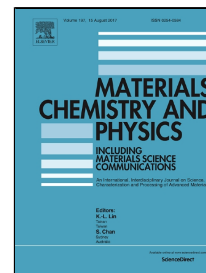


Accepted Manuscript

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

Shuo Huang, Xiaoqing Li, He Huang, Erik Holmstrom, Levente Vitos



PII: S0254-0584(17)30684-3
DOI: 10.1016/j.matchemphys.2017.08.061
Reference: MAC 19959
To appear in: *Materials Chemistry and Physics*
Received Date: 30 March 2017
Revised Date: 15 June 2017
Accepted Date: 21 August 2017

Please cite this article as: Shuo Huang, Xiaoqing Li, He Huang, Erik Holmstrom, Levente Vitos, Mechanical performance of FeCrCoMnAl_x high-entropy alloys from first-principle, *Materials Chemistry and Physics* (2017), doi: 10.1016/j.matchemphys.2017.08.061

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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

Shuo Huang ^{a,*}, Xiaoqing Li ^{a,b,**}, He Huang ^{a,c}, Erik Holmström ^d, Levente Vitos ^{a,b,e}

^a *Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-100 44, Sweden*

^b *Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75120 Uppsala, Sweden*

^c *Science and Technology on Surface Physics and Chemistry Laboratory, Mianyang 621900, PR China*

^d *Sandvik Coromant R&D, 126 80, Stockholm, Sweden*

^e *Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, H-1525 Budapest, P.O. Box 49, Hungary*

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.

* Corresponding author.

** Corresponding author.

E-mail addresses: shuoh@kth.se (S. Huang), xiaoqli@kth.se (X. Li).

Download English Version:

<https://daneshyari.com/en/article/7921857>

Download Persian Version:

<https://daneshyari.com/article/7921857>

[Daneshyari.com](https://daneshyari.com)