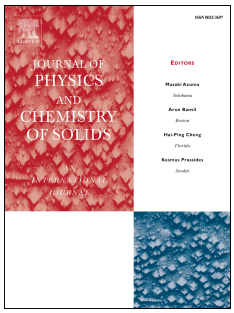
Accepted Manuscript



Stabilization of ferromagnetism and high spin polarization ratio in Cr-doped Fe_2VSi

Xingmiao Guo, Ni Zhaoning, Li Qingshuai, Luo Hongzhi

PII: S0022-3697(18)30023-4

DOI: 10.1016/j.jpcs.2018.03.022

Reference: PCS 8492

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 4 January 2018

Revised Date: 12 March 2018

Accepted Date: 13 March 2018

Please cite this article as: X. Guo, N. Zhaoning, L. Qingshuai, L. Hongzhi, Stabilization of ferromagnetism and high spin polarization ratio in Cr-doped Fe_2VSi, *Journal of Physics and Chemistry of Solids* (2018), doi: 10.1016/j.jpcs.2018.03.022.

Stabilization of ferromagnetism and high spin polarization ratio in Cr-doped Fe_2VSi

Xingmiao Guo[1], Zhaoning Ni[1], Qingshuai Li[1], Hongzhi Luo[1 *]

[1] School of Materials Science and Engineering, Hebei University of Technology, Tianjin 300130, P R China

* Corresponding author. Tel. 86-22-6020-4765; Fax. 86-10-6256-9068;

Email: luo_hongzhi@163.com

Abstract

Effect of Cr doping on the magnetic structure and electronic properties of Fe_2VSi has been investigated by experimental measurement and first-principles calculations. In $Fe_2V_{1-x}Cr_xSi$, ferromagnetism can be stabilized with 10% Cr substitution. The Curie temperature T_C increases rapidly with increasing Cr content and reaches 365K when x = 0.4. The saturation magnetization M_s also increases with increasing Cr content. A small amount of A15 secondary phase is observed with increasing Cr content at x = 0.4, indicating that the solid solubility of Cr in Fe_2VSi has been reached. In $Fe_2V_{1-x}Cr_xSi$, high spin polarization ratio is predicted when $x \geq 0.25$, and half-metallic character is observed when x = 0.5, 0.75 and 1.0. The calculated total spin moment M_t also increases with increasing x. When x is larger than 0.2/0.25, the experimental/theoretical total moment gets close to the Slater-Pauling curve of M = Z - 24 for half-metallic Heusler alloys. All this makes $Fe_2V_{1-x}Cr_xSi$ promising candidates for spintronic applications.

Keywords: A: Magnetic materials; C: ab initio calculations; D: Magnetic properties; Electronic structure.