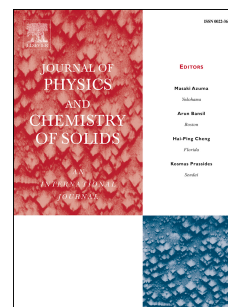


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Stabilization of ferromagnetism and high spin polarization ratio in Cr-doped Fe₂VSi

Xingmiao Guo¹, Zhaoning Ni¹, Qingshuai Li¹, 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 Fe₂VSi has been investigated by experimental measurement and first-principles calculations. In Fe₂V_{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 Fe₂VSi has been reached. In Fe₂V_{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 Fe₂V_{1-x}Cr_xSi promising candidates for spintronic applications.

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

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