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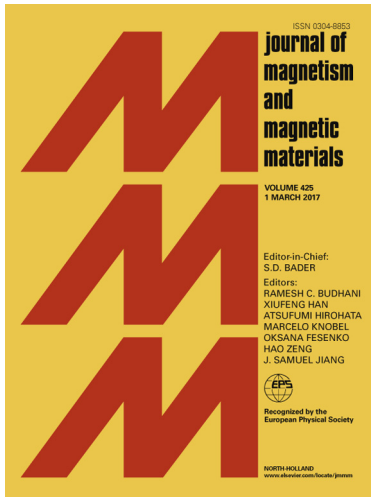

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PII: S0304-8853(17)32153-4
DOI: https://doi.org/10.1016/j.jmmm.2017.12.018
Reference: MAGMA 63487

To appear in: *Journal of Magnetism and Magnetic Materials*

Received Date: 10 July 2017
Revised Date: 30 October 2017
Accepted Date: 4 December 2017

Please cite this article as: V.D. Buchelnikov, M.A. Zagrebin, V.V. Sokolovskiy, Magnetic states of Ni_2MnZ and Ni_2CrZ (Z = Al, As, Bi, Ga, Ge, In, P, Pb, Sb, Si, Sn, Tl) Heusler alloys, *Journal of Magnetism and Magnetic Materials* (2017), doi: https://doi.org/10.1016/j.jmmm.2017.12.018

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Magnetic states of Ni_2MnZ and Ni_2CrZ (Z = Al, As, Bi, Ga, Ge, In, P, Pb, Sb, Si, Sn, Tl) Heusler alloys

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Abstract

In this work we study the magnetic states of ternary Ni_2CrZ (Z = Al, As, Bi, Ga, Ge, In, P, Pb, Sb, Si, Sn, Tl) Heusler alloys in comparison with Ni_2MnZ ones by *ab initio* methods. It is shown that the Ni-Mn based alloys are ferromagnetic. Contrary, the Ni-Cr based alloys with Z = Ga, In, Tl, Si, Ge, Sn, Pb are compensated aniferromagnets and with Z = Al, P, As, Sb, Bi are ferromagnets. The formation energy of alloys studied is calculated and stable compounds are predicted. The possible martensitic transitions in Ni-Mn and Ni-Cr based Heusler alloys are estimated. Within the Heisenberg model and Monte Carlo tecnique, the Curie temperatures are obtained. Theoretical results are compared with other theoretical end experimental results.

Keywords: Heusler alloys, *ab initio* methods, martensitic transformations, magnetic states

1. Introduction

The physical effects such as magnetically and thermally induced shape memory effect (SME), the large magnetoresistance and giant magnetocaloric effect (MCE) are promise properties of magnetic Heusler alloys [1, 2, 3]. Ones of the

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