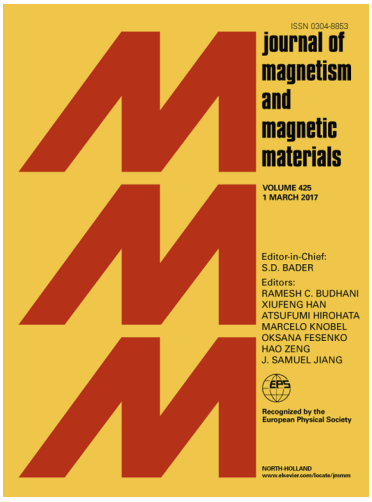

First-principles investigation of the martensitic transition and magnetic properties in Heusler alloys Mg_2YZ (Y=Sc, Ti, V, Z=Al, Ga, In)

C.S. Jiang, Wenyi Peng, Cong Liu, Xiaohua Deng, Jun Yuan, Yuren Wen

PII: S0304-8853(18)31052-7
DOI: https://doi.org/10.1016/j.jmmm.2018.09.051
Reference: MAGMA 64333

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

Received Date: 10 April 2018
Revised Date: 4 September 2018
Accepted Date: 12 September 2018

Please cite this article as: C.S. Jiang, W. Peng, C. Liu, X. Deng, J. Yuan, Y. Wen, First-principles investigation of the martensitic transition and magnetic properties in Heusler alloys Mg_2YZ (Y=Sc, Ti, V, Z=Al, Ga, In), *Journal of Magnetism and Magnetic Materials* (2018), doi: https://doi.org/10.1016/j.jmmm.2018.09.051

First-principles investigation of the martensitic transition and magnetic properties in Heusler alloys Mg_2YZ (Y=Sc, Ti, V, Z=Al, Ga, In)

C.S. Jiang [a, b], Wenyi Peng [a,*], Cong Liu [a], Xiaohua Deng [c], Jun Yuan [a], Yuren Wen [a]

[a] School of materials science and Engineering, Nanchang University, Nanchang 330031, China

[b] School of Science, Jiujiang University, Jiujiang 332005, China

[c] Institute of Space Science and Technology, Nanchang University, Nanchang 330031, China

[*] Corresponding author. E-mail address: wypeng@ncu.edu.cn

Abstract

Crystal structure, magnetism, martensitic transition, electronic structure and mechanical properties of Heusler compounds Mg_2YZ (Y=Sc, Ti, V, Z=Al, Ga, In) were studied by carrying out first-principles calculations based on density functional theory. All compounds in the cubic phase have an inverse Heusler structure with Hg_2CuTi as the prototype. Mg_2ScZ is paramagnetic and does not undergo a martensitic transition, while Mg_2Ti(or V)Z undergoes a martensitic transition and shows ferromagnetism, which is basically unchanged (or smaller) with the phase transition. Y and Z atoms play major and minor roles, respectively, in the electronic structure, which directly affects the magnetism of the two phases. The calculated mechanical properties indicate that Mg_2TiZ is ductile in the cubic phase and brittle in the tetragonal phase, while Mg_2VZ has a similar brittleness in both the cubic and tetragonal phases. It is predicted that Mg_2TiZ and Mg_2VAl (or Ga) are prone to tetragonal distortion, with Mg_2VIn tending towards further phase transition because of mechanical instability.

Keywords:

Heusler compound; martensitic transition; first-principles; magnesium alloy; ferromagnetism

1. Introduction

Heusler compounds have received considerable attention because of their rich physical properties, such as ferromagnetism [1-4], shape memory effect [5-11], half-metal [12-17] and thermoelectric [18-20] properties. Moreover, these properties can be regulated by changing the material components or ratios. At present, more than 1000 types of Heusler compounds have been found, and possible compositions for these materials have been summarized in a previous report [21]. The general formula for a Heusler compound is given as X_2YZ (full Heusler compound) or XYZ (half Heusler compound); such compounds show a high degree of order. The crystal structure of a full Heusler compound consists of four FCC sublattices, which move 1/4 of the distance along the diagonal line of the body [22,23]; the structure shows four equidistant sites, with Wyckoff positions of A(0,0,0), B(1/4,1/4,1/4), C(1/2,1/2,1/2) and D(3/4,3/4,3/4). If the valence electrons of X are higher than the valence electrons of Y, the Heusler compound crystallizes in the cubic space group $Fm\bar{3}m$, with $Cu_2MnAl(L2_1)$ as prototype with an atomic site occupation of X^A-Y^B-X^C-Z^D. Otherwise, the inverse Heusler structure is crystallized, with an atomic site occupation of X^A-X^B-Y^C-Z^D in the cubic space group $F\bar{4}3m$, with Hg_2CuTi(XA) as prototype [24].

In 2016, Ogawa et al. found that Mg-20.5 at% S_C alloy in the space group $IM\bar{3}M$ is a superelastic alloy at 120 K and that Mg-18.3 at% Sc shows an obvious shape memory effect [25]; in 2017, Natarajan et al. investigated the phase stability of binary alloy Mg-Sc using a first-principles method [26]. The atomic site occupation of the BCC Mg-Sc supercell is the same as that for the Heusler compound, which provides evidence for the possibility of investigating Mg-based Heusler compounds with a shape memory effect.

In this paper, the stability, martensitic transition, mechanical properties, magnetism and electronic structures