Journal of Alloys and Compounds 647 (2015) 573–577

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: http://www.elsevier.com/locate/jalcom

Pressure dependence of structural, elastic and electronic of Mg_2Y: A first principles study

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ARTICLE INFO

Article history:
Received 8 September 2013
Accepted 17 May 2015
Available online 19 June 2015

Keywords:
First principles
Mg_2Y
Structural
Elastic
Electronic

ABSTRACT

The first-principles calculations are applied to investigate the structural, elastic constants and electronic of Mg_2Y alloy with increasing pressure in a range of 0–50 GPa. These properties are based on density functional theory (DFT) method within the generalized gradient approximation (GGA) for exchange and correlation. The anisotropy, the shear modulus, and Young's modulus are also studied. It is found that pressure can significantly improve the ductility of Mg_2Y. Moreover, elastic constants, anisotropies of Mg_2Y increase monotonically with the increasing pressure. Furthermore, when external pressure reaches a high level (50 GPa), the structure phase transition of Mg_2Y may be happened. Finally, results of density of state (DOS) reveal the structural stability decreased as compressed.

1. Introduction

Mg and its alloys are potential engineering materials duo to light weight and high specific stiffness [1,2]. While pure Mg and most commercial wrought Magnesium alloys exhibit a low room-temperature ductility the addition of rare earth elements in solid solution causes a significant increase in ductility: Mg–Y alloys show an increase in room-temperature ductility by about 5 times, while maintaining comparable strength and well-balanced work hardening, through the addition of 3 wt.% Y [3–6]. Therefore, investigation on the Mg–Y phases has drawn great academic attention.

In recent decades, a large number of theories and experiments on trinary Mg–Y based alloys such as Mg–Y–Zn(Al, Cd, Mn, Gd, Li, Nd) have been reported. Some investigations focused on the structure and electronic properties of the compounds i.e. $Mg_{97}ZnY_2$, $Mg_3Zn_3Y_2$, $MgAl_4Y$, MgY, $Mg_{24}Y_5$ and $Mg_{24+x}Y_5$ by theoretical and experiment methods [7–10]. However, up to now very little fundamental information (i.e. elastic properties) can be found on the Mg_2Y compound. Its variations of crystal structure, electronic structure and mechanical properties under external condition like pressure have not been studied yet. In order to obtain deeper insight into Mg_2Y compound, density functional theory (DFT)-based methods [11,12] provide a new tool to quantitatively address possible effects of pressures on relevant physical and mechanical properties in this compound.

In this work, we present the first-principles calculations to investigate the properties of Mg_2Y crystal in the pressure range 0–50 GPa with a step of 10 GPa, by using first-principles calculation based on DFT. The change of Lattice parameters, elastic properties and band structure from 0 to high pressure are analyzed. The mechanical properties for Mg_2Y compound at different pressures are also estimated.

2. Method of calculation

In this paper, the calculations are performed with the CASTEP [13,14] code which is based on DFT. In the DFT method, the generalized gradient approximation (GGA) [15] is widely used for the first-principles prediction of the ground-state properties of crystalline solids, and it's known to give many of these properties to high accuracy. Moreover, the exchange correlation potential is described by the Perdew–Burke–Ernzerh (PBE) [15] version of the GGA. The cut-off energy of atomic wave function, E_{cut}, is set at 380 eV. The Monkhorst-Pack grid with $5 \times 5 \times 4$ $k-$ points is used for structure optimization and self-consistent energy computations. The Brodyden–Fletcher–Goldfarb–Shanno (BFGS) [16] minimization scheme is used in geometry optimization. The settings about tolerances of the geometry optimization are as follows: the difference of the total energy 5×10^{-6} eV/atom, and maximum stress within 0.02 GPa.

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http://dx.doi.org/10.1016/j.jallcom.2015.05.132
0925-8388/

3. Results and discussion

3.1. Structural properties and pressure effects

Mg_2Y is a hexagonal close-packed (hcp) structure with space group P63/mmc. Two Mg atoms occupy the 2a site (0,0,0), six Mg atoms occupy the 6h site (0.8409,0.6818,0.25) and four Y atoms occupy the 4f site (0.3333,0.6667,0.626) in a 12 atoms unit cell, respectively. The structure of Mg_2Y is shown in Fig. 1. At the first step, the geometrical structure is optimized by approach of GGA with the PBE function. The results of the optimized lattice constants are shown in Table 1. It's found that the most stable structure of Mg_2Y at P = 0 GPa and T = 0 K corresponds to the ratio c/a of 1.62, and the calculated results are in good agreement with the previously experimental data (Table 2).

Fig. 2 shows the pressure dependence of the normalized lattice parameters a/a_0, c/c_0 and primitive cell volume V/V_0 in the range of from 0 to 50 GPa (where a_0, c_0 and V_0 are the zero pressure equilibrium structural parameters). As pressure increasing, the equilibrium ratio a/a_0 decreases more quickly than c/c_0, indicating that the compression along the a-axis is much larger than that along the c-axis. This result is in agreement with the comparatively stronger (Mg–Y) bonds which determine the c-axis length. Unfortunately, there are no experimental data compared with our data (Fig. 3).

3.2. Elastic properties of the Mg_2Y

Elastic properties determine the stiffness of a crystal against the external strain, so they are important for understanding the structure stability and the strength of materials such as bulk modulus (B), shear model (G), Young's modulus (E) and Poisson's ratio (σ).

According to the mechanical stability criteria of the elastic constants in hcp structure [18] as $C_{12} > 0$, $C_{33} > 0$, $C_{66} = (C_{11} - C_{12})/2 > 0$, $C_{44} > 0$, $(C_{11}+C_{12})(C_{11}+C_{12})\,C_{33} - 2C_{13}^2 > 0$, it is obvious that the structure of this material is not stable when P = 50 GPa ($C_{66} = -12.081 < 0$). It suggests that its structure phase transition of Mg_2Y may be happened. We try to cut down to 45 GPa, and found that $C_{66} = 0.258$, near the critical point.

The mechanical anisotropy of Mg_2Y can be calculated by using the bulk module B_a along the a-axis and B_c along the c-axis, which are defined as [19,20]:

$$B_a = \alpha \frac{dP}{d\alpha} = \frac{\Lambda}{2+\alpha} \tag{1}$$

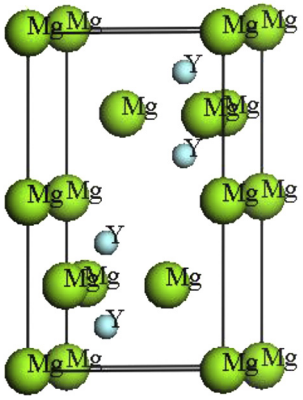

Fig. 1. The crystal structure if the Mg_2Y compound.

Table 1
The optimized parameters at 0 GPa, 0 K.

Structure	Experimental study [17]	This work
a_0(Å)	6.037	6.080
c_0(Å)	9.752	9.858
v_0(Å^3)	307.799	315.638

Table 2
The elastic constant C_{66} at various pressure.

P (GPa)	10	20	30
C_{66}	31.063	31.991	27.797
P (GPa)	40	45	50
C_{66}	17.747	0.258	−12.081

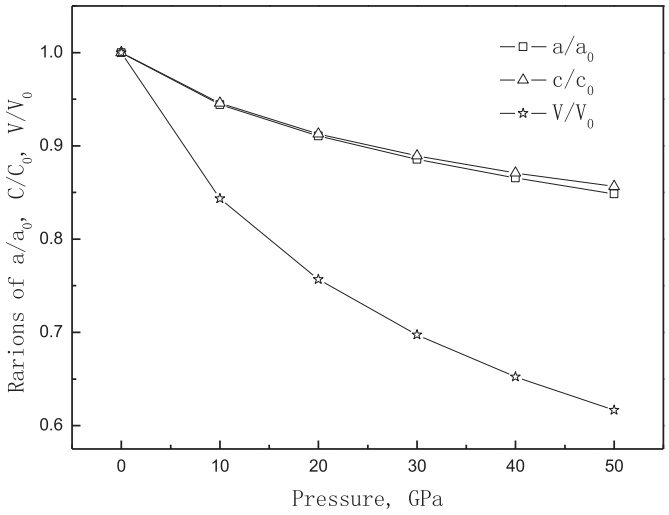

Fig. 2. The lattice parameters a/a_0, c/c_0 and primitive cell volume V/V_0 as a function of pressure of Mg_2Y at 0 K.

$$B_c = c\frac{dP}{dc} = \frac{B_a}{\alpha} \tag{2}$$

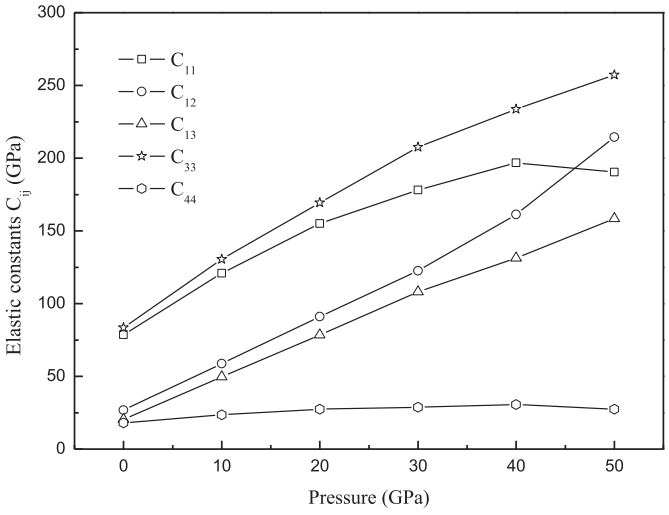

Fig. 3. The calculated elastic constants C_{ij} as a function of pressure.