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Ab initio study of the structural, elastic, thermodynamic, electronic and vibration properties of TbMg intermetallic compound

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ABSTRACT

The structural, elastic, thermodynamic, electronic and vibrational properties of CsCl-type TbMg have been studied by performing ab initio calculations based on density functional theory using the Vienna Ab initio Simulation Package (VASP). The exchange correlation potential within the generalized-gradient approximation (GGA) of projector augmented wave (PAW) method is used. The calculated structural parameters, such as the lattice constant, bulk modulus, its pressure derivative, formation energy and second-order elastic constants are presented in this paper. The obtained results are compared with related experimental and theoretical studies. The electronic band calculations, total density of states (DOS), partial DOS and charge density are also presented. Formation enthalpy and Cauchy pressure are determined. In order to obtain more information the elastic properties such as Zener anisotropy factor, Poisson's ratio, Young modulus, isotropic shear modulus, Debye temperature and melting point have been carried out. The elastic constants are calculated in zero and different pressure ranges (0–50 GPa) with bulk modulus. We have performed the thermodynamic properties of TbMg by using quasi-harmonic Debye model. The temperature and pressure variation of the volume, bulk modulus, and thermal expansion coefficient have been predicted over a pressure range of 0–25 GPa for of TbMg. Pressure dependence of the anisotropy factors, Young's modulus, Poisson's ratios, bulk modulus and axis compressibility of TbMg are

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presented along different directions and planes. Finally, the phonon dispersion curves are presented for TbMg.

1. Introduction

Magnesium and magnesium alloys have been attracted considerable attention due to their unique physical properties, particularly, the low density, high specific strength, Young's modulus and good stiffness. Magnesium alloys are of prominence technological importance, especially in the automobile industry and aircraft industry. Magnesium (periodic group IIA) being a normal metal has a larger metallic radius than others and bears no d electrons. Hence, a different magnetic behavior has been expected for REMg and MgRE (RE: Rare Earth) compounds. There are many studies about magnetic properties of these types of compounds. The magnetic properties of the CsCl-type compound TbMg have been studied by means of neutron diffraction and magnetization measurements by Schafer et al. [1]. Aleonard et al. [2] have investigated the magnetic properties of GdMg and TbMg, as well as the magnetic structure of TbMg by neutron diffraction. Aleonard et al. [3] have studied the magnetic properties of RMg compounds by magnetization measurements on single crystals (R = Tb, Dy, Ho, Er, Tm) and neutron diffraction and seen that magnetic structures are antiferromagnetic with Ce, Pr, Nd, but result from a competition between ferromagnetisim and antiferromagnetism with heavy rare earths. The magnetic properties of rare earth–magnesium compounds with the CsCl structure have been determined in the temperature range 4.2–300 K by Buschow et al. [4]. Magnetic properties of intermetallic compounds of rare earth metals are given in handbook by Kirchmayr et al. [5]. Intermetallic compounds of rare earths and non-magnetic metals have been investigated by Buschow et al. [6]. Aleonard et al. [7] have presented magnetization measurements on single crystals of RMg compounds (R = Tb, Dy, Ho, Er) and have explained the magnetization anisotropy in terms of crystal field (CEF) effects in their work. TbMg appeared to us a very suitable system for testing the X-ray multipolar scattering technique applied to the determination of a magnetic structure. The brittle and elastic properties of the B2-MgRE (RE = Sc, Y, Ce, Pr, Nd, Gd, Tb, Dy, Ho, Er) intermetallics have been investigated using first-principles density functional calculations by Wu and Hu [8]. Villars et al. [9] have presented intermetallic phases in their handbook of crystallographic data. The elastic properties of B2-MgRE (RE = Sc, Y, La–Lu) intermetallic compounds have been calculated at $T = 0$ K by using first principles within the generalized gradient approximation (GGA) and The characteristic of elastic constants of B2-MgRE are explained by the insight of electronic structures under deformation by Tao et al. [10]. Wang et al. [11] present the third-order elastic constants for the magnesium-rare-earth alloys MgY, MgTb, MgDy, and MgNd with CsCl-type B2 structure. The generalized-stacking-fault energy (GSFE) surfaces for MgRE (RE = Y, Tb, Dy, Nd) intermetallics with B2-type structures have been presented using ab initio calculations by Wu et al. [12]. Wang et al. [13] have performed an ab initio study of the thermodynamic properties of rare-earth–magnesium intermetallic compounds MgRE (RE = Y, Dy, Pr, Tb) with B2-type structures. The temperature-dependent elastic modulus of MgRE (RE = Y, Dy, Pr, Sc, Tb) intermetallics with B2-type structure are presented from first-principles quasistatic approach, in which the static volume-dependent elastic constants are obtained by the first-principles total-energy method within density functional theory and the thermal expansion is obtained from the quasiharmonic approach based on density-functional perturbation theory by Wang et al. [14]. Luca et al. [15] have presented that earlier neutron powder diffraction experiments showed the existence at low temperature of a canted magnetic structure, with antiferromagnetic wavevectors and several models were found to be consistent with experiments and the actual structure remained undetermined. Moreover, the compounds in the rare-earth magnesium series show an unusual, among rare-earth intermetallics, reluctance to oxidize [15]. This reduces the contribution of the oxidized surface to the scattering phenomena and favors the observation of weak multipolar reflections [15]. Thus, Luca et al. [15] have recalled firstly, the magnetic properties of TbMg and the models of magnetic structures consistent with the neutron powder diffraction experiment and