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Full length article

# Theoretical study of elastic, mechanical and thermodynamic properties of MgRh intermetallic compound

S. Boucetta*

*Université SETIF 1, Laboratoire d'Elaboration de Nouveaux Matériaux et Caractérisations (ENMC), Département de Physique, 19000 Sétif, Algeria*

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**Abstract**

In the last years, Magnesium alloys are known to be of great technological importance and high scientific interest. In this work, density functional theory plane-wave pseudo potential method, with local density approximation (LDA) and generalized gradient approximation (GGA) are used to perform first-principles quantum mechanics calculations in order to investigate the structural, elastic and mechanical properties of the intermetallic compound MgRh with a CsCl-type structure. Comparison of the calculated equilibrium lattice constant and experimental data shows good agreement. The elastic constants were determined from a linear fit of the calculated stress−strain function according to Hooke's law. From the elastic constants, the bulk modulus $B$, shear modulus $G$, Young's modulus $E$, Poisson's ratio $\sigma$, anisotropy factor $A$ and the ratio $B/G$ for MgRh compound are obtained. The sound velocities and Debye temperature are also predicted from elastic constants. Finally, the linear response method has been used to calculate the thermodynamic properties. The temperature dependence of the enthalpy $H$, free energy $F$, entropy $S$, and heat capacity at constant volume $C_v$ of MgRh crystal in a quasi-harmonic approximation have been obtained from phonon density of states and discussed for the first report. This is the first quantitative theoretical prediction of these properties.
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*Keywords:* Intermetallics; Elastic properties; Mechanical properties; Thermodynamic properties; Computer simulations

## 1. Introduction

Magnesium (Mg), with its abundance in the Earth is becoming an important engineering material. The last years, significant progress was made on the science, technology and application of magnesium and its alloys. Research on Mg based alloys is of particular interest due to its low density (~1.74 g/cm$^3$) and high specific strength and stiffness than many other engineering materials, including aluminum, steel and polymer-based composites. Magnesium also possess many other attractive properties, such as a high damping capacity, electromagnetic shielding, thermal conductivity, good machinability and high recycling potential [1]. Magnesium alloys are among the lightest structural materials known and are used in a variety of applications, particularly in automobile industry and aerospace manufacturing [2]. The above-mentioned features motivated us to study these alloys.

Magnesium forms a wide range of ordered intermetallic compounds with the 4d transition metals (TM), for example the compound MgRh was prepared by heating the elements in stoichiometric proportion and the reaction was carried out in fused quartz tube at 1000 °C. The crystal structure of MgRh compound was determined by X-ray powder diffraction, and it crystallizes in B2 type structure [3]. To the best of our knowledge, the intermetallic compound MgRh has not been

* Tel.: +213 36 87 35 51.
*E-mail addresses:* boucetta_said02@yahoo.fr, sd.boucetta@gmail.com.
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studied neither experimentally nor theoretically. Thus, in this work we have carried out a theoretical investigation on the structural, elastic, mechanical and thermodynamic properties of MgRh alloy, in order to provide a sounder basis for further experimental and theoretical studies. Ab initio methods offer one of the most powerful tools carrying out theoretical investigation of an important number of physical and chemical properties of materials with a great accuracy. The rest of this paper is organized as follows: the computational method is described in Section 2, the numerical results and discussions are given in Section 3, and finally a conclusion is presented in Section 4.

## 2. Computational method

Our first-principles quantum mechanics calculations are performed with the plane-wave pseudo-potential (PW-PP) total energy method implemented with the CASTEP (Cambridge Serial Total Energy Package) simulation program [4]. This is based on the density functional theory (DFT) [5,6] which is, in principle, an exact theory of the ground state. We have used two approximations. First, the local density approximation (LDA) developed by Ceperley and Adler and parameterized by Perdew and Zunger [7,8], as well as the generalized gradient approximation (GGA), with the new functional of Perdew–Burke–Ernzerhof (PBE), known as PBEsol [9], are made for electronic exchange-correlation potential energy. Second, Coulomb potential energy caused by electron–ion interaction is described using the Vanderbilt-type ultrasoft scheme [10], in which the orbitals of Mg ($2p^6 3s^2$), Rh ($4d^8 5s^1$), are treated as valence electrons. The cut-off energy for the plane-wave expansion was chosen at 340 eV and the Brillouin zone sampling was carried out using the $8 \times 8 \times 8$ set of Monkhorst–Pack mesh [11].

The structural parameter ($a$) of MgRh was determined using the Broyden–Fletcher–Goldfarb–Shenno (BFGS) minimization technique [12]. This method usually provides the fast way of finding the lowest energy structure.

In the structural optimization process, the energy change, maximum force, maximum stress and maximum displacement are set as $1.0 \times 10^{-5}$ eV/atom, 0.03 eV/Å, 0.05 GPa, and 0.001 Å, respectively.

The elastic constants were determined from first-principles calculations by applying a given homogeneous strain (deformation) with a finite value and calculating the resulting stress according to Hook's law [13]. The total energy is converged to $2.0 \times 10^{-6}$ eV/atom in the self-consistent calculation.

The thermodynamic properties of a crystal in a quasi-harmonic approximation have been predicted using phonon calculations with the linear response method.

## 3. Results and discussion

### 3.1. Structural properties

The atomic structure of MgRh intermetallic compound is known to crystallize in a cubic lattice of CsCl-type structure (B2) with the space group Pm-3m (221) and the equilibrium lattice parameter has a value of (3.099 ± 0.002) Å [3]. The unit cell structural model of the MgRh compound is built according to the experimental data [3], as shown in Fig. 1. The crystal structure was optimized at first. The obtained results of calculated lattice parameter $a$ of MgRh intermetallic compound using the (PW-PP) method within both the LDA and the GGA-PBEsol approximations are 3.053 Å and 3.101 Å respectively. One can see from the present results that the calculated lattice constant $a$ is 1.4% smaller than the experimental value using LDA and it is only 0.06% higher than the experimental value using GGA-PBEsol. Our calculated equilibrium lattice parameter agrees very well with the experimental data, above all in GGA approximation.

### 3.2. Elastic and mechanical properties

Elastic constants are very important material parameters. Evident and direct application of elastic constants is in the evaluation of elastic strains or energies in materials under stresses of various origins: external, internal and thermal [14]. The elastic constants can also provide information on the stability, stiffness, brittleness, ductility, and anisotropy of a material and propagation of elastic waves and normal mode oscillations. Moreover, knowledge of the values of elastic constants is crucial for a sound understanding of the mechanical properties of the relevant material.

The elasticity of a cubic crystal is specified by the three independent elastic constants $C_{11}$, $C_{12}$ and $C_{44}$. In this work, the calculated elastic constants of MgRh compound at zero pressure and temperature are presented in Table 1. For a cubic crystal, the obtained elastic constants meet the requirements of mechanical stability criteria: $C_{11} > 0$, $C_{44} > 0$, $C_{11} - C_{12} > 0$, $C_{11} + 2C_{12} > 0$ and $C_{11} > B > C_{12}$. From Table 1, one can see that the elastic constants of MgRh compound satisfy all of these conditions, suggesting that the structure of MgRh is mechanically stable. The elastic constants values calculated using the LDA approximation are slightly higher than those obtained with the GGA-PBEsol approximation. To the best of our knowledge, there are no experimental and other theoretical data in literature for the elastic constants ($C_{ij}$) of MgRh for comparison, so we consider the present results as prediction study which still awaits an experimental confirmation. The

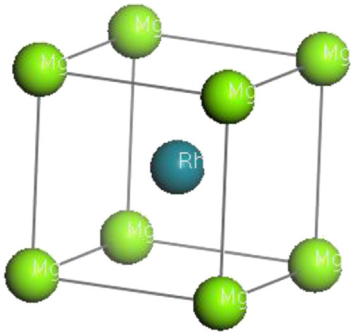


Fig. 1. Crystal structure of MgRh.

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