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First principles study of structural, electronic and magnetic properties of magnesium

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Abstract. We investigated the structural, electronic, and magnetic properties of Mg, in the CS (simple cubic), NiAs (Nickel arsenide), FCC (rock-salt), R (Rhombohedral), Diamond and WZ (wurtzite) phases. Calculations were performed using the first-principles pseudo-potential method within the framework of spin-density functional theory (DFT).

1. Introduction

Previous studies with Mg in the hcp phase show that it is a fragile metal at room temperature with a strong surface irregularity which to date has not been surpassed [1-5]. However, in the NaCl and CsCl phases it has been mixed with Li at room temperature, obtaining an alloy that can change from ductile to brittle, depending upon the amount of Li in the mixture [5]. Today, the industry is interested in this alloy, Mg-Li, due to its low density and dent resistance for the construction of automobile parts [6]. Several theoretical and experimental papers have shown that Mg is stable in the CsCl and NaCl phases, both in bulk and in the form of thin films. Mg in the CsCl phase is stable at pressures $P \sim 50$ GPa, but it is unstable at room temperature. The stability of the alloy Mg-Nb in the CsCl phase at room temperature allows forming multilayer films of Mg-Nb. Mg is combined with other materials to form ions of Mg and achieve the construction of rechargeable and non-rechargeable batteries, in order to replace Li batteries with Mg ones, since Mg is 10^4 times more abundant in the earth's crust than Li [7].

2. Method

Calculations were performed using the first-principles pseudo-potential method in the framework of spin density-functional theory (DFT) by means of Quantum Espresso Code [8]. Exchange and correlation effects were dealt with using the generalized gradient approximation (GGA) implemented in the Perdew–Burke–Ernzerhof functional (PBE) [9]. Ultrasoft pseudo-potentials were employed [10]. The wave function was expanded in plane waves up to a cutoff of 40Ry. A gamma-centered Monkhorst–Pack [10] k-point grid of $10 \times 10 \times 10$ was used in the First Brillouin zone. The convergence for the energy was 0.0001Ry. For determining the properties of Mg in this configuration, a supercell model was implemented. For example, in WZ a $1 \times 1 \times 2$ supercell was used, and a $\sqrt{2} \times \sqrt{2} \times 2$ supercells was used in the simple cubic phase.

3. Structural properties

Figure 1 show the energy of the compound versus volume (E vs. V) by unit formula of Mg. It can be seen that each curve has minimum energy, which indicates that the phase is metastable. The energies



and volumes are given by unit formula.

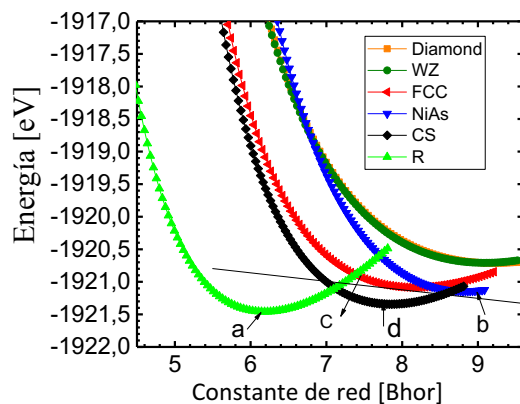


Figure 1. Energy vs. volume for the Mg compound in six structures.

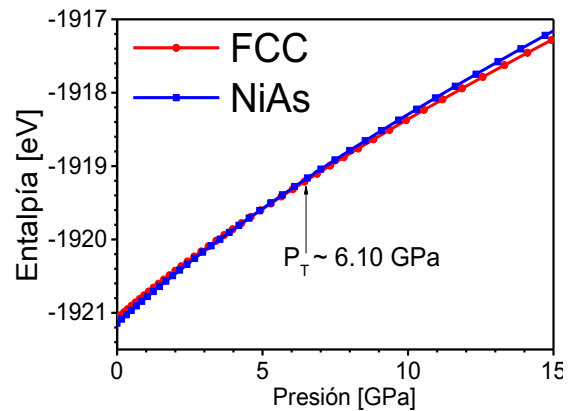


Figure 2. Enthalpy vs. pressure for the Mg compound in two structures.

These graphics (Figure 1 and 2) are fit to the Murnaghan equation of state [11] for each phase. In this way, the equilibrium lattice constant, the bulk modulus, and other structural parameters can be obtained (see Table 1).

Figure 1 shows the cohesion energy as a function of the Mg for the R, CS, NiAs, FCC, Diamond, and WZ structures. In this superimposition it can be seen that the ground state crystallization is R (Rhomboidal) in a hexagonal cell, since it is the lowest energy with respect to the other phases (Table 1), but there is also a local minimum in the CS structure with energy of ~ 0.12 eV/unit formula. In this Figure 1, four points, labeled a, b, c, and d, correspond to: a) R phase in conditions of minimum energy $P=0$. b) NiAs phase before a phase transition FCC, $P < P_T$. c) FCC phase after the phase transition from NiAs, $P > P_T$. d) CS phase in conditions of minimum energy $P=0$.

Figure 2 depicts enthalpy versus pressure and shows an intersection between the phases NiAs and FCC at $P_T \sim 6.10$ GPa. We found that there is no transition of the R phase nor of the other five phases, but possible transitions from the NiAs phase to the WZ and diamond phases were found.

Table 1 The structural parameters of Mg in the R, CS, NiAs, FCC, Diamond and WZ-like structure. Cohesive energies and volumes are given per unit cell (containing eight atoms). The parameter a_o (Bhor) in the cubic structure is taken as a (Bohr) $= a_o(\text{Bohr})/\sqrt{2}$ where a (Bohr) is the lattice constant.

Structural Parameter	R	CS	NiAs	FCC	Diamond	WZ
	Our results	Our results	Our results	Our results	Our results	Our results
a_{\min} [Bohr]	6.18	7.85	8.83	8.15	9.23	9.09
Volume [Bhor ³]	258.87	342.51	374.91	191.43	277.78	266.53
c/a	5.05	2.8284	2.51	2.8282	2.8284	3.28
B [GPa]	19.00	15.91	16.73	22.08	13.06	15.96
B'	2.95	2.98	2.68	2.99	2.67	2.53
E cohesion [eV]	-1921.46	-1921.34	-1921.14	-1921.08	-1920.71	-1920.71

Table 1 reports the structural parameters obtained. These parameters are determined by fitting the curves of E vs. V to Murnaghan's state equation [11]. In the tables, c/a is the relationship between lattice parameters, V is the volume of the unitary cell, B is the bulk modulus, and E_0 is the cohesion energy.

4. Electronic properties

The electronic properties of Mg in this configuration were studied for the R and CS phases. Figures 3 and 4 show the total and partial density of states for each of these phases at zero pressure, respectively. The first thing we observe is that the Mg is composed of orbitals $3s$ and $2p$. The presence of states near the Fermi level indicates that this material behaves as a metal. In the calculations, the polarization of the spin was taken into account, but it was not necessary to include how the density of up-spin states was equal to that of the down-spin states. Therefore, we can also say that the material is not magnetic in any of these phases.

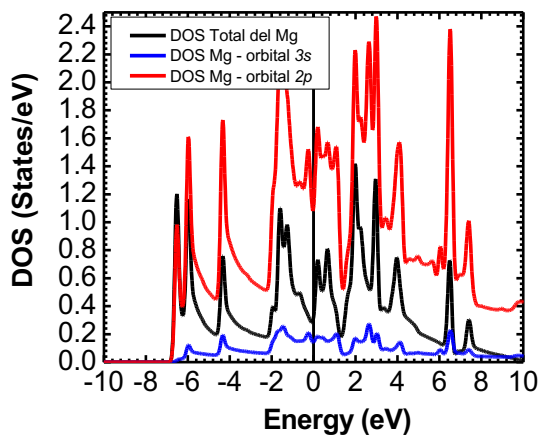


Figure 3. Partial and total DOS of Mg in the R phase in conditions of minimum energy $P=0$.

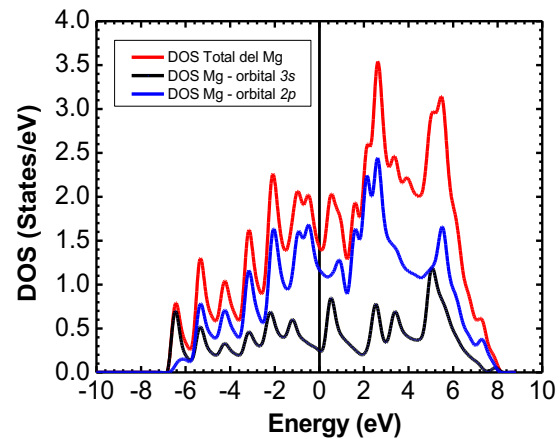


Figure 4. Partial and total DOS of Mg in the CS phase in conditions of minimum energy $P=0$.

5. Phase transition

We studied the electronic properties Mg in dots immediately before and after the transition point. Figure 5 shows the partial and total DOS in the NiAs phase before a phase transition FCC, $P < P_T$, and as in the two previous figures a metallic behavior is observed. Figure 6 shows the partial and total DOS of Mg in the FCC phase after the phase transition NiAs, $P > P_T$, showing a metallic behaviour. For both, electronic contributions are due to hybridization of orbitals s and p of the Mg.

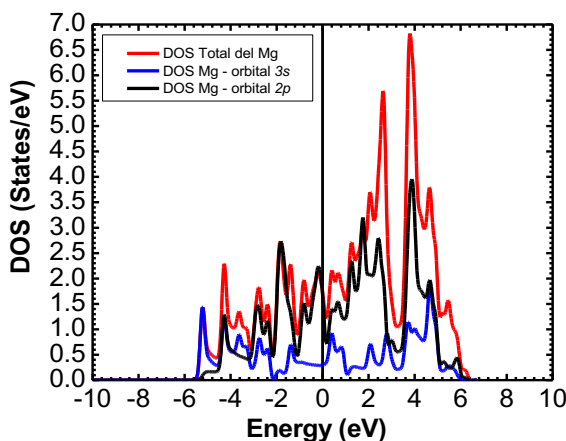


Figure 5. Partial and total DOS of Mg in the NiAs phase before a phase transition FCC, $P < P_T$.

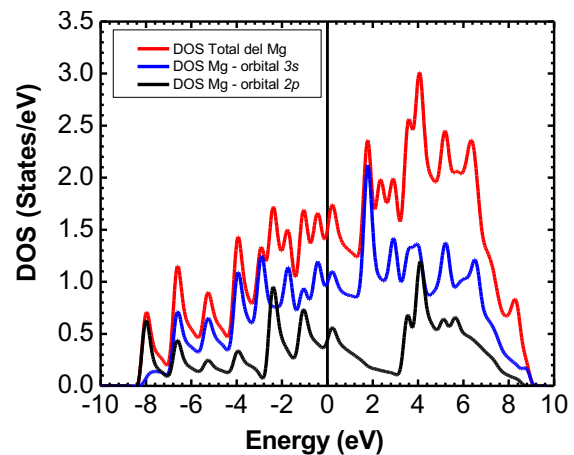


Figure 6. Partial and total DOS of Mg in the FCC phase after the phase transition NiAs, $P > P_T$.

6. Conclusions

We calculated the structural, electronic and magnetic properties of Mg, carried out by means of DFT using the Wu-Cohen GGA approximation. Our calculations predict that in a hexagonal $1 \times 1 \times 2$ supercell and $\sqrt{2} \times \sqrt{2} \times 2$ supercell in the simple cubic phase, Mg crystallizes in the R (Rhombohedral) phase in a hexagonal supercell. The volume module in the six phases is not greater than ~ 22.08 GPa, indicating that the metal is not very rigid compared with Si in the diamond structure. Furthermore, for a transition pressure of ~ 6.10 GPa, Mg changes from NiAs to FCC. Finally, Mg in this configuration behaves as a metallic, nonmagnetic material.

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