Le 3ème Séminaire International sur les Energies Nouvelles et Renouvelables
The 3nd International Seminar on New and Renewable Energies

Unité de Recherche Appliquée en Energies Renouvelables,
Ghardaïa – Algérie 13 et 14 Octobre 2014

Theoretical studies of elastic properties of cubic FeTi and orthorhombic FeTiH

K. Benyelloul[1], H. Aourag[2], HI. Faraoun[2], Y.Bouhadda[1]

[1]*Unité de Recherche Appliquée en Energies Renouvelables, URAER, Centre de Développement des Energies*

Renouvelables, CDER, 47133, Ghardaïa, Algeria

[2] *Department of physics, University of Tlemcen 13000 Algeria*
[1]benyelloul_kamel@yahoo.fr

[1]H.Aourag@dgrsdt.dz

[3]Bouhadda@yahh.com

[*]Second Company
Address Including Country Name

Abstract— In this paper, a first-principles calculations based on the density functional theory (DFT) within the generalized gradient approximation (GGA) was used. The single crystal elastic constants for the intermetallics FeTi and FeTiH, are successfully obtained from the stress-strain relationship calculations and the strain energy-strain curves calculations, respectively. The shear modulus, Young's modulus, Poisson's ratio and shear anisotropic factors are also calculated. The bulk modulus derived from the elastic constants calculations of cubic FeTi, orthorhombic P2221 FeTiH are calculated. For cubic FeTi compounds bulk modulus is a good agreement with theoretical results and experimental data available. It is found that, the insertion of hydrogen into the structure FeTi causes an increasing bulk modulus. From analysis of the ratio of shear to bulk modulus, it is found that FeTi and its hydrides compounds are ductile. This ductibility, change with change the concentration of hydrogen.

Keywords— Hydrogen storage, Elastic constants, First-principles calculations

I. INTRODUCTION

Hydrogen is a handy energy carrier and can be used in a variety of ways. In future, it could potentially replace petroleum products in a long term [1]. The major challenges in the development of new hydrogen storage materials, with particular reference to batteries and fuel cells, are improved energy storage density, kinetics and cycle life, using readily available elements at reasonable cost [2]. Different compounds have been used for hydrogen storage, mainly are hydrides such as rare earths, mish-metals, Mg based compounds and FeTi [3, 4, 5]. Mg has shown great results as hydrogen carrier for vehicles purposes with hydrogen content of 7.6%. This metal is cheap, fairly accessible and it is available easily [6]. Research on intermetallic compounds for hydrogen storage was already attempted more than 25 years ago, they opened new possibilities for industrials developments [7]. The use of intermetallic FeTi has been pushed due to its good storage properties as well as its inexpensive price and great availability of elements involved [6].

FeTi equiatomic intermetallic compound has attracted a large number of experimental and theoretical studies recently, partly due to the fact that it is one of the important materials for hydrogen storage [8]. l.-F.Zhu et al [9] have studied pressure dependences of selected thermodynamic, structural and elastic properties as well as electronic structure of equiatomic B2 FeTi using the density functional theory. They have computed the free energies, the thermal expansion coefficients, the heat capacities at constants pressure and volume and the isothermal bulk modili at finite temperatures. E.Gonzalez et al [6] have applied first-principles calculation of hydrogen interaction with Platinum on the B2 FeTi (111) surface, they have determine the optimal location for Pt and then for adsorbed hydrogen. Reilly and Wiswall [10] have observed, when hydrogen interacts with the FeTi intermetallic compounds, two hydrides are produced FeTiH and FeTiH2. Kinaci et all [11] have calculated the formation energies of FeTiHx (x=1-6) by using the ab initio pseudopotentiel within the generalised gradient approximation (GGA), and the results are in best agreement with experimental data. Zhi-Sheng Nong et al [12] have studied the structural, elastic properties and electronic structural of FeTi and its hydrides by the first principles calculations. Except, the work reported by Zhi-Sheng Nong et al [12], on the elastic properties of B2 FeTi and its hydrides, these constants of orthorhombic structure of P2221 FeTiH has been not yet calculated or measured. We therefore think it is worthwhile to perform these calculations using the different methods for the computation of elastic properties within density functional density (DFT), in order to complete the exciting experimental and theoretical works these compound.

The main goal of this work is to investigate the elastic properties of cubic FeTi and orthorhombic $P222_1$ FeTiH.

Le 3ème Séminaire International sur les Energies Nouvelles et Renouvelables
The 3nd International Seminar on New and Renewable Energies

Unité de Recherche Appliquée en Energies Renouvelables,
Ghardaïa – Algérie 13 et 14 Octobre 2014

The rest of the paper is organized as follows. In section 2, details of the theory and computational are presented. In section 3, we presented and analyzed the results obtained by different methods. Finally, a conclusion of the present work is given.

II. Computational methods

We perform Density Functional Theory DFT [13] calculations using the Vienna ab initio simulation package (VASP) [16,17] code with the projector augmented wave (PAW) scheme [14,15]. We adopted the generalized gradient approximation (GGA) [18] of the Perdew and Wang (PW91) functional to describe the exchange-correlation interaction [19].The optimisation of the structural parameters was performed until the forces on the atoms were less than 0.02 eV/Å and all stress components less than 0.003 eV/Å3 . The calculations are converged at an energy cut-off of 450 eV and 600 eV for FeTi, FeTiH respectively. The Brillouin zone was sampled with a mesh of 13x13x13 and 11x11x11 generated by Monkhorst-Pack method [20] for FeTi and FeTiH structures, respectively.

In order to fit the first-principles calculated total energy E as a function of volume V. we employ the four-parameter Birch-Murnaghan equation of state (EOS) with its linear from given by [21].

$$E(V) = a + bV^{-2/3} + cV^{-4/3} + dV^{-2} \qquad (1)$$

Where a, b, c, and d are fitting parameters. Using expressions derived from fitting parameters, we can obtain the physical properties of the alloys such a equilibrium volume (V_0), energy (E_0), bulk modulus (B) and its pressure derivative (B') [22]. Inversely, based on the fitted equilibrium properties, the fitting parameters can also be determined, see details in [21].

Below, two approaches were discussed to calculate the different elastic constants. One by (stress-strain relationship) [23] is to use IBRION = 6 and ISIF = 3 to calculate the elastic constants, as implemented in the VASP [16,17]. The elastic tensor is determined by performing six finite distortions of the lattice parameters and deriving the elastic constants from stress-strain relationship. The final elastic moduli include both, the contributions for distortions with rigid ions and the contributions from the ionic relaxations [24].

The other way (strain energy-strain curve), the constants elastics were calculated as a second derivatives of the internal energy with respect to strain tensor (ε) [25]. The total energy calculations can be done based on the density functional theory (DFT) [13]. Elastic constants were deduced from the total energy calculations by applying small strains to the equilibrium lattice and analysing the change in the total energy of the unit cell. We express the energy of the strained system by means of a Taylor expansion in the distortion parameters [26].

$$E(V,\delta) = E(V_0,0) + V_0 \left(\sum_{i=1}^{6} \tau_i \delta_i + \frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} C_{ij} \delta_i \delta_j + 0(\delta^3) \right) \qquad (2)$$

Where τ_i are related to the strain on the crystal, C_{ij} are the elastic constants and V_0 is the volume of unstrained orthorhombic system.

The symmetry of the lattice reduces the number of the independent components of the elastic constants tensor. Three independent elastic constants for cubic phase FeTi and nine for orthorhombic phases of FeTiH were calculated as mentioned before. For each calculation, energies were calculated for at seven strains with $\delta = \pm 0.005, \pm 0.01, \pm 0.02$. Each strain was parametrized by a single variable δ, and the total energy was calculated for each distortion. The calculated total energies were fitted to a polynomial in δ and then equated to appropriate elastic constant coefficient expression given for each matrix in cubic and orthorhombic phases

For the cubic FeTi, the three independent elastic constants namely C_{11}, C_{12} and C_{44} have been calculated using volume conserving distortions [27]. The elastic stability criteria for a cubic crystal at ambient condition are $C_{11} + 2C_{12} > 0$; $C_{44} > 0$ and $C_{11} - C_{12} > 0$ [28]. Also, it is important to maintain high accuracy in the calculations since the total energy depends strongly on volume than on the distortions [29].

Two of these can be derived from the bulk modulus

$$B = \frac{C_{11} + 2C_{12}}{3} \qquad (3)$$

And the so-called Zener's elastic constants C',

$$C' = \frac{C_{11} - C_{12}}{2} \qquad (4)$$

The C_{11} and C_{12} elastic constants are derived from Eqs (3) and (4). The C' elastic constant was obtained using the orthorhombic deformation,

$$I + D_0 = \begin{pmatrix} 1+\delta & 0 & 0 \\ 0 & 1-\delta & 0 \\ 0 & 0 & \dfrac{1}{1-\delta^2} \end{pmatrix} \qquad (5)$$

Yielding the following change in the total energy:

Le 3ème Séminaire International sur les Energies Nouvelles et Renouvelables
The 3nd International Seminar on New and Renewable Energies

Unité de Recherche Appliquée en Energies Renouvelables,
Ghardaïa – Algérie 13 et 14 Octobre 2014

$$\Delta E/V = 2C'\delta^2 + \theta(\delta^4) \tag{6}$$

The C_{44} elastic constants can be calculated from the monoclinic distortion,

$$I + D_M = \begin{pmatrix} 1 & \delta & 0 \\ \delta & 1 & 0 \\ 0 & 0 & \dfrac{1}{1-\delta^2} \end{pmatrix} \tag{7}$$

Corresponding to the energy change in

$$\Delta E/V = 2C_{44}\cdot\delta^2 + \theta(\delta^4) \tag{8}$$

III. RESULTS AND DISCUSSION

A. Structural properties

All physical properties are related to the total energy. For instance, the equilibrium lattice constant of a crystal is the lattice constant that minimizes the total energy. If the total energy is calculated, any physical property related to the total energy can be determined.

The optimized lattice parameters and the corresponding volumes of unit's cells, along with available experimental values for FeTi and FeTiH, are due to [30] and [31] respectively, and are reported in Table 1.

Table I, shows the properties obtained for the structural optimization of the cubic FeTi, using the experimental value reported by A.M. Vanderkraan et al [30] the lattice parameter is 2.972 Å. It can be found that the GGA values of the lattice constant match fairly well with the experimental value, it can show a contraction of about 0.94%. The error of LSDA is bigger that the GGA (the errors less than 2.93%). It is seen that the lattice parameter values of GGA calculation implanted in VASP code compared to experimental values are better than values obtained by LSDA implanted in Wien2k code.

The structure parameters for orthorhombic phase from experimental observation [31] were optimized and then listed in Table 1. The calculated cell parameters for the orthorhombic structure compare well the corresponding experimental values, the theoretical lattice parameters a, b, c for FeTiH are smaller with relative error of -1.56%, -0.78% and -2.37% respectively. Thus, the theoretical results of our calculations are credible. The atom positions for the orthorhombic structure for FeTiH are also in good agreement with the experimental values. The bulk modulus, obtained by fitting the total energy-volume data to the universal equation of state [21] are 194.45 GPa and 195.43 GPa for FeTi and FeTiH respectively.

B. Elastic constants Polycrystalline elastic moduli

Elastic properties play a key role in the materials science and technology, they provides a link between the mechanical and dynamical behaviour of crystals, and give important information concerning the nature of the forces operating in solids. In particular, they provide information on the stability and stiffness of materials [32,33]. She define how a material undergoes stress deforms and then recovers and returns to its original shape after stress ceases [34].

The calculated elastic constants of FeTi compound are listed in Table II, along with the previous theoretical calculations using the volume conserving distortions technique [27] and the stress-energy relationship methods [23] for VASP calculations. The elastic constants for two techniques are basically consistent. But the calculated value of C_{12} for stress-energy relationship is lower than the result of volume conserving distortions technique. Whereas C_{11} and C_{44} have almost same values for the two techniques calculations. All results are compared with experimental data and previous theoretical calculations.

TABLE I
CALCULATED LATTICE PARAMETERS (A, B, C) (Å), OPTIMIZED ATOMIC POSITIONS, CALCULATED BULK MODULUS B (IN GPA) AND DERIVATIVE OF BULK MODULUS B'.

Perov.		Parameter		SG		Atomic position		B	B'
	Exp.	GGA	LDA		Site	Exp.	GGA		
FeTi	a=2.972 [30]	a=2.944	a=2.885	221	Fe(1a)	(0, 0, 0)	(0, 0, 0)	194.45	4.16
					Ti(1b)	(0.5, 0.5, 0.5)	(0.5, 0.5, 0.5)		
FeTiH	a=2.956	a=2.909			Fe (2c)	(0, 0.206, 0.25)	(0, 0.3037, 0.25)	195.43	4.32
	b=4.543	b=4.507		17	Ti (2d)	(0.5, 0.25, 0.75)	(0.5, 0.25, 0.75)		
	c=4.388 [31]	c=4.284			H (2a)	(0, 0, 0) [32]	(0, 0, 0)		

TABLE II
ELASTIC CONSTANTS (IN GPA) OF THE CUBIC FeTi. THE RESULTS ARE COMPARED WITH OTHER THEORETICAL RESULTS AND EXPERIMENTAL DATA

System	C_{11}	C_{12}	C_{44}	Ref.
FeTi				
Volume conserving	375.79	98.12	65.15	Present

Le 3ème Séminaire International sur les Energies Nouvelles et Renouvelables
The 3nd International Seminar on New and Renewable Energies

Unité de Recherche Appliquée en Energies Renouvelables,
Ghardaïa – Algérie 13 et 14 Octobre 2014

Stress-energy relationship	371.26	89.53	62.86	Present
Theory	385	95	72	Ref.[9]
Exp.	325	121	69	Ref. [38]

Since the calculated elastic constants for cubic FeTi given by the stress-strain relationship calculation for VASP approach are satisfactory results compared with experimental and others works, its can further be extended to determine the different elastic constant for orthorhombic structure FeTiH. It can be seen that the calculated elastic constants C_{ij} from the strain energy-strain and the stress-strain relationship calculations for orthorhombic FeTiH are listed from Table III. The elastic constants obtained by two methods are basically consistent. The deviations are party due to the calculation methods and fitting errors. And stability conditions [35] are all satisfied, which indicate, the orthorhombic FeTiH is mechanically stable.

$C_{ij} > 0$ (i=1-6), $(C_{11} + C_{22} - 2C_{12} > 0)$,

$(C_{11} + C_{33} - 2C_{13} > 0)$

$(C_{22} + C_{33} - 2C_{23} > 0)$

and $(C_{11} + C_{22} + C_{33} + 2C_{12} + 2C_{13} + 2C_{23} > 0)$ (9)

The value of C_{11}, C_{22} and C_{33} for FeTiH are all very large, suggesting that it is hard to be compressed under the uniaxial stress along the X, Y or Z axis in these compounds.

For orthorhombic $P222_1$ structural FeTiH, it can be seen that $C_{11} > C_{22} > C_{33}$. The implication of this is that the atomic bonds along the (1 0 0) plane between nearest neighbours are stronger than those along (0 1 0) plane and the (0 0 1) plane. The shear elastic constants C_{11}, C_{22}, C_{33} which are related to the unidirectional compression along the principle crystallographic directions are greater than C_{44}, C_{55} and C_{66} which reflect the resistance to shear deformation. This indicates the weaker resistance to the unidirectional compression compared to the resistance to shear deformation. Unfortunately, to our best knowledge, there are no experimental and theoretical data for the elastic constants of orthorhombic structure FeTiH available for a direct comparison.

TABLE III
CALCULATED ELASTIC CONSTANTS CIJ (IN GPA) FOR THE P2221 FETIH.

FeTiH	Strain energy-strain curve	Stress-energy relationship
C_{11}	346.49	359.23
C_{22}	328.89	325.96
C_{33}	298.58	306.25
C_{44}	83.81	59.98
C_{55}	66.53	80.73
C_{66}	62.86	65.96
C_{12}	103.62	105.61
C_{13}	106.14	111.92
C_{23}	192.75	195.79

C. Polycrystalline elastic moduli

In case of polycrystalline aggregates, it is not possible to calculate or measure individual elastic constants (C_{ij}). Nonetheless, average elastic properties such as polycrystalline bulk modulus (B), shear modulus (G), Young's modulus (E) and Poisson's ratio (ν) can be determined [26]. In the Voigt and Reuss schemes [36]. For the cubic structure, the Voigt and Reuss bulk moduli are equivalent with the single crystal bulk modulus from equation $B = (C_{11} + 2C_{12})/3$. The Voigt and Reuss shear moduli are given by [26].

TABLE IV
THE CALCULATED ELASTIC MODULUS (IN GPA) AND POISSON'S RATIO N FOR FETI AND ITS HYDRIDES BY USING VOIGT-REUSS-HILL APPROXIMATION

System	B_V	B_R	B_H	G_V	G_R	G_H	E	ν	B/G
FeTi (PAW)	190.67	190.67	190.67	94.62	82.70	88.66	230.28	0.298	2.15
Stress-energy relationship	183.44	183.44	183.44	94.06	80.74	87.40	226.27	0.305	2.09

Le 3ème Séminaire International sur les Energies Nouvelles et Renouvelables
The 3nd International Seminar on New and Renewable Energies

Unité de Recherche Appliquée en Energies Renouvelables,
Ghardaïa – Algérie 13 et 14 Octobre 2014

| FeTiH | 197.66 | 196.50 | 197.08 | 80.74 | 74.37 | 77.55 | 205.68 | 0.326 | 2.54 |

$$G_V = \frac{(3C_{44} + C_{11} - C_{12})}{5} \quad (10)$$

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{(4C_{44} + 3(C_{11} - C_{12}))} \quad (11)$$

For the orthorhombic structure, the Voigt and Reuss bulk moduli are different and defined by [26]

$$B_R = \frac{1}{(s_{11} + s_{22} + s_{33}) + 2(s_{12} + s_{13} + s_{23})} \quad (12)$$

$$B_V = \frac{1}{9}(C_{11} + C_{22} + C_{33} + 2C_{12} + 2C_{13} + 2C_{23}) \quad (13)$$

The Voigt and Reuss shear moduli are defined as follows [26]

$$G_R = \frac{15}{4(s_{11} + s_{22} + s_{33}) - 4(s_{12} + s_{13} + s_{23}) + 3(s_{44} + s_{55} + s_{66})} \quad (14)$$

$$G_V = \frac{1}{15}(C_{11} + C_{22} + C_{33} - C_{12} - C_{13} - C_{23}) + \frac{1}{5}(C_{44} + C_{55} + C_{66}) \quad (15)$$

In Eqs. (14) and (16), the s_{ij} are the elastic compliance constants. The elastic moduli of polycrystalline material can be approximated by Hill's averages for shear modulus (G_H) and bulk modulus (B_H) are [26]

Then, the Young's modulus E and Poisson's ratio ν are related to the hardness of polycrystalline materials. These quantities are given by [26];

$$E = \frac{9BG}{3B + G} \quad , \quad \nu = \frac{3B - 2G}{2(3B + G)} \quad (16)$$

Based on the available standard relations, bulk modulus, shear modulus, Poisson's ratio and Young's modulus are determined using the elastics constants, they are listed in Table IV. It can be seen that FeTiH display larger bulk modulus than FeTi, and lower shear modulus than FeTi. It can be suggested that the bulk modulus increase gradually with increase of number of hydrogen atom, indicating that the FeTi alloy becomes more difficult to compress with the increasing the number of hydrogen atom, this relative "hardening" is due to the formation of increasing number of hydrogen-metal bonds within the alloy lattice.

Poisson's ratio ν are determined from the following expression (Eq.(19)), it is generally accepted that the values of Poisson's ratio smaller than 0.1 are associated with covalent material, whereas ionic materials have typical values close to 0.25 [37]. In our case all values of ν are greater then 0.25, and listed in Table IV, suggest a considerable ionic character in our compounds. Other that Poisson's ratio can usually used to evaluate the stability of the crystal against shear [35,38]. The calculated results show that compared with the FeTi and his hydrides. FeTi has a lower tenacity it has smaller value of Poisson's ratio, and the absorption of hydrogen increase the Poisson's ratio and improve the plasticity.

To predict the brittle and ductile behaviour of solids, Pugh [39] introduced a simple relationship that the ratio of bulk to shear modulus (B/G) is associated with ductile or brittle of materials. If B/G < 1.75, the materials behaves in a brittle manner, otherwise, the material performs in a ductile manner. The values of B/G are presented in Table IV is indicated the FeTi and its hydrides are ductile. We can see that the variation of B/G increasing with increasing the number of hydrogen atom, indicating that the concentration of hydrogen atom can change the ductibility. A right description of an anisotropic behaviour has an important implication in engineering science and in crystal physics [40]. Zener anisotropy A is an indicator of the degree of anisotropy in the solid structure compared to the isotropic material [41]. For the cubic phase, the Zener anisotropy is given as [36];

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \quad (17)$$

The Zener anisotropy factors in the orthorhombic phase are three, firstly, A_1 which is the shear anisotropic factor for the $\{100\}$ shear planes between $\langle 0\,1\,1\rangle$ and $\langle 0\,1\,0\rangle$ directions. Secondly, A_2 which is the shear factor in the $\{0\,10\}$ shear planes between $\langle 1\,0\,1\rangle$ and $\langle 0\,0\,1\rangle$ directions. Lastly, for $\{001\}$ direction the shear plane between $\langle 1\,10\rangle$ and $\langle 0\,1\,0\rangle$ is given as A_3 [42]. These factors are given as follows;

$$A_1 = \frac{4C_{44}}{C_{11} + C_{33} - 2C_{13}} \quad (18)$$

$$A_2 = \frac{4C_{55}}{C_{22} + C_{33} - 2C_{23}} \quad (19)$$

and

$$A_3 = \frac{4C_{66}}{C_{11} + C_{22} - 2C_{12}} \quad (20)$$

5

Le 3ème Séminaire International sur les Energies Nouvelles et Renouvelables
The 3nd International Seminar on New and Renewable Energies
Unité de Recherche Appliquée en Energies Renouvelables,
Ghardaïa – Algérie 13 et 14 Octobre 2014

The calculated A_1, A_2 and A_3 for $P222_1$ FeTiH are listed in Table V .A value of unity means that the crystal exhibits isotropic properties, why value other than unity represents varying degrees of isotropy. From our result, it can be seen only FeTiH exhibit larger anisotropic in the (0 1 0) plane.

TABLE V

THE ANISOTROPIC FACTORS A_1, A_2 AND A_3, ANISOTROPY IN THE COMPRESSION AND SHEAR (%) FOR $P222_1$ FeTiH

System	Methods	A_1	A_2	A_3	A_{comp}(%)	A_{shear} (%)
FeTi	Volume conserving	0.469	0.46	0.46	0	6.72
	Stress-energy relationship	0.446	0.44	0.44	0	7.62
FeTiH	Strain energy-strain curve	0.775	1.10	0.53	0.274	4.10
	Stress-energy relationship	0.543	1.34	0.55	-	-

Another way of measuring the elastic anisotropy proposed is given by the percentage of anisotropy in the compression and shear [33];

$$A_{comp} = \frac{B_V - B_R}{B_V + B_R} \times 100\% \qquad (21)$$

$$A_{shear} = \frac{G_V - G_R}{G_V + G_R} \times 100\% \qquad (22)$$

For these two expressions, a value of zero is associated with elastic isotropy; while a value of 1 (100%) is the largest possible anisotropy. The percentage anisotropy values have been computed for FeTi and FeTiH, and are shown in Table V. It can be seen that the anisotropy in compression is small and the anisotropy in shear is high.

IV. CONCLUSION

We have performed ab-initio calculations to predict structural and elastic properties of the two compounds (FeTi and FeTiH). Elastic constants are calculated by first-principles calculation within the generalized gradient approximation based on density functional formalism. For cubic FeTi the elastic properties were obtained from volume conserving distortions methods and stress-strain relationship calculated based on VASP code and is compared. Good agreement with experimental values has been archived. Bulk modulus is determined by fitting using the 4 parameters Birch-Murnaghan equation of state, the different is approximately 0.88% between theory and experimental value. Our calculations have given B/G ratio than 2.00 these suggesting a mostly ductile behaviour.

The elastic constants for orthorhombic $P222_1$ FeTiH were determined from the stress-strain relationship calculations and the strain energy-strain curves calculations respectively. The calculated lattice parameters are in excellent agreement with the experimental data for the hydrides of FeTi compounds. Our calculated results on the elastic constants satisfy the traditional mechanical stability conditions. The mechanical properties like bulk modulus, shear modulus, Young's modulus, Poisson's ratio and shear anisotropic factors are also calculated. For $P222_1$ FeTiH the values of ratio B/G is larger than 1.75, and therefore FeTiH can be classified is a ductile materials. We can see that the variation of ratio B/G increase with increasing the number of hydrogen atom, indicating that the concentration of hydrogen atom can change the ductibility. Since there are no experimental elastic data available for the orthorhombic structures FeTiH compound, we think that the quantum mechanical simulation estimation is the only reasonable tool for obtaining such important information.

REFERENCES

[1] A. Izanlou, AK. Aydinol. An ab initio study of dissociation adsoption of H_2 on FeTi surfaces. International Journal of Hydrogen Energy 2010; 35:1681-92.

[2] M. Bououdina, D. Grant, G. Walker. Review on hydrogen absorbing materials-structure, microstructure, and thermodynamic properties. Int J Hydrogen Energy 2006;31:177-82

[3] JM. Marchetti, HL. Corso, JL. Gervasoni. Experimental and theoretical study of the behaviour of hydrogen in rare earths. International Journal of Hydrogen Energy 2005;30:627-30.

[4] JM. Marchetti, E. Gonzalez, P. Jasen, G. Brizuela, A. Juan. Interaction of hydrogen and platinum over a B2FeTi(110) slab. International journal of Hydrogen Energy 2011;36:9037-44.

[5] IP. Jain, C. Lal, A. Jain. Hydrogen storage in Mg: a most promising material. International journal of Hydrogen Energy 2010;35:5133-44.

[6] E. Gonzalez, P. Jasen, JM. Marchetti, G. Brizuela, A. Juan. Density functional and bonding study of hydrogen and platinum adsorption on B2-FeTi(111) slab. International journal of Hydrogen Energy 2012;37:2661-68.

[7] B. Sakintuna, F. Lamari-Darkrim, M. Hirscher. Metal hydride materials for solid hydrogen: A review. International journal of Hydrogen Energy 2007; 32:1121-40.

[8] M. Gupta. The electronic structure of hydrogenated intermetallic compounds: Theory. Journal of the Less-Common Metals. 1984; 101: 35-51.

[9] LF. Zhu, M. Friak, A. Udyansky, D. Ma, A. Schlieter, U. Kuhn, J. Eckert, Neugebauer J. Intermetallics 2014;45:11-17.

[10] JJ. Reilly, RH. Wiswall. Formation and properties of iron titanium hydride. Inorg Chem 1974; 13(1): 218-22.

[11] A. Izanlou, MK. Aydinol. Ab-initio investigation of FeTi-H system. International Journal of Hydrogen Energy 2007; 32: 2466-74

[12] N. Zhi-Sheng, Z. Jing-Chuan, Y. Xia-Wei, C. Yong, L. Zhong-Hong, L. Yong. First-principles study of hydrogen storage and diffusion in B2 FeTi alloy. Computational Materials Science 2014; 81:517-23

[13] W. Kohn, L. Sham. self-consistent equations including exchange and correlation effects. Phys.Rev. 1965;140:1133-40.

Le 3ème Séminaire International sur les Energies Nouvelles et Renouvelables
The 3nd International Seminar on New and Renewable Energies

Unité de Recherche Appliquée en Energies Renouvelables,
Ghardaïa – Algérie 13 et 14 Octobre 2014

[14] G. Kresse, D. Joubert. Form ultrasoft pseudopotontials to the projector augmented-wave method. Phys.Rev B 1999; 59: 1758-75.

[15] PE. Blochl. Projector augmented-wave method. Phys.Rev B 1994;50:17953-79.

[16] G. Kresse, J. Furthmuller. Efficient iterative schemes for ab initio total energy calculation using a plane-wave basis set. Phys.Rev B 1996; 54:11169-86.

[17] G. Kresse, J. Hafner. Ab-initio molecular dynamics for liquid metals. Phys.Rev B 1993; 47:558-61.

[18] JP. Perdew, Y. Wang. Accurate and simple analytic representation of the electron-gas correlation energy. Phys.Rev B 1992;45(23):13244-49.

[19] JP. Perdew, JA. Chevary, SH. Vosko, KA. Jackson, MR. Pederson, DJ. Singh, C. Fiolhais, Atoms, molecules, solids, and surfaces: Application of the generalized gradient approximation for exchange and correlation. Phys.Rev B 1992;46(11)6671.

[20] HJ. Monkhorst, JD. Pack. Special points for Brillouin-zone integrations. Phys.Rev. B 1976;13:5188-92.

[21] SL. Shang, Y. Wang, DE. Kim, ZK. Liu. First-principles thermodynamics from phonon and Debey model: application to Ni and Ni3Al. Comp.Mate.Sci.2010;47:1040-48.

[22] DE. Kim, SL. Shang, ZK. Liu. Effects of alloying elements on elastic properties of Ni3Al by first-principles calculations. Intermetallics 2010;18:1163-71.

[23] Y. Le Page, P. Saxe. Symmetry general least-squares extraction of elastic data for strained materials from ab-initio calculations of stress. Phys. Rev B. 2002;65:104104-117.

[24] S. Li, X. Ju, C. Wan. Theoretical studies of elastic properties of orthorhombic LiBH4. 2014;81:378-85.

[25] DC. Wallace. Thermodynamics of crystals. Wiley 1972.

[26] P. Ravindran, L. Fast, PA. Korzhavyi, B. Johansson. Density functional theory for calculation of elastic properties of orthorhombic crystals: Application to TiSi2. Journal of Applied Physics. 1998; 84:4891-4904.

[27] M. Rajagopalan. Full potential linear augmented plane wave study of the elastic properties of XPt3 (X=V,Cr,Mn,Fe,Co,Ni). Physica B 2010; 405: 2516-18.

[28] M. Rajagopalan, S. Praveen Kumar, R. Anuthama. FP-LAPW study of the elastic properties of Al2X (X=Sc,Y,La,Lu). Physica B 2010; 405: 1817-20.

[29] C. Asker, L. Vitos, IA. Abrikosov. Elastic constant and anisotropy in FeNi alloys at high pressures from first-principles calculations. Physical Review B 2009;79:214112-9.

[30] AM. Vanderkraan, KHJ Buschow. The Fe-57 mossbauer isomer shift in intermetallics compounds of iron. Physica B & C. 1986; 138(1-2): 55-62.

[31] P. Thompson, MA. Pick, F. Reidinger, LM. Corliss, JM. Hasting, JJ. Reilly. Neutron diffraction study of β iron titanium deuteride. J Phys F 1978; 8(4): L75-80.

[32] R. Golesorkhtabar, P. Pavone, J. Spitaler, P. Puschnig, C. Draxl. ElaStic: A tool for calculating second-order elastic constants from first-principles. Computer Physics Communication. 2013; 184:1861-73.

[33] H. Koc, AM. Mamedov, E. Deligoz, H. Ozisik. First principles prediction on the elastic, electronic, and optical properties of Sb_2S_3 and Sb_2Se_3 compounds. Solid State Sciences 2012;14:1211-20.

[34] AH. Reshak, J. Mosteza. DFT calculation for elastic constants of orthorhombic structure within WIEN2K code: A new package (ortho-elastic). Journal of Alloys and Compounds. 2012; 543: 147-51.

[35] QJ. Liu, ZT. Liu, LP. Feng, H. Tian. First-principles study of structural, elastic, electronic and optical properties of orthorhombic GaPO4. 2011; 13: 1076-82.

[36] VI. Razumovskiy, EI. Isaev, AV. Ruban, PA. Korzhavyi. Ab initio calculations of elastic properties of Pt-Sc alloys. Intermetallics. 2008; 16: 982-86.

[37] A. Sekkal, A. Benzair, H. Aourag, HI. Faraoun, G. Merad. Structural and thermoelastic properties of B2-YX (X=Cu, Mg and Rh) intermetallic compounds. 2010; 405:2831-35.

[38] ZS. Nong, JC. Zhu, HI Yu, ZH. Lai. First principles calculation of intermetallic compounds in FeTiCoNiVCrMnCuAl system high entropy alloy. Transaction of Nonferrous Metals Society of China. 2012; 22: 1437-44.

[39] SF. Pugh. Relation between the elastic moduli and plastic properties of polycrystalline pure metals. Philosophycal Magazine. 1954;45:823-43.

[40] XL. Yuan, MA. Xue, W. Chen, TQ. An, Y. Cheng. Investigations on the structural, elastic and electronic properties of the orthorhombic Zirconium-Nickel alloy under different pressure. 2012; 65: 127-32.

[41] SQ. Wang, HQ. Ye. Ab initio elastic constants for the lonsdaleite phases of C, Si and Ge. Journal of Physics: Condensed Matter. 2003; 15: 5307-14.

[42] PWO. Nyawere, NW. Makau, GO. Amolo. First-principles calculations of the elastic constants of the cubic, orthorhombic and hexagonal phases of BaF_2. Physica B. 2014; 434: 122-28.