

Density functional investigation on structural, elastic, thermal and mechanical properties of NiTi intermetallic compound

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Abstract. Theoretical study of structural, elastic, mechanical and thermal properties of B₂-type binary intermetallic NiTi is performed using full-potential linearized augmented plane wave (FP-LAPW) method. In this approach the generalized gradient approximation and local density approximation is used for exchange-correlation (XC) potential. We have calculated the ground state properties such as lattice constant ($a_0 = 3.0140 \text{ \AA}$ and 2.9439 \AA), bulk modulus ($B = 161.58 \text{ GPa}$ and 191.92 GPa) and pressure derivative of bulk modulus ($B' = 4.21$ and 4.15) using PBE-GGA and LDA approximations respectively for NiTi. Our calculated lattice constants are in good agreement with the experimental data available. A special attention has been paid to the determination of the second order elastic constants. The second order elastic constants ($C_{11} = 308.58 \text{ GPa}$, $C_{12} = 87.97 \text{ GPa}$ and $C_{44} = 57.90 \text{ GPa}$) have been calculated using PBE-GGA at ambient condition. In addition Poisson's ratio (σ), Young's Modulus (E), Shear modulus (G_H) and the ratio of anisotropy factor (A) are also reported. Ductility/brittleness of this compound is further analyzed by calculating the B/G_H ratio and Cauchy pressure ($C_{12}-C_{44}$). The studied compound is found to be ductile in nature. Sound wave velocities with Debye Temperature (θ_D) are also investigated.

1. Introduction

The B₂ structured (CsCl-type structure) intermetallic compounds have been extensively studied for several decades due to their high oxidation resistance, high stiffness and high strength for elevated temperature for engineering applications [1]. Intermetallics are the compounds prepared with the combination in the certain proportions of two or more metals may be non-metals and react to produce a solid-state phase which is completely different from its elements of combination. A brief discussion is mentioned concerning the experimental and theoretical work carried out related to these kinds of intermetallic compounds in the literature till now. Due to their above-mentioned properties, these intermetallics are used in aircraft engine. Cheng et. al. [2] presented the first principles study of elastic properties and electronic structure of NiTi, CoTi and FeTi. Baranov [3] predicted structural stability of pure elements and binary intermetallic compounds assuming the density of atoms as stationary and undeformable in internal and external spherical symmetrical shell. The B₂-type NiTi intermetallic compound motivated our interest because B₂-type is the simplest and most common cubic structure and there is no systematic study of mechanical and thermal behaviour of NiTi is found in the literature. In the present paper, we have performed theoretical FP-LAPW study of structural, elastic, mechanical and thermal properties of NiTi intermetallic compound using GGA and LDA approximation. The paper is organized as follows. The method of calculation is briefly described in Section 2. Section 3 deals with the results with discussion of the present work.



2. Method of calculation

For the calculations of total energy and electronic structure, FP-LAPW method based on density functional theory is used. It is implemented in the WIEN2k code [4]. PBE-GGA [5] and LDA [6] was used as exchange correlation energy calculations. All the calculations were performed with the non-spin polarized density functional theory. Generally, the convergence is achieved by expanding the basis function up to $R_{MT} \cdot K_{max} = 7$, where R_{MT} is the smallest atomic radius in the unit cell and K_{max} gives the magnitude of the largest k vector in the plane wave expansion. The maximum value for partial waves inside the atomic sphere is $l_{max} = 10$ while the charge density is Fourier expanded up to $G_{max} = 12$ (Ryd)^{1/2}. The self-consistent calculations are converged when the total energy of the system is stable within 10^{-4} Ry. A dense mesh of 1000 k points and the tetrahedral method [7] have been employed for the Brillouin zone integration. The total energies are fitted to third order Birch equation of state [8] to obtain the ground state properties.

3. Results and discussions

3.1 Structural properties

In order to calculate the ground state properties of NiTi, the total energy is calculated as a function of reduced volume in B₂-type (CsCl) structure using full potential linearized augmented plane wave (FP-LAPW) method. The plot of total energy with the reduced volume is shown in figure 1. The calculated total energies are fitted to the Birch equation of state [8] to investigate the volume-energy relationship. The ground state properties, such as equilibrium lattice constant (a_0), bulk modulus (B) and pressure derivative of bulk modulus (B') for NiTi have been calculated using GGA and LDA approximations. The calculated values for these properties are presented and compared with available experimental [9] and other theoretical [3] data in table 1. As a comparison of our calculated lattice constants with the available experimental and other previous theoretical calculations, we found PBE-GGA overestimate the lattice constants while LDA underestimate the same [10]. The over binding in LDA underestimate the volume and overestimate the bulk modulus while the enhancement factor $F_x(s)$ for PBE-GGA rises more rapidly, give more accurate atomization energy [11]. Since the lattice constants obtained by PBE-GGA is more realistic and closer to experimental results and because of its advantage over LDA, the further calculations have been carried out using only PBE-GGA. It is also observed that our calculated bulk modulus (B) overestimates the other theoretical data [9] for the same compound which may be due to the different approximations used in the calculation. Due to the unavailability of any data both experimental and theoretical regarding B', it could not be compared.

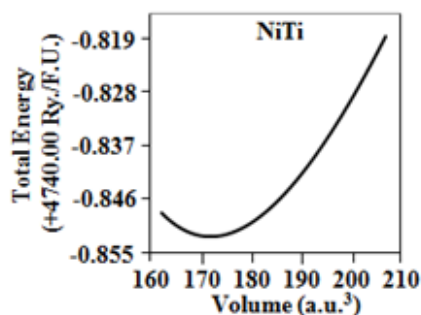


Figure 1. Energy vs Volume Curve

3.2 Electronic properties

In the present work, the self-consistent band structures (BS) along the high symmetry directions, total and partial density of states (TDOS and PDOS) are presented in figure 2(a) and figure 2(b) to have insight into electronic behaviour of NiTi. In figure 2(a), one can see that the Fermi level is fixed at the origin. In the same figure the lowest lying band is observed due to 's'-like states of Ti atom at Γ -point. From the Figure 2(b), it is very clear that some of states are crossing Fermi level from valence band to conduction bands, means there is no band gap at E_F , fulfil the metallic character of NiTi compound.

The peaks are observed at -2 eV and -4 eV in valence band due are to 'd' like state of Ni. The metallicity of NiTi is due to the hybridization 'd' like states of Ni and Ti at the Fermi level. The conduction band is mainly dominated by 'd' like state of Ti. As can be seen from the Table 1 that due to metallic character the value of finite DOS at Fermi level for NiTi is obtained 1.57 states/eV/F.U.

Table 1. The calculated ground state properties and density of states at the Fermi level $N(E_F)$ for NiTi at ambient pressure.

Solid	Work	Approx.	a_0 (Å)	B (GPa)	B'	$N(E_F)$ (States/eV)
NiTi	Present	PBE-GGA	3.0140	161.58	4.21	-
		LDA	2.9439	191.92	4.15	1.57
	Exp.	-	3.013 ^a	-	-	-
	Oth. The.	-	2.985 ^b	139.00 ^b	-	-

Exp. - Experimental, Oth.The. - Other Theory, Approx. – Approximations

^aRef [9], ^bRef [3]

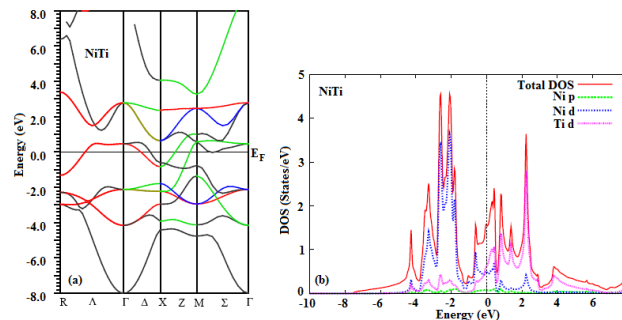


Figure 2. (a) Band Structure and (b) Density of States of NiTi using PBE-GGA

3.3 Elastic properties

The elastic constants provide a link between the mechanical and dynamical behavior of crystal. We have calculated the elastic constants for NiTi using PBE-GGA at ambient pressure using the method developed by Thomas Charpin and integrated it in the WIEN2k package. The calculated values of elastic constants at ambient pressure are given in table 2. We have also analyzed the ductility of investigated compound using Pugh's criteria [12] and Cauchy's pressure. If the value of B/G_H is greater than 1.75, the investigated compound is predicted as ductile in nature. Our calculated result indicates that the studied compound is ductile in nature with B/G_H ratio as 4.90. The ductile nature of NiTi can also be correlated to the positive Cauchy pressure and thereby metallic nature of the studied compound. It can be noted that our calculated elastic constants satisfy the stability criterions: $C_{11} - C_{12} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{12} < B < C_{11}$, which clearly indicate the stability of NiTi in CsCl structure.

Table 2. Calculated elastic properties of NiTi.

Solids	Approx.	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B/G_H	$C_{12}-C_{44}$
NiTi	PBE-GGA	308.58	87.97	57.90		
	LDA	207.53	186.15	85.61	4.9	100.54

3.4 Mechanical properties

Elastic constants can be used to determine mechanical properties such as Density (ρ), anisotropic factor (A), shear modulus (G_H) Young's modulus (E) and Poisson's ratio (σ) for useful applications.

These are fundamental parameters which are closely related to many physical properties like internal strain, thermo-elastic stress, sound velocity, fracture, toughness etc. We have calculated these properties of NiTi and presented in Table 3. The calculated value of Poisson's ratio reveals the metallic nature of the studied compound. Neither experimental nor theoretical results of these properties are available for NiTi, so we could not compare our results with other measured or theoretical values.

Table 3. The calculated mechanical properties of NiTi at ambient pressure using LDA.

Solids	$\rho \times 10^3$ (kg/m ³)	A	G_H	E	σ
NiTi	6.935	8.00	39.07	109.82	0.40

3.5 Thermal properties

We have calculated the Debye temperature (θ_D) by using the average sound velocity v_m and elastic constants. The values of v_m and (θ_D) for B₂ phase are found to be 3190.50 m/s, 240.65°K respectively. In the absence of any measured data in the literature, they could not be compared. Hence, our results can be considered as a prediction for these properties of intermetallic compounds and it will testify future experimental work.

4. Conclusions

We have systematically performed the FP-LAPW calculations to evaluate the structural and electronic properties of NiTi binary intermetallic compound using density functional theory (DFT). We have applied generalized gradient approximation of PBE-GGA and local density approximation (LDA) for the exchange correlation calculations. The total energy is fitted to the Birch equation of state. The ground state properties like lattice constant, bulk modulus and pressure derivative of bulk modulus are calculated and compared. The obtained lattice constants are in good agreement with the available experimental and theoretical values. Due to the overlapping of valence band and conduction band the metallic nature of NiTi is satisfied. The calculated elastic constants show that NiTi is elastically stable in B₂ phase. Using these elastic constants, the shear modulus (G_H), Poisson's ratio (σ), Young's modulus (E) and anisotropy factor (A) are also reported. In the present study, we found $B/G_H > 1.75$ and $C_{12}-C_{44} > 0$ which implies that all these compounds are ductile in nature and NiTi have an excellent ductility.

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