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Comparison on Ground State Properties of Modeled TiV_3 And TiV_3N Compounds using TB-LMTO Method

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Abstract: The influence of pressure on the Magnetic and Electronic structure of modeled TiV_3 and TiV_3N compounds using Tight Binding Linear Muffin Tin Orbital Method. From several lattice parameters,the equilibrium volume of these compounds has been obtained using total energy calculation. The present approach indicates thatTiV_3N is nonmagnetic and TiV_3 shows a ferromagnetic order at low pressure and becomes nonmagnetic at high pressures(lower volume).The band structure and density of states has been plotted for both compoundsto analyze the electronic contribution.

Keywords: Electronic structure; Magnetic properties; Total energy calculations; Bulk moduli; LMTO.

1. Introduction

The 3d-transition metal nitrides are important for technological applications because of their physical properties such as very high melting point, extreme hardness, and metallic conductivity. Interestingly, the transition metal nitrides in the nanostructured form has been most attractive for magnetic storage devices, catalytic studies, superconducting applications, and for technological tasks arising within the semiconductor industries. Titanium Vanadium Nitride has been significant alternative forbinary nitride coatings in industrial applications involving wear protection, cutting tools and machinery components. It has also been used in various kind of areas such as the packaging industry, transparent barrier coatings and micro-electronics.[1-4]It gives better film properties like high hardness, low coefficient of friction, good wear resistance and excellent corrosion protection, high melting point etc.[5] A nanostructured composite of Titanium Vanadium Nitride render low cost, high molar density and superior chemical resistance makes it a required material for the succeeding age band of lithium batteries and super capacitors.[6-7]Because of many experimental problems to obtain orderly substituted iron nitrides, some ternary iron nitrides (Me_xFe_{4-xN}) can be obtained by mechanical alloying and the effects of different substitutions on $Me_xFe_{4-x}N$ ternary Perovskite nitrides (where M = Fe, Mn, Au, Ag, Sn, Pd, Ni, Pt, In, Zn, Cu, Cr, V, Co, Al) has been reported on the electronic structure of fully ordered substituted iron nitrides by means of self-consistent band structure calculations within the Local Spin Density Approximation (LSDA).[8-21] C. A. Kuhnen et al[9] studied the behavior of the magnetism of the cobalt, chromium and titanium in place of Fe atom on Fe_4N compound with pressure using LMTO method. Hence our effort continues on finding the effects of nitrogen in the electronic structure of alloy with V–Ti.

2. Methodology

O.K. Anderson in 1971 introduced linear methods in band theory to solve many self-consistent electronic structure problems. One of the most effective linear methods used to estimate the ground state properties of infinite crystals and real materials is Tight Binding Linear Muffin Tin Orbital Method

(TB-LMTO) with Atomic Sphere Approximation (ASA). Simplest and most widely usedone-electron Hamiltonian is tight-binding with minimal base. Within ASA, the Muffin Tin spheres replaces Wigner SeitzSpheres in which the energy dependence has been canceled and provides accurate electronic structure.[22-24]The modeled TiV_3 and TiV_3N compounds has been crystallized in the simple cubic structure with space group *Pm-3m* where in each case the metal atoms occupy the corner sites and the face-centered position, while the nitrogen atoms occupy the body-centered site. The structural stability of these compounds is found from total energy calculations and calculated values has been fitted with Birch Murnaghan equation of state.[25-26]The ferromagnetic and nonmagnetic calculations has been performed to investigate the magnetic behavior of the compounds.The exchange correlation energy of the electron gas with scheme of Von Barth and Hedin[27]has been employed.Therefore the most important relativistic correction namely the Darwin's correction, mass velocity terms and spin–order coupling has alsobeen included.The one-electron potentials has been self-consistently obtained using reciprocal space sums with **216** k-points. The self-consistent cycles were carried out until energy convergence on a scale better than **0.1**mRy has been achieved. The density of states (DOS) has been calculated as a sum of delta functions for **6 x 6 x 6** mesh points.

3. Result and Discussion

The binding curves between total energy and lattice parameters of TiV_3 and TiV_3N compounds has been displayed in figure1. It has been obtained through an analytical fitting of the calculated total energies to fourth degree polynomial in each case. The Bulk moduli for respective equilibrium lattice parameters of all the compounds has been shown in the table 1.It shows that the inclusion of nitrogen increases the elastic effect of TiV_3.

Table 1. Estimated lattice parameters and Bulk moduli of the compounds TiV_3, $VTi_3$and TiV_3N.

Compounds	Lattice Constant 'a' (a.u)	B (Mbar)
TiV_3(NM)	7.2690	1.7848
TiV_3(FM)	7.2672	1.7891
TiV_3N	7.4977	2.2487

Under pressure the ferromagnetic calculations of TiV_3 provides nearly null local magnetic moments at Ti and V sites represents that the magnetic phase is nonmagnetic for lower volumes(below a=8.2185 a.u). Contrarily, the FM calculation gives local magnetic moments -0.0762 μ_B at titanium sites and 2.6706 µB at Vanadium sites for slightly higher volumes (negative pressures) with lattice parameter a = 8.9858a.u. Hence, the ordered TiV_3 exhibits a ferromagnetic order with a total magnetic moment per unit cell of 7.9356 μ_B. Figure.2 represents two separated but crossing branches overlap at a region of co-existence, where magnetic moment approaches zero.A discussion on the structural and magnetic properties of TiV_3N is given with a comparison of the TiV_3, disorder to get insights of the Nitrogen substitution effects. The electronic structures analyzed from projected density of states for both compounds (shown in figure.4) are also reported.

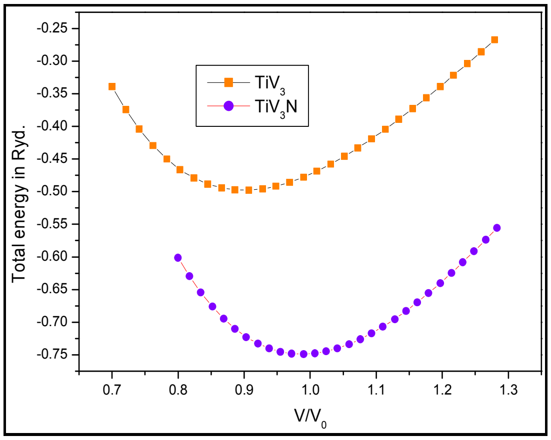

Figure 1 (a).Binding curves between total energies +7391(in Rydberg) versus lattice spacing 'a' (atomic units) for the compounds TiV_3 in NM & FM states.

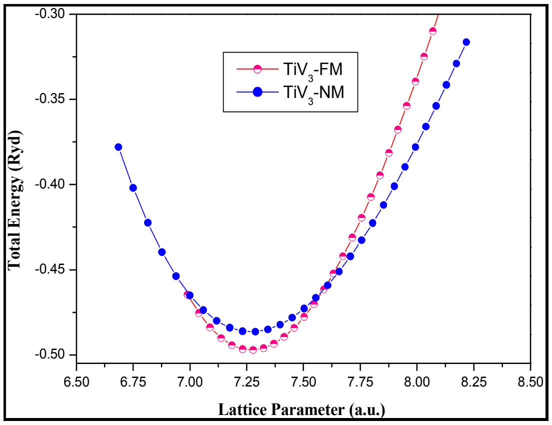

Figure 1(b).Binding curves between total energies +7391 & +7500(in Rydberg) versus relative volume V/V_o for the compounds TiV_3& TiV_3N.

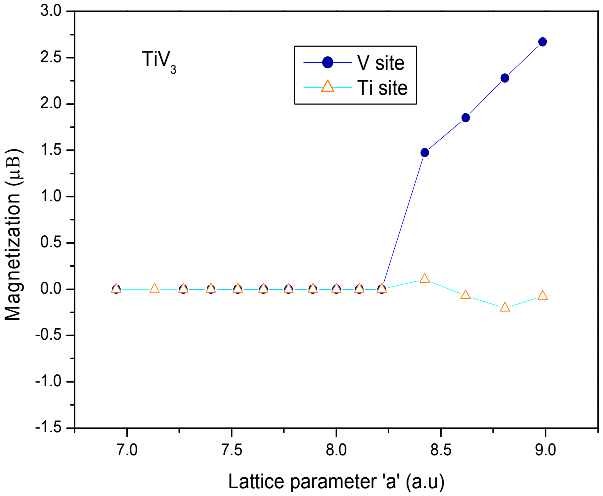

Figure 2.The magnetic moments (in Bohr magnetrons) as a function of lattice parameter (in atomic units) at V and Ti sites for the TiV_3 ordered alloy.

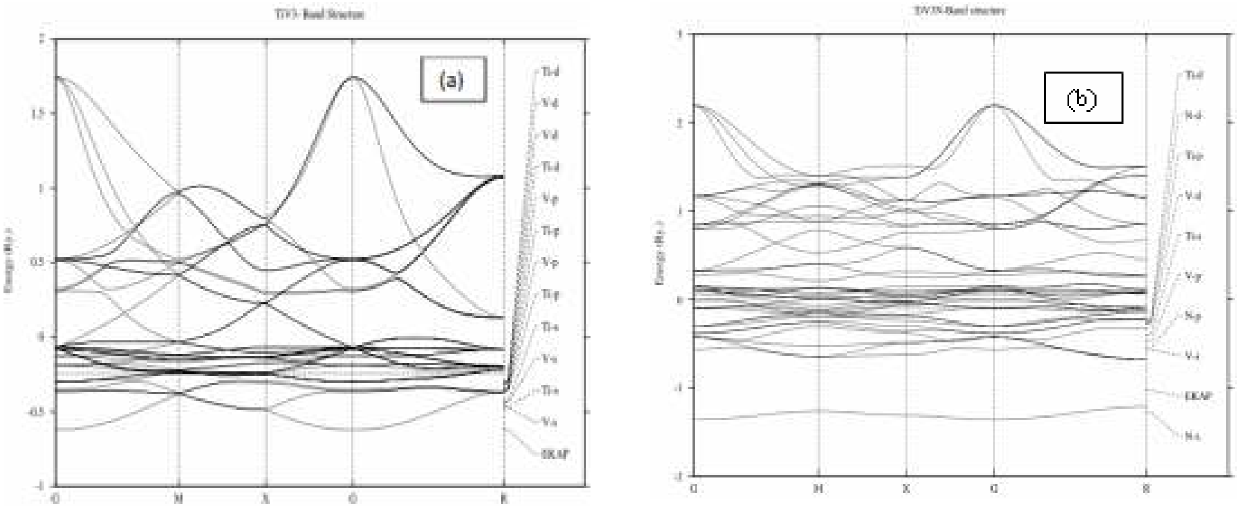

Figure.3(a)

Figure.3(b)

Figure 3.Band structure for the compounds TiV_3 and TiV_3N respectively.

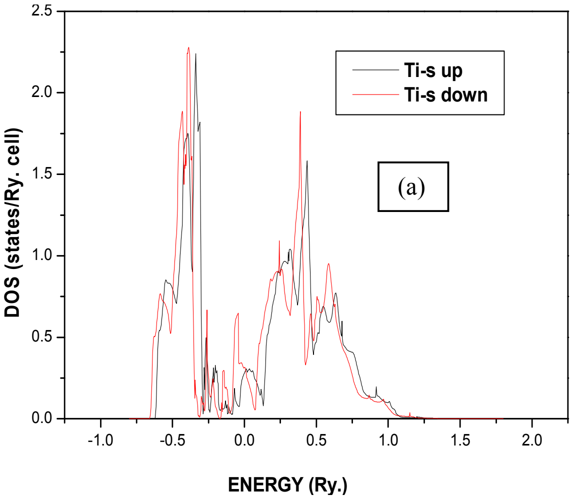

Figure.4(a).

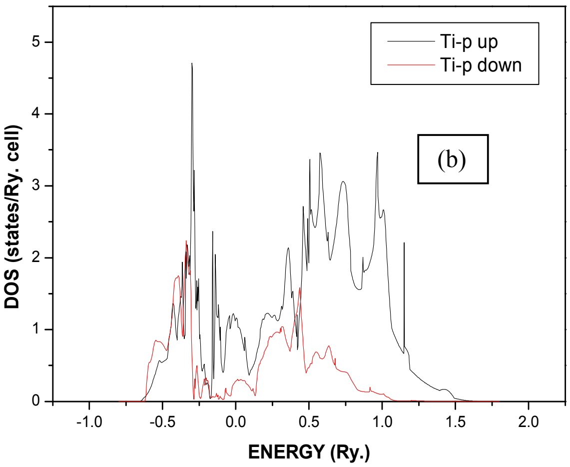

Figure.4(b).

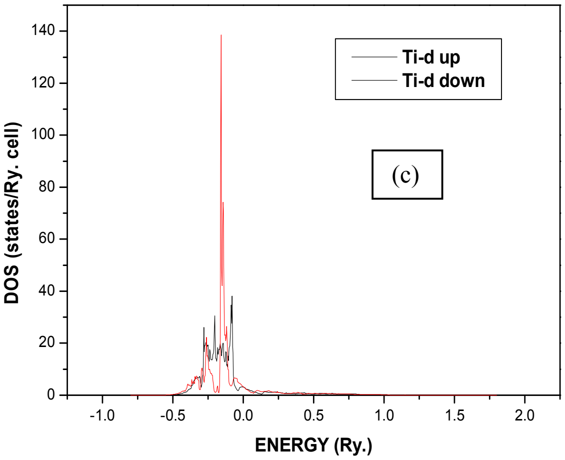

Figure.4(c).

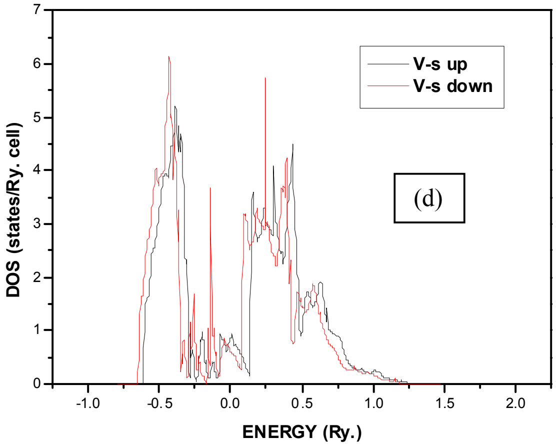

Figure.4(d).

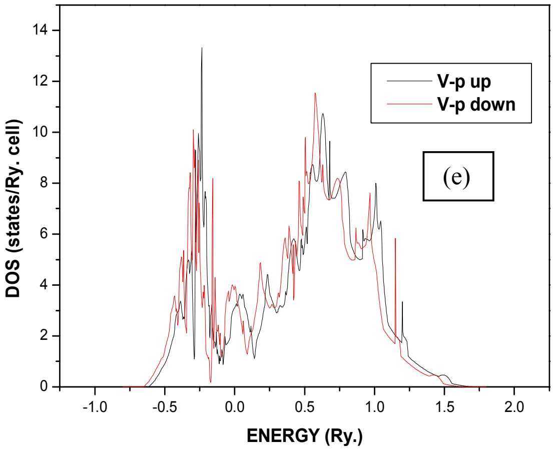

Figure.4(e).

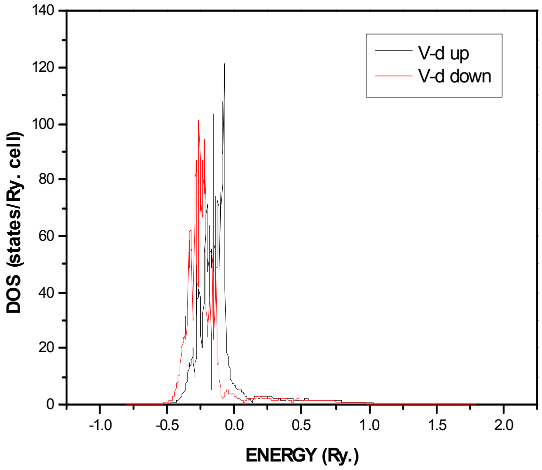

Figure.4(e).

Figure 4. Projected Density of state of spin up and spin down electrons for TiV_3 compound (a) Ti-s (b) Ti-p (c) Ti-d (d) V-s (e) V-p (f) V-d

4. Conclusions

Analyzing the electronic structure and magnetic behavior of the ordered compounds TiV_3 and TiV_3N well known due to several industrial applications. Using LMTO method, the total energies has been calculated to determine the equilibrium lattice parameters. The ferromagnetic calculations gives a null local magnetic moments for TiV_3N at V and Ti sites which implies that the stable phase is nonmagnetic. Spin polarized results at theoretical equilibrium indicates that the ground state of TiV_3 is ferromagnetic with a high moment at higher volumes (at negative pressure) verified by band structure calculation. The *l*-projected DOS to investigate the trends of chemical bonds from an itinerant point of view has been calculated. The inclusion of nitrogen in TiV_3 alloy destroys its ferromagnetic order due to vanadium atoms that populates mainly the spin down d-states giving equal occupation numbers for both spin directions has been investigated from the s, p and d projected density of states for corresponding Ti, V and N states (not shown).Since the Nitrogen strongly interacts with metal atom at face centered position,it contributes high values to bulk moduli of TiV_3N compound.

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