ORIGINALE ARTICLE

A COMPUTATIONAL STUDY ON THE MAGNETIC PROPERTIES OF VANADIUM LAYERS ON NIOBIUM SUBSTRATES: EFFECTS OF SURFACE ORIENTATION, RELAXATION, AND ELECTRONIC STRUCTURE

| Dimbimalala, Randrianasoloharisoa [1] | Andry Nirina, Randrianarisoa [1] | and | Fils, Lahatra Razafindramisa [1] |

[1.] Laboratoire de Physique de la Matière et du Rayonnement | Université d'Antananarivo | Département de Physique | Antananarivo | Madagascar |

| DOI: 10.5281/ZENODO.10029598 | | Received September 02, 2023 | | Accepted September 17, 2023 | | Published October 21, 2023 | | ID Article | Dimbimalala-Ref3-4-17ajiras171023 |

ABSTRACT

Background: The investigation of magnetism in transition metals is a pivotal aspect of studying artificial systems, particularly ultrathin metallic films. The magnetic properties of transition metals, especially vanadium, either independently or in conjunction with other transition metals, have consistently captivated researchers in this domain. **Objectives**: This study aims to explore the magnetic characteristics of vanadium on a niobium substrate using Density Functional Theory (DFT) with the DACAPO code. **Methods**: We examined systems comprising a single layer of vanadium or niobium, as well as vanadium on niobium. Our investigation encompassed the influence of layer relaxation, surface orientation, and the coupling of V/Nb. The analysis and interpretation of results were grounded in the study of atom positions and density of states for each atom. **Results**: The relaxation of layers composed solely of vanadium or niobium generally resulted in a reduction of the magnetic moments of atoms within those layers. Similarly, altering the surface orientation from (100) to (110) led to a decrease in the magnetic moment, reaching 0. This reduction is attributed to the increased proximity of atoms, facilitating the recovery of d orbitals for these atoms. In the V/Nb system, for the (100) surface orientation, relaxation also led to a moment reduction. Conversely, for the (110) orientation, each layer became antiferromagnetic after relaxation. The emergence of the antiferromagnetic moment is primarily attributed to the Body-Centered Cubic (BCC) structure of vanadium and niobium. **Conclusions**: Our findings indicate that, for the relaxed system, the magnetic moment of vanadium on the V/Nb surface is higher than that of vanadium in an isolated V system. Therefore, the practical utility of vanadium in conjunction with niobium surpasses that of vanadium alone.

Keywords: *vanadium, niobium, ab-initio calculation, DFT, relaxation, magnetic moment.*

1. INTRODUCTION

Over the past two centuries, condensed matter physics has played a pivotal role in metallurgy, chemistry, and the synthesis of artificial materials. The emergence of this modern scientific discipline has empowered researchers to manipulate and control the magnetic properties of materials at their discretion. Comprehending the magnetic characteristics of materials based on their electronic structures represents a significant challenge in both theoretical and experimental fundamental research. The evolution of microcomputers, driving exploration at the nanoscale through innovations like scanning electron microscopes, has propelled physicists into the realm of nanoscience. Concurrently, the continuous refinement of precise ab initio calculations, coupled with advancements in simulation algorithms such as density functional theory (DFT), has enabled predictions regarding the behavior of atoms in bulk materials.

The magnetism of transition metals stands as a central and compelling theme in the examination of artificial metallic systems, including ultrathin films, atomic clusters (aggregates of tightly bound atoms or molecules with distinct properties), and magnetic nanoparticles. Due to their unique characteristics, the investigation into the magnetism of transition metals, exemplified by vanadium, through numerical calculation methods continues to captivate researchers in this field. Notably, the apparent contradiction between experimental results and theoretical studies on the magnetic moment of V, in conjunction with other transition metals, serves as a driving force for our current work.

Furthermore, the underutilization of the V/Nb coupling in ab initio simulations for a monolayer of vanadium has spurred our interest. We could only identify the studies of Kim and Lee (2001) [1] and Khalifeh (1997) [2] delving into this system. Our calculations will employ DFT implemented in the DACAPO code (Danish Ab-initio Pseudo Potential Code), utilizing the pseudo-potential method with the correlation exchange function provided through the generalized gradient approximation (GGA). This choice ensures a more accurate estimation of magnetic properties compared to the local spin density approximation (LSDA). In the present study, we will delve into the theoretical foundations of ab-initio calculations for resolving many-body problems.

2. COMPUTATIONAL METHOD

All simulations presented in this study were conducted using the Dacapo package [3,4], a computational framework grounded in Density Functional Theory (DFT) employing a plane wave basis set. The ionic cores are characterized by ultrasoft pseudopotentials developed by Vanderbilt [5]. The self-consistent solution of the Kohn-Sham one-electron equations was pursued, employing the Generalized Gradient Approximation parameterized by Perdew-Wang (GGA-PW91) for the exchange-correlation part [6,7]. In our calculations, the plane wave basis set was constrained by a 350

eV energy cutoff. Brillouin zone sampling utilized a (4x4x1) k-point Monkhorst-Pack grid [8]. To aid convergence, Fermi broadening corresponding to kBT=0.1 eV was applied. Total energies were extrapolated to T=0 K.

Six systems were considered for simulation: a 7-layer slab of V(100), a 7-layer slab of Nb(100), a configuration with a 1-layer slab of V deposited on a 6-layer slab of Nb(100), a 7-layer slab of V(110), a 7-layer slab of Nb(110), and a configuration with a 1-layer slab of V deposited on a 6-layer slab of Nb(110). The slab was periodically reproduced in the perpendicular direction, with images separated by a vacuum region 10 Å thick. Only the V (respectively Nb) surface plane was allowed to relax freely, while the other layers were held in the bulk configuration. The simulations commenced with the determination of the bulk lattice constant for vanadium and niobium. Subsequently, individual analysis was carried out for systems composed of Nb(100) (respectively Nb(110)) and V(100) (respectively V(110)), permitting relaxation of each surface atom simultaneously. This was followed by calculations for the hybrid systems V/Nb, considering both orientations.

The variation of inter-layer distance in percent value was calculated from the following formula:

$$\Delta d_{ij}(in\ \%) = \frac{d_{ij}(relaxed) - d_{ij}(cc)}{d_{ij}(cc)} \times 100 \qquad \textbf{(1)}$$

With:
$\boldsymbol{d_{ij}(cc)}$ the distance of two adjacent layers in centered cubic system,
$d_{ij}(relaxed)$ the distance of two adjacent layers in relaxed system,
i and **j** are the indexes of the layers with j=i+1,
We took **i=1** the index of the top layer, the surface,
j=2 the index of the layer just below or subsurface.

3. RESULTS

3.1 Structure Analysis

The equilibrium calculated lattice parameter of niobium bulk of 3.31 Å is in good agreement with the experimental value which is 3.3 Å [9]. For vanadium bulk, we found a lattice parameter of 3.0 Å. This value is also in good agreement with the experimental value of 3.03 Å from [9].

According to Table 1, the relaxation of the Nb(100) provided a contraction of 10.30% over the distance between the surface layer and the one just below. This result is in good agreement with that obtained by Ramanathan et al. [10] of 10.11% performed with the LSDA method. Methfessel et al. [11] also confirmed this result with a contraction of 9.3% using the FP-LMTO (Full Potential Linear-Muffin Tin Orbital) method. Shein et al. [12] found a contraction of 13.1% with VASP-PAW (Plane Augmented Waves) for this same configuration. The experimental study by Fang et al. [13] by electronic photo diffraction of the Nb (001), using K_α radiation as excitation source provided a contraction of 13 ± 5% between the top layer and the subsurface.

By changing the orientation of the niobium surface plane into (110), the contraction became 4.32%. The latter is the result of the particular arrangement of the atoms for forming the (110) plane of niobium. Each atom is no longer on the same plane but only half of the atoms that make up the surface.

Table 1: Variation in % of the interatomic distances for the different niobium slabs. Minus sign indicates contraction.

System	Δ_{12}(%)
Nb (100)	-10.30
Nb (100) [10]	-10.11
Nb (100) [11]	-9.30
Nb (100) [12]	-13.10
Nb experiment [13]	-13±5

Table 2 shows the geometric optimization of the slab of V(100). The surface skilled a strong contraction of 13.18%. According to Ramanathan et al [14] the calculation with a GGA pseudo potential for the top V–V provided a contraction of 9.8% from its initial position. The FLAPW result of Bihlmayer et al. [15] is close to ours with 11.10% contraction. The LEED experience of Jensen et al. [16] gives a contraction of 7.0%.

Table 2. Variation in % of the interatomic distances for the different vanadium slabs. Minus sign indicates contraction.

System	Δ_{12}(%)
V (100)	-13.18
V (100) [14]	-9.80
V (100) [15]	-11.10
V (100) [16]	-7.00
V experiment [17]	-6.7±1.5

According to table 3 below we obtained a contraction of 5.85% between the top layer and the subsurface for the V/Nb(100) system. This value is in good agreement with that found by Ramanathan et al. [14] of 4.80%. For the V/Nb(110) system, a contraction of 5.42% has been calculated for the distance between the vanadium and the first layer of niobium with respect to its initial position.

Table 3. Variation in % of the interatomic distances for the different V/Nb slabs. Minus sign indicates contraction.

System	Δ_{12}(%)
V/Nb (100)	-5.85
V/Nb (100) [14]	-4.80
V/Nb (110)	-5.42

3.2 Magnetic Analysis

3.2.1. The Vanadium system

3.2.1.1. The Position Effect: We have obtained the magnetic moments of atoms at the surface and at the subsurface in a non-relaxed vanadium slab (100) as shown in Table 4. The surface of V alone presents a very significant ferromagnetic moment of 3.24 μ_B per atom. We have a result in good agreement compared with the calculation made by Ramanathan et al. [18] of 3.40 μ_B for the vanadium on the surface (100). The sub surface of V has a magnetic moment induced of - 2.22 μ_B per atom. Its absolute value has decreased relative to the outer surface.

Table 4: Magnetic Moment per Atom in Surface of Non-Relaxed V(100).

Position	Moment(μ_B)
Surface	3.24
Sub-surface	-2.22

In Figure 1(a), the local densities of states (LDOS) for a vanadium atom are depicted, comparing its surface (dotted line) and subsurface (solid line) configurations. Transitioning from the surface to the subsurface results in a reduction of peaks near the Fermi level, leading to a slightly more dispersed density of states. This broadening primarily arises from the contribution of spin-down states, as illustrated in Figure 1(b). Figure 1(b) illustrates that for the surface atom, spin-up states dominate, resulting in a positive momentum. Conversely, for the subsurface atom, spin-down states prevail, although the disparity between spin-up and spin-down states is less pronounced. Consequently, the subsurface atom exhibits a negative momentum, with an intensity lower than that of the surface atom.

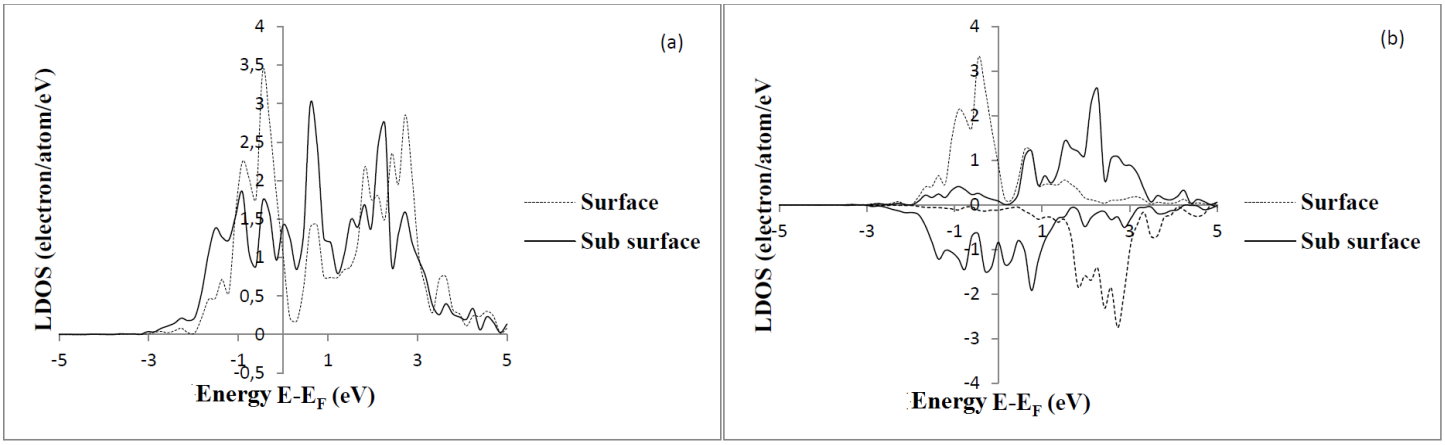

Figure 1: The figure presents the local density of state (ldos) of d-band of vanadium in surface (dotted line) and subsurface (solid line). (a) total ldos, (b) ldos with spin up and spin down.

The magnetic moment holds significance at the surface, diminishing and altering its sign upon transitioning to the subsurface. This change is attributed to the altered atomic environment in the subsurface, where the atom becomes surrounded by neighboring atoms. In this subsurface context, the redistribution of spin-up and spin-down states occurs through the overlapping of d orbitals with adjacent atoms, allowing the atom to rebalance its density distribution.

3.2.1.2. The Relaxation Effect

Upon examination of Table 5, the impact of relaxation on the V(100) system becomes evident. Our calculations reveal a magnetic moment of 3.24 μB for the non-relaxed surface of V, contrasting with 0.91 μB for the relaxed surface. A similar reduction is observed in the subsurface of vanadium. Specifically, a magnetic moment of -2.22 μB is evident for the non-relaxed subsurface, while only -0.21 μB is observed for the relaxed subsurface.

Table 5: Effect of Relaxation in the Magnetic Moment (in μ_B)per Atom of the V(100) System

Position	Non-relaxed	Relaxed
Surface	3.24	0.91
Sub-surface	-2.22	-0.21

The reduction in momentum is corroborated by Figure 2(b), illustrating a decline in spin-up density peaks and a concurrent rise in spin-down density, resulting in a diminished difference between the densities of spin up and down states, and consequently, a decrease in magnetic moment. Figure 2(a) reveals a broadening of 1eV extending toward the negative energies of the d-band.

The primary impact of relaxation is the attenuation of the magnetic moment. Following relaxation, atomic distances contract, enabling electrons to redistribute their distribution through the overlap of d-orbitals. This mechanism facilitates the rebalancing of electron distribution among the atoms, contributing to the observed decrease in magnetic moment.

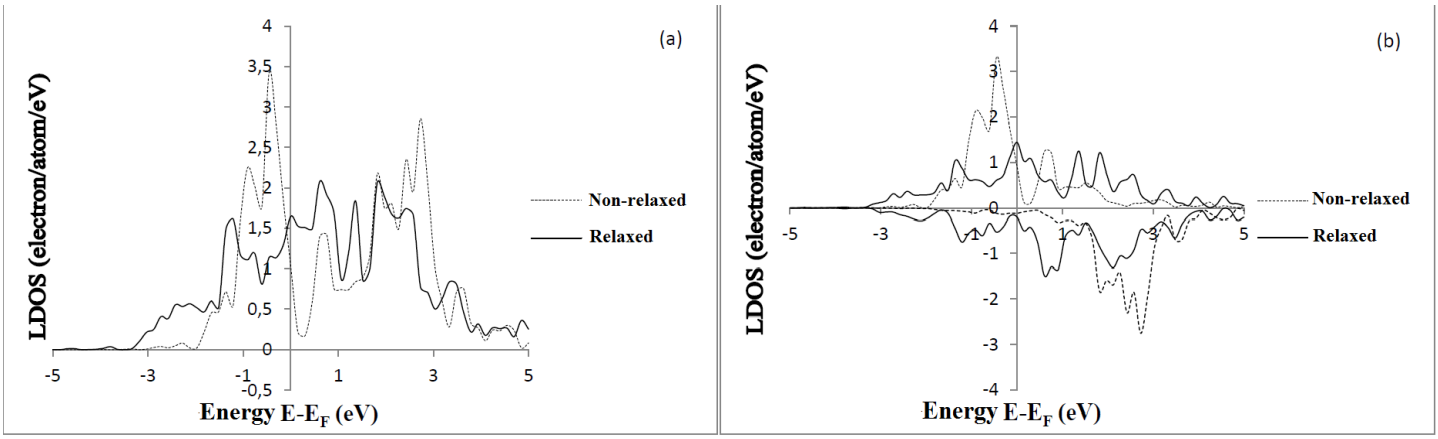

Figure 2: The figure presents the local density of state (ldos) of d-band of vanadium in non-relaxed surface (dotted line) and relaxed surface (solid line). (a) total ldos, (b) ldos with spin up and spin down.

3.2.1.3. The Orientation Effect

Table 6 indicates that altering the surface orientation from (100) to (110) results in a reduction or complete cancellation of the magnetic moment. Figure 3 illustrates an expansion of the d-band and a realignment in the distribution of spin-up and spin-down densities when transitioning from the (100) to (110) orientation.

Table 6. Effect of orientation in the Magnetic Moment (in μ_B)per Atom of the V(100) System

Orientation	Non-relaxed	Relaxed
100	3.24	0.91
110	0	0

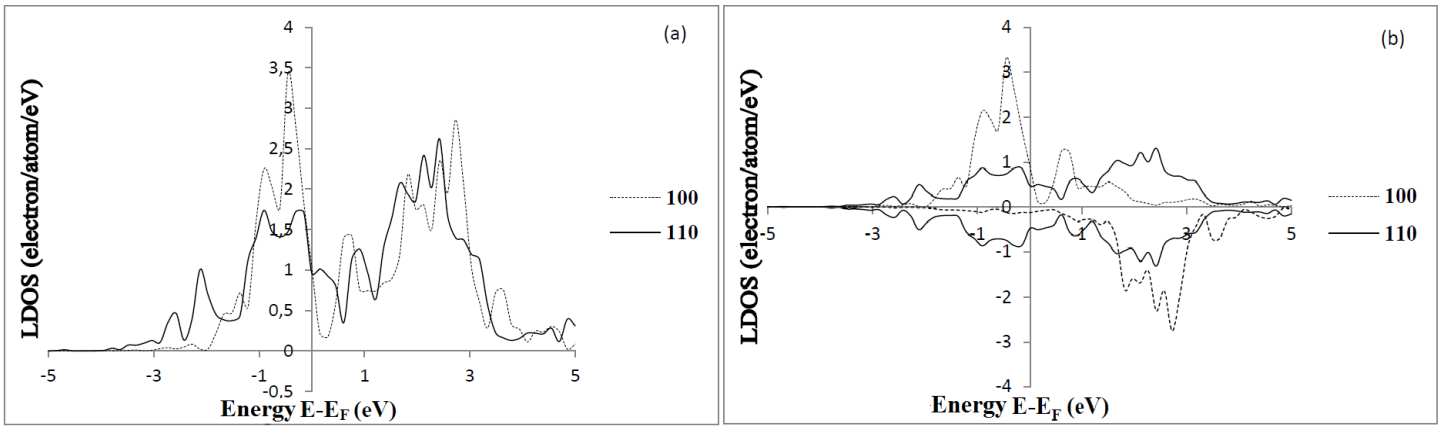

Figure 3: The figure presents the local density of state (ldos) of d-band of vanadium in 100 surface (dotted line) and 110 surface (solid line) of non-relaxed surface. (a) total ldos, (b) ldos with spin up and spin down.

On the other hand, in figure 4 where the surfaces are relaxed, the densities of states have almost the same shape for the two orientations. Orientation effects are screened by relaxation effects.

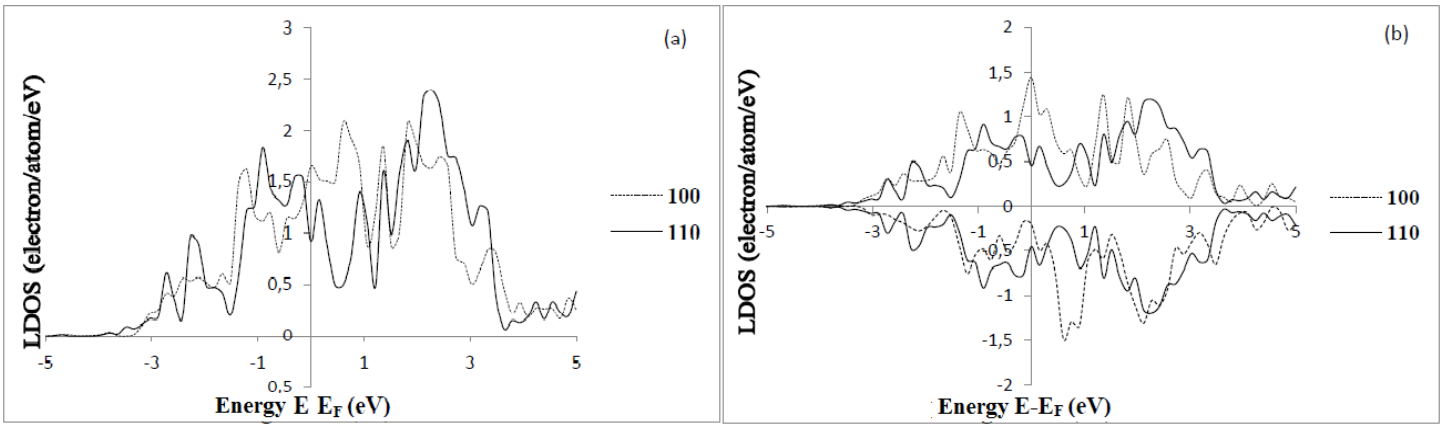

Figure 4: The figure presents the local density of state (ldos) of d-band of vanadium in 100 surface (dotted line) and 110 surface (solid line) of relaxed surface. (a) total ldos, (b) ldos with spin up and spin down.

Altering the orientation from (100) to (110) typically results in a decrease in the magnetic moment. Specifically, in the (110) orientation, the distance between closely neighboring atoms within the same plane is smaller compared to that in the (100) orientation. This distance measures 2.60 Å for V(110) as opposed to 3 Å for V(100). The reduced interatomic distance in V(110) allows for a more facile overlap of d-orbitals among surface atoms, facilitating the rebalancing of electron spin distributions and consequently leading to a reduction in magnetic moment

3.2.2. The V/Nb system

3.2.2.1. Relaxation Effect: According to table 7, as for the results we have obtained so far, the relaxation has the effect of decreasing the moment of V at the surface for the orientation 100. On the other hand for the orientation 110, the vanadium surface ferromagnetic deposited on niobium becomes antiferromagnetic when allowed to relax.

Table 7. Magnetic Moment (μ_B) per Atom in Surface of Vanadium Deposited on Niobium

Orientation	Non-relaxed	Relaxed
100	2.47	1.85
110	1.67	+1.32/-1.32

Figure 5 shows that for orientation 100, the relaxation does not change the shape of the ldos much, but we observed a small increase in the spin down population, which causes the magnetic moment to decrease.

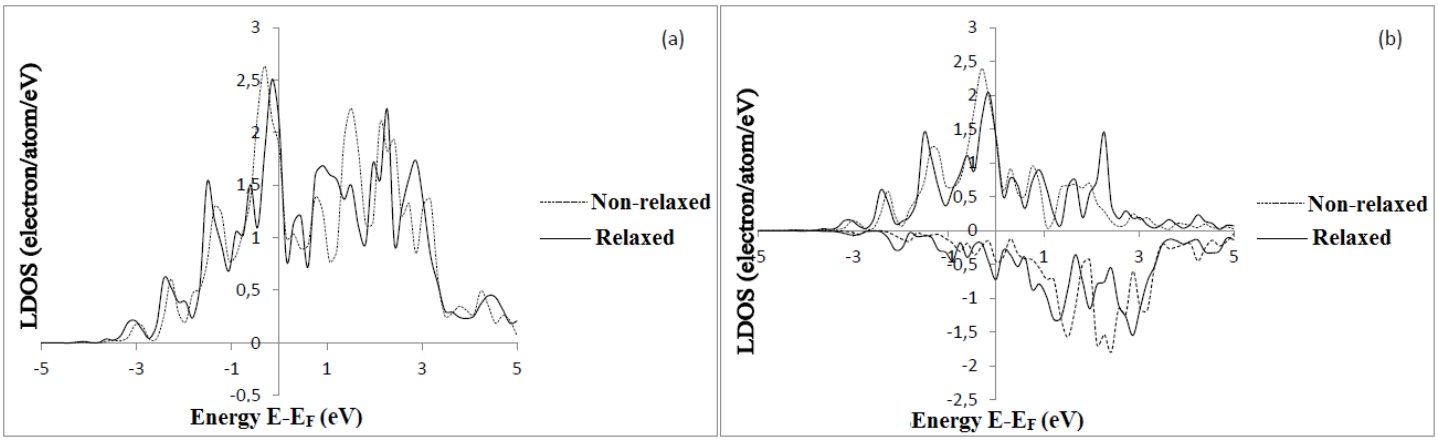

Figure 5: The figure presents the local density of state (ldos) of d-band of vanadium on niobium 100 in non-relaxed surface (dotted line) and relaxed surface (solid line). (a) total ldos, (b) ldos with spin up and spin down.

Figure 6(a) reveals that post-relaxation, the overall structure of the local density of states (LDOS) for V(110) undergoes only a minor modification, particularly in the vicinity of the Fermi level. Conversely, an examination of the spin-up and spin-down density distributions in Figure 6(b) shows a reversal of this distribution. Spin-up, which was the majority density prior to relaxation, transitions to a minority density post-relaxation. This inversion is observed for half of the vanadium atoms, resulting in a shift from a positive to a negative magnetic moment.

For the other half, not explicitly shown in the figures, there is no inversion in the distribution, but rather a change in the shape of the spin-up and spin-down LDOS. This alteration contributes to a reduction in the magnetic moment, although it remains positive.

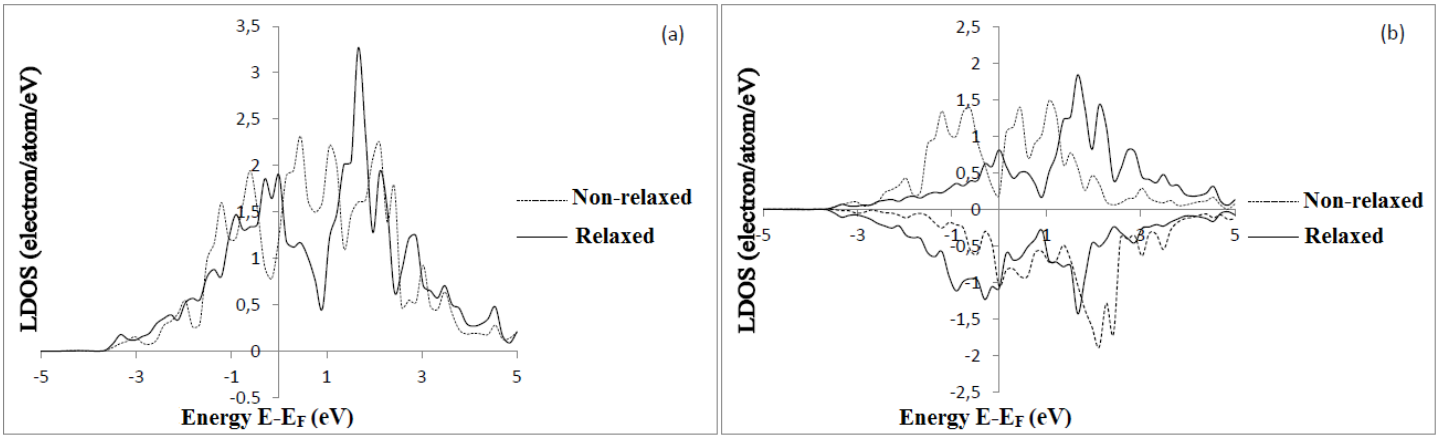

Figure 6: The figure presents the local density of state (ldos) of d-band of vanadium on niobium 110 in non-relaxed surface (dotted line) and relaxed surface (solid line). (a) total ldos, (b) ldos with spin up and spin down.

3.2.2.2. Orientation Effect: The change of orientation from 100 to 110 leads to a decrease in the magnetic moment of vanadium for a non-relaxed system (table 7). The ldos in Figure 7(b) shows that below the Fermi level, the density of states for spin down did not vary much by changing orientation while the density of states for spin up decreased when going from orientation 100 to orientation 110.

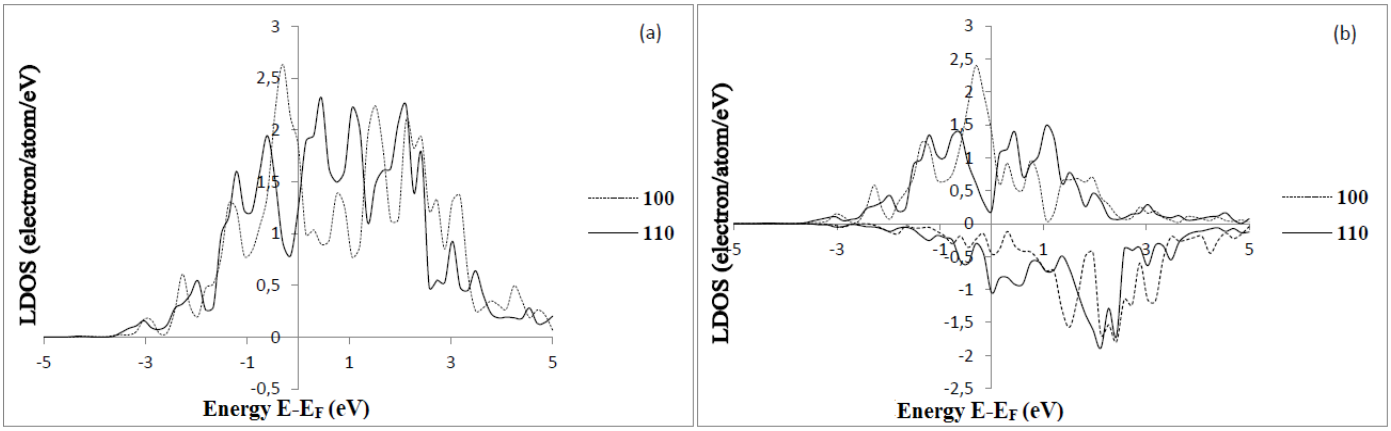

Figure 7: The figure presents the local density of state (ldos) of d-band of vanadium in V/Nb non relaxed system in 100 surface (dotted line) and 110 surface (solid line). (a) total ldos, (b) ldos with spin up and spin down.

When the layers are relaxed, the ferromagnetic layers with the 100 orientation become antiferromagnetic with the 110 orientation (table 7). Figure 8(b) shows that the up and down spin densities are reversed. The majority spins up with the 100 orientation become a minority when moving to the 110 orientation.

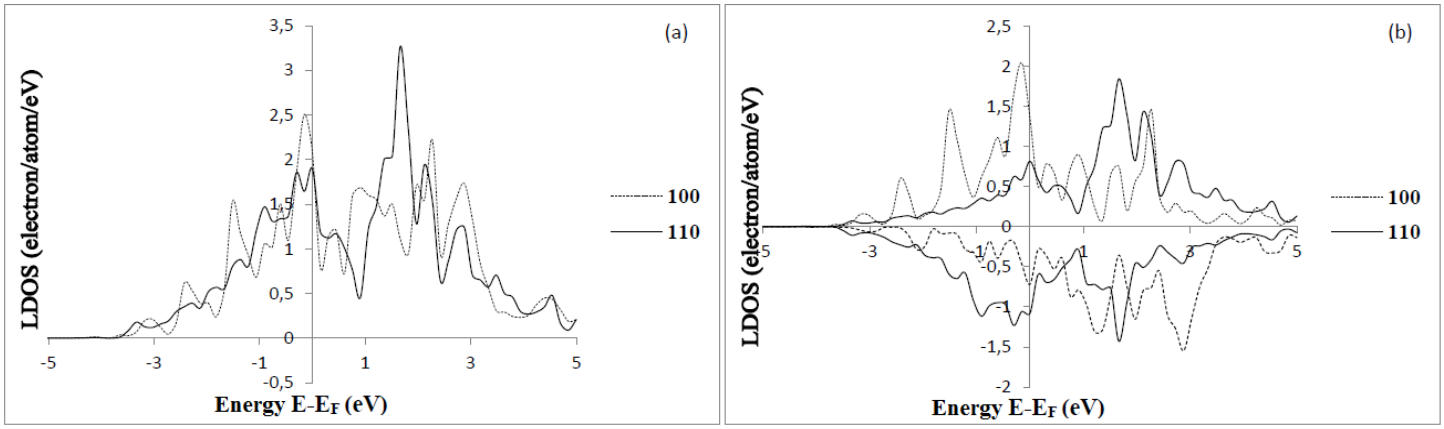

Figure 8: The figure presents the local density of state (ldos) of d-band of vanadium in V/Nb relaxed system in 100 surface (dotted line) and 110 surface (solid line). (a) total ldos, (b) ldos with spin up and spin down.

In general, relaxation tends to decrease the magnetic moment of the surface layer for the (100) orientation. For the (110) orientation, relaxation induces the surface layer to transition into an antiferromagnetic state. This oscillating relaxation mode is a characteristic feature observed in low Miller index transition metal surfaces.

The Centered Cubic (CC) structure significantly influences these results. In a CC structure, atoms at the summits of the cube exhibit a moment opposite to that at the center of the cube. Consequently, for the (100) orientation, the surface atoms, corresponding to the summits of the CC cell cube, possess a positive moment, while the sub-surface layer atoms, corresponding to the center of the CC cell cube, exhibit a negative moment.

For the (110) orientation, the atoms within a layer originate simultaneously from the summits and the center of the CC cell cube, resulting in each layer having atoms with opposite moments, rendering it antiferromagnetic. However, this transition to the antiferromagnetic state of each layer is contingent upon relaxation. The antiferromagnetic state becomes apparent only after relaxation. In this condition, the reduced distances between atoms intensify interactions, facilitating the emergence of the antiferromagnetic state.

3.2.2.3. Coupling V/Nb Effect

Table 8. Magnetic Moment (μ_B) per Atom in Surface of V(100) system and V/Nb(100) system

Orientation	Non-relaxed	Relaxed
V(100)	3.24	0.91
V/Nb(100)	2.47	1.85

For orientation 100, changing the substrate from vanadium to niobium has the effect of decreasing the moment of the vanadium surface deposited on the substrate when the system is not relaxed. On the other hand, when we relaxed the system, the moment of the vanadium surface increases when the substrate is changed from vanadium to niobium as shown in table 8.

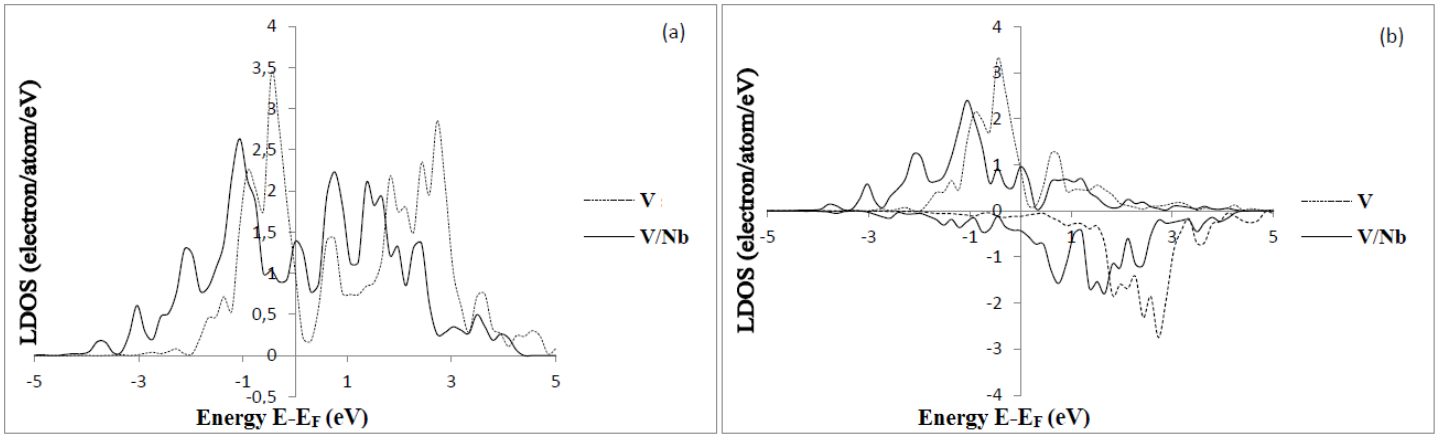

Figure 9: The figure presents the local density of state (ldos) of d-band of vanadium in V(100) non relaxed system (dotted line) and V/Nb(100) non relaxed system (solid line). (a) total ldos, (b) ldos with spin up and spin down.

The analysis of the local density of states (LDOS) reveals that in non-relaxed systems, transitioning the substrate from V to Nb results in an expansion of the d-band width, particularly influenced by the density of spin-up states (Figure 9(a)). Simultaneously, there is an increase in spin-down density (Figure 9(b)). This combined effect of increased bandwidth and spin-down density contributes to a reduction in the magnetic moment of the vanadium at the surface.

In contrast, for relaxed systems, changing the substrate to Nb does not lead to an increase in the width of the d-band (Figure 10(a)). However, there is an elevation in spin-up density accompanied by a decrease in spin-down density, resulting in an overall increase in the magnetic moment of vanadium.

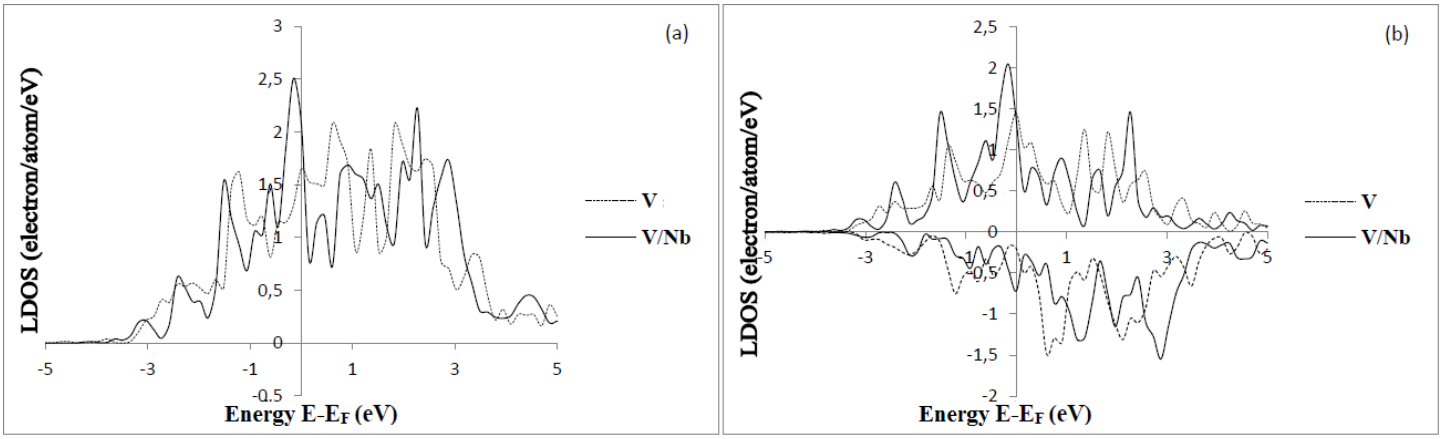

Figure 10: The figure presents the local density of state (ldos) of d-band of vanadium in V(100) relaxed system (dotted line) and V/Nb(100) relaxed system (solid line). (a) total ldos, (b) ldos with spin up and spin down.

For orientation 110, the system formed by V alone has zero magnetic moment. On the other hand, the V at the surface acquires a moment when the substrate has been changed to Nb. If the system is not relaxed, the surface of V is ferromagnetic and if left relaxed, the surface of V becomes antiferromagnetic as shown in table 9.

Table 9. Magnetic Moment (μ_B) per Atom in Surface of V(110) system and V/Nb(110) system

Orientation	Non-relaxed	Relaxed
V(110)	0	0
V/Nb(110)	1.67	1.32/-1.32

Altering the substrate to Nb does not induce a change in the width of the d-band; however, it does result in a modification of the distribution of spin-up and spin-down densities. In the non-relaxed system, the spin-up density increases while the spin-down density decreases for each surface atom of V (Figure 11(b)). In the relaxed system, a more intricate pattern emerges, where the spin-up density decreases and the spin-down density increases for some atoms within a shell (Figure 12(b)). Conversely, for other atoms in the same shell, there is an increase in spin-up density accompanied by a decrease in spin-down density.

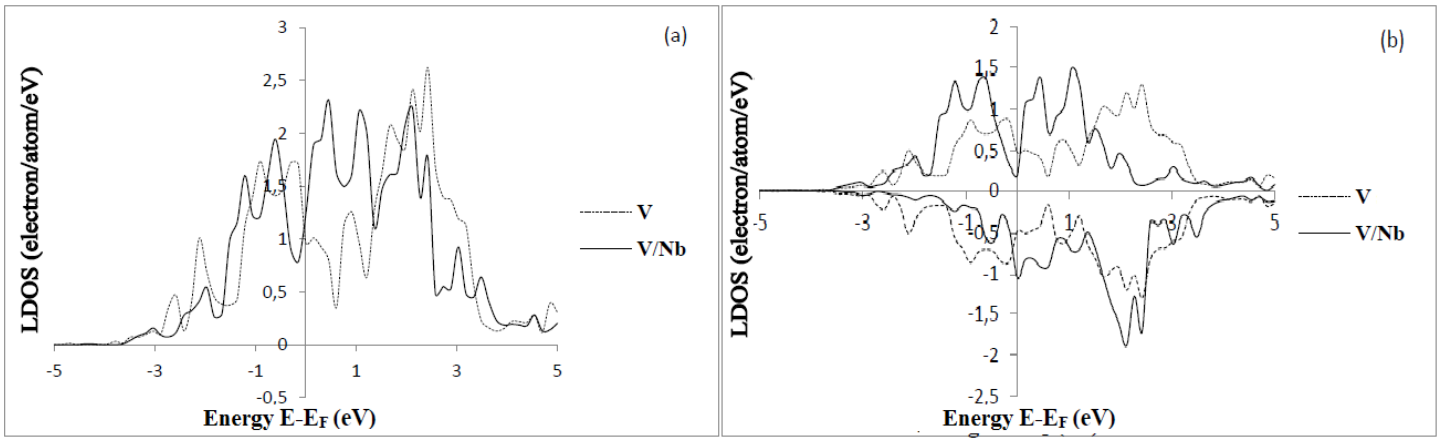

Figure 11: The figure presents the local density of state (ldos) of d-band of vanadium in V(110) non relaxed system (dotted line) and V/Nb(110) non relaxed system (solid line). (a) total ldos, (b) ldos with spin up and spin down.

In the 110 orientation, when the layers are not relaxed, the V/Nb coupling induces the emergence of magnetic moments for both V and Nb. Notably, these moments exhibit opposite signs. Conversely, upon relaxing the layers, the observation reveals the formation of antiferromagnetic layers. These findings can be rationalized by considering the magnetic properties inherent in CC meshes, akin to the patterns observed in previous cases.

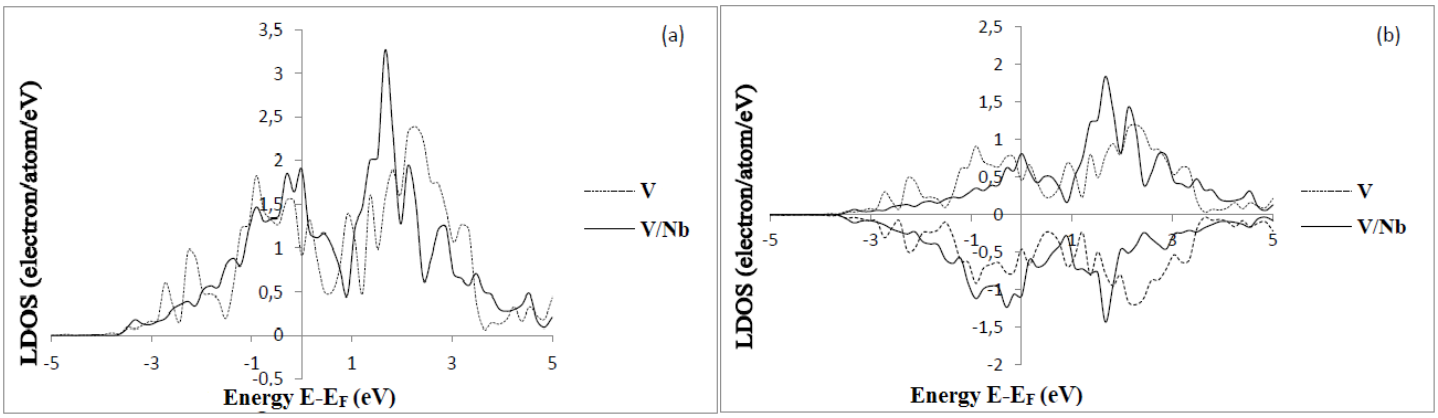

Figure 12: The figure presents the local density of state (ldos) of d-band of vanadium in V(110) relaxed system (dotted line) and V/Nb(110) relaxed system (solid line). (a) total ldos, (b) ldos with spin up and spin down.

In the non-relaxed 100 orientation, the coupling of V/Nb leads to a reduction in the absolute value of the magnetic moment for both V and Nb. Conversely, when the V/Nb system undergoes relaxation, the magnetic moments of both V and Nb increase compared to the values observed for V alone or Nb alone. The crucial factor influencing this behavior is the atomic radius. Given that the atomic radius of V is smaller than that of Nb, the relaxation of V atoms on Nb results in a less compact V layer compared to a system comprising V alone. In this scenario, the magnetic moment of V in the

V/Nb system increases in comparison to the moment of V in the system with V alone. Additionally, it is noted that the magnetic moment of Nb is primarily induced by the moment generated by V.

4. CONCLUSION

The investigation of Vanadium magnetism oriented along the (100) and (110) directions, coupled with the transition metal niobium, was conducted using density functional theory in this thesis. Calculations were performed utilizing the DACAPO code, facilitating structural analysis through layer relaxation, magnetic moment calculations, and the study of local density of states (LDOS) for the surfaces.

The supercell technique, involving the representation of surfaces by associating a metal plane with an empty space, was employed to model the studied surfaces. This approach maintains symmetry throughout space, satisfying the periodicity condition stipulated by Bloch's theorem.

Geometric optimization yielded results consistent with the literature, revealing an oscillating relaxation mode for the V and Nb slabs in both orientations studied. Subsequent to the structural analysis, magnetic moments of the layers were computed with and without supercell relaxation. It was observed that the magnetic moment per atom of the single element closely approximates that of the isolated atom reported in the literature, but undergoes a rapid reduction post-surface optimization. Significant ferromagnetic moments were identified for the V (100) and V (110) layers, aligning well with results obtained using alternative methods. Relaxation effects decreased magnetic moments by 25% for the (100) orientation and 20% for the (110) orientation for V or Nb alone at the surface. Conversely, an increase in the magnetic moment was noted for the V (100) surface and V in the V/Nb system compared to the surface of V alone, highlighting the impact of realistic surface relaxation. The investigation of local density of states (LDOS) confirmed the magnetic properties of the layers. Systems composed of V and Nb with antisymmetric LDOS exhibit hybridized d-bands, giving rise to significant magnetic moments on the external surface. Slabs with symmetric spins do not manifest macroscopic magnetic properties due to orbital charge cancellation. Supercell geometry optimization attenuates the amplitude of LDOS curves for different layers, consequently reducing the magnetic moment depending on the considered orientation.

The CC structure emerges as a critical factor in LDOS analysis, as surface properties are influenced by the positions of atoms forming the layers. This study affirms that V on the Nb substrate exhibits a magnetic moment irrespective of the orientation considered. Addressing this intrinsic magnetic property of vanadium helps reconcile discrepancies with results obtained through other methods, such as experimental analyses using LEED or TB.

5. REFERENCES

1. Kim I.G., Lee J.I. A precise first-principles study on the non-existence of ferromagnetism in V monolayer on the Nb(001) surface. *Current Applied Physics*. 2001; 1(2-3):183-185.
2. Khalifeh J.M. Magnetic structure of vanadium overlayers on semi-infinite Nb substrate. *Journal of Magnetism and Magnetic Materials*. 1997; 168(1-2):25-30.
3. Hammer B., Hansen L.B., Nørskov J.K. Improved adsorption energetics within density-functional theory using revised Perdew-Burke-Ernzerhof functionals. *Physical Review B*. 1999; 59 (11): 7413-7421.
4. Ab initio pseudopotential code Dacapo (version 2.7.3, 2003), developed at CAMPOS (Center for Atomic-Scale Materials Physics, Department of Physics, Technical University of Denmark, Lyngby; see http://www.fysik.dtu.dk for details).
5. Vanderbilt D. Soft self-consistent pseudopotentials in a generalized eigenvalue formalism. *Physical Review B*. 1990; 41 (11): 7892-7895.
6. Perdew J.P., Wang Y. Accurate and simple analytic representation of the electron-gas correlation energy. *Physical Review B*. 1992; 45 (23): 13244-13249.
7. Perdew J.P., Chevary J.A., Vosko S.H., Jackson K.A., Perderson M.R., Singh D.J., Fiolhais C. *Physical Review B*. 1992; 46 (11): 6671-6687.
8. Monkhorst H.J., Pack J.D. Special points for Brillouin-zone integrations. *Physical Review B*. 1976; 13 (12): 5188-5192.
9. Kittel C. Introduction to Solid State Physics. 7th ed., vol. 23. New York: Wiley; 1996.
10. Ramanathan A.A., Khalifeh J.M., Hamad B.A. A DFT study of substrate effect on the magnetism of V(001) surface. *Surface Science*. 2011; 605(11-12): 1074-1076.
11. Methfessel M., Hennig D., Scheffler M. Trends of the surface relaxations, surface energies, and work functions of the 4d transition metals. *Physical Review B*. 1992; 46 (8): 4816-4829.
12. Shein K.I, Shein I.R., Medvedeva N.I., Shalaeva E.V., Kuznetsov M.V., Ivanovskii A.L. Effects of Atomic Relaxation and the Electronic Structure of Niobium (100) and (110) Surfaces. *The Physics of Metals and Metallography*. 2006; 102(6): 604-610.
13. Lo W.S., Chien T.S., Fang B.S., Wei C.M., Mei W.N. Photoelectron-diffraction studies of Nb(001). *Surface Review and Letters*. 1998; 5(5): 1035-1041.
14. Ramanathan A.A., Khalifeh J.M., Hamad B.A. Structure and magnetism of the V/Ta(0 0 1) surface: A DFT calculation. *Journal of Magnetism and Magnetic Materials*. 2009; 321(22): 3804-3807.
15. Bihlmayer G., Asada T., Blügel S. Electronic and magnetic structure of the (001) surfaces of V, Cr, and V/Cr. *Physical Review B*. 2000; 62 (18): R11937-R11940.
16. Jensen V., Andersen J.N., Nielsen H.B., Adams D.L. The surface structure of V(100). *Surface Science*. 1982; 116(1): 66-84.
17. Bartynski R.A., Heskett D., Garrison K., Watson G.M., Zehner D.M., Mei W.N., Tong S.Y., Pan X. Photoelectron diffraction determination of the geometry of a clean metal surface: Ta(100). *Physical Review B*. 1989; 40 (8): 5340- 5343.

18. Ramanathan A.A., Khalifeh J.M., Hamad B.A. Evidence of surface magnetism in the V/Nb(0 0 1) system: A total energy pseudopotential calculation. *Surface Science*. 2008; 602(2):607–613.

How to cite this article: Dimbimalala Randrianasoloharisoa, Andry Nirina Randrianarisoa, and Fils Lahatra Razafindramisa. A COMPUTATIONAL STUDY ON THE MAGNETIC PROPERTIES OF VANADIUM LAYERS ON NIOBIUM SUBSTRATES: EFFECTS OF SURFACE ORIENTATION, RELAXATION, AND ELECTRONIC STRUCTURE. *Am. J. innov. res. appl. sci. 2023;17(4): 266*-276. DOI: 10.5281/zenodo.10029598