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Study of the Physical, Mechanical, Thermodynamic and Electronic Properties in volume of TiN

Alain second DZABANA HONGUELET[1,2,4*], Abel Dominique EBOUNGABEKA[1,2,] and Timothee NSONGO[1,2,3]
[1]Faculty of Science and Technology, Marien Ngouabi University, Congo Brazzaville
[2]Groupe de Recherche sur les Propriétés Physiques et Chimiques des Matériaux, Congo Brazzaville
[3]Center for Geological and Mining Research, Congo Brazzaville
[4]Association Alpha Sciences Beta Technologies, Congo Brazzaville
second_alain@yahoo.fr

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Abstract

In this study, we investigated the mechanical and electronic properties of cubic-phase titanium nitride (TiN) using Density Functional Theory (DFT) with the Generalized Gradient Approximation (GGA). The geometric optimization results reveal that the lattice parameter a is 3.003738 Å and the volume V is 56.440305 Å³. The calculated elastic constants, C11 = 602.57615 GPa and C12 = 115.48060 GPa, confirm the stability of the cubic phase of TiN. The compressibility modulus B is 277.84578 GPa, and Young's modulus E is 469.62823 GPa, indicating significant mechanical rigidity. The Debye temperature is 558.56408 K, reflecting strong lattice vibrations and high thermal stability. Additionally, our analysis shows that cubic TiN exhibits anisotropy in the transverse propagation mode, particularly in the [100] and [110] directions. The electronic structure reveals a band gap of 0.642 eV, characteristic of a semiconductor. These results underscore TiN's mechanical robustness, thermal stability, and semiconducting nature.

Keywords: Band structure, density of states, elastic constants, titanium nitride, DFT, elastic moduli, elastic constants, electronic structure, temperature of debye.

Introduction

Titanium, a metal of considerable significance, is extensively used across various industries, including aeronautics and medicine[1]. Discovered in 1791 by British mineralogist William Gregor, who isolated it from ilmenite sand found in Cornwall's Helford River, titanium is renowned for its remarkable purity and strength despite its relative abundance in the Earth's crust[2]. Ranking 4th in abundance among metals, titanium's use is characterized by its high technology demands, purity, rarity, and exceptional strength.

The interest in titanium has notably expanded, particularly in the realm of titanium nitride (TiN)[3]. Research conducted by Professor Timothée NSONGO from Marien NGOUABI University has explored titanium thin films, emphasizing their importance in various industrial applications[4]. This includes investigations into the structural and adhesive properties of titanium thin films, as well as related work by Stéphane GROSSO on Ti architectural[5] coatings and experimental study on titanium alloys[6].

The research group at Marien NGOUABI University has recently undertaken a series of studies to delve into the mechanical properties of TiN for diverse applications. Abel EBOUNGABEKA, under the guidance of Professor NSONGO, has focused on TiN dental implants, aiming to understand and enhance their performance[7]. In addition, MIMBOUI Yhan has utilized LAMMPS with the Modified Embedded Atom Method in simulations directed by Dr. Alain DZABANA to investigate TiN's properties[8].

Our current objective is to conduct a Density Functional Theory (DFT) study to analyze the electronic properties of TiN. This study aims to build on existing research to elucidate the electronic structure of TiN and understand the origins of its mechanical properties, contributing to a more comprehensive understanding of this important material.

Methodology

This study employs Density Functional Theory (DFT) with Generalized Gradient Approximation (GGA) to model the mechanical and electronic properties of cubic titanium nitride (TiN)[9]. Leveraging the success of DFT in similar material simulations, this approach provides a robust framework for both geometric optimization and the evaluation of elastic constants[10]. Calculations are performed with a plane wave cutoff energy of 500 eV to ensure precise modeling of atomic interactions[11].

The simulation was conducted on a Windows 10 64-bit operating system using an Intel processor. A preliminary study established the optimal cutoff energy and k-point sampling, setting the plane wave cutoff energy at 500 eV and k-points at 1×1×1 in the Brillouin zone. The self-consistent convergence method was used for optimizing the cubic TiN structure.

For geometric optimization, the Perdew-Burke-Ernzerhof (PBE) pseudo potential was employed to calculate crystalline parameters, while the Perdew-Burke-Ernzerhof for solids (PBEsol) pseudo potential was used for evaluating elastic constants. This methodological setup ensures accurate and detailed insights into the mechanical and electronic properties of TiN.

Results and Discussion

In this work, we present a comprehensive analysis of cubic TiN, covering crystalline parameters, mechanical properties, and electronic properties obtained through Density Functional Theory (DFT). We detail the lattice parameter and volume, which align well with experimental data, validating the DFT calculations.

The mechanical properties are examined through elastic constants, modulus of elasticity, and compressibility, demonstrating TiN's significant mechanical stability and resistance to deformation and compression. Additionally, the electronic properties are explored using Density of States (DOS) and Partial Density of States (PDOS) analyses, providing insight into the material's electronic structure and behavior. Thermodynamic properties are also assessed, offering a deeper understanding of TiN's performance under various thermal conditions. This comprehensive study underscores TiN's robustness and its suitability for high-performance applications, supported by accurate DFT results.

Choice of Cutoff energy: The cutoff energy is a crucial parameter in Density Functional Theory (DFT) calculations using plane waves. It defines the upper limit of the kinetic energy of plane waves included in the expansion of the electronic wave functions. Essentially, it sets the maximum energy of the plane waves considered in the calculations of a material's electronic structure.

In DFT simulations, the choice of cutoff energy directly affects both the accuracy and computational cost of the calculations. A higher cutoff energy allows for a more precise description of electronic interactions by including higher-energy wave functions, which can improve the accuracy of the results. However, this also increases the computational demand, making simulations more resource-intensive.

Therefore, it is essential to select an appropriate cutoff energy to achieve accurate results while maintaining reasonable computational efficiency. Typically, convergence tests are performed to determine the optimal cutoff energy by checking that calculated properties (such as lattice parameters, elastic constants, or total energies) stabilize when the cutoff energy is increased.

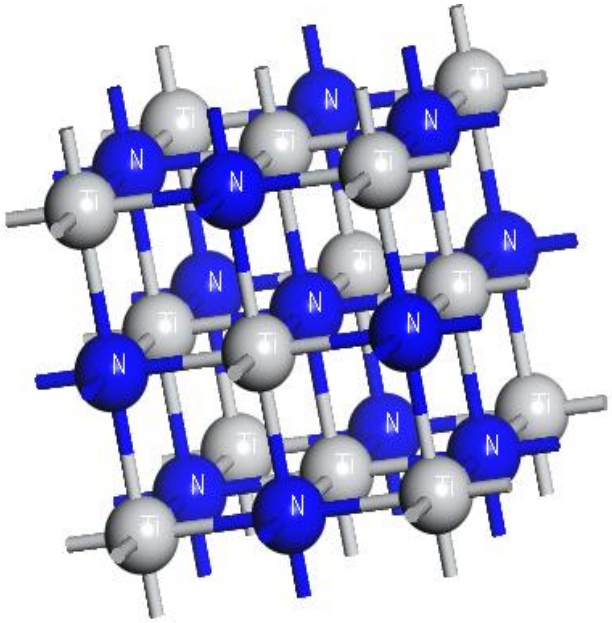

Figure-1: Titanium nitride.

The graph provided illustrates the evolution of energy as a function of k-points in the Brillouin zone, with calculations conducted using a plane-wave cutoff energy Ecut = 550 eV and a k-point mesh of 7*7*7 The data indicates that, at this cutoff energy and k-point range, the computed energy values have stabilized, showing that further increases in Ecut or adjustments in the k-point mesh do not significantly alter the results.

This stability suggests that the chosen parameters are sufficient to accurately capture the electronic structure of the material. The graph effectively demonstrates the convergence of the calculation with respect to the k-point sampling and cutoff energy, confirming the reliability of the results obtained.

Crystalline parameters: The Table-1 presents the crystallographic parameters for the cubic phase of TiN trioxide calculated using Density Functional Theory (DFT). The results obtained for the lattice constants a = b = c are in close agreement with theoretical values, exhibiting a margin of error of approximately 2%. This small deviation indicates that the DFT calculations are highly accurate and reliable for predicting the structural properties of cubic TiN. The consistency with theoretical expectations confirms the effectiveness of the computational approach in modeling the crystalline structure of this material.

Table-1: Cristalline Parameters.

Parameters	Our study
a=b=c in A	3,003738
$\alpha=\beta=\gamma$	60.00
Volume A^3	56.440305
$d_{Ti)N}$ in A	1,98

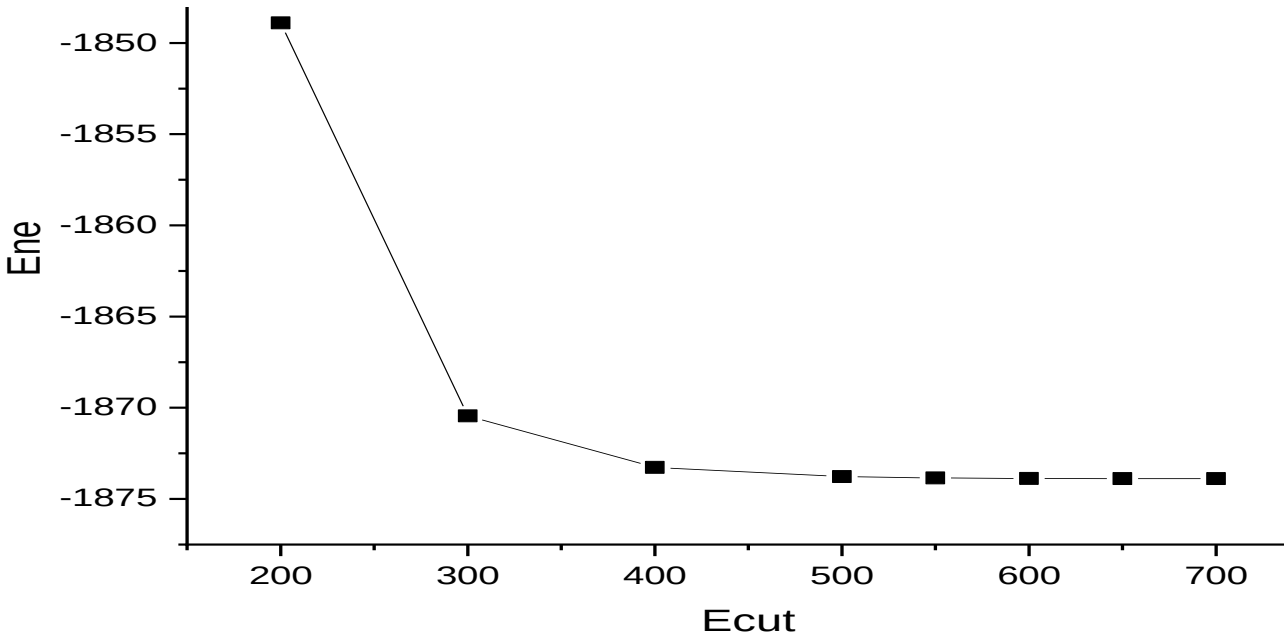

Figure-2: Cutoff Energy.

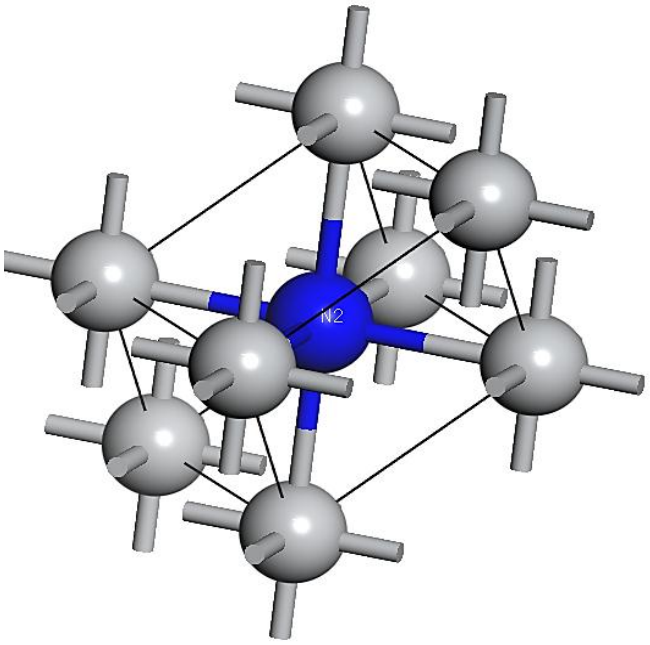

Figure-3: TiN elementary cell.

Mechanical properties: Mechanical properties are expressed in terms of elastic constants and functional elastic moduli. Mechanical properties are essential parameters for predicting the elastic properties and mechanical stability of materials.

The mechanical properties of the cubic structure of TiN have been calculated and compared with experimental results. We have shown that TiN is quite stable, this stability being verified by the condition given by the elastic constants C_{12} -C_{22}>0.

Elastic constants: The elastic and mechanical properties of solids reflect their reactions to certain external factors. In the simplest case, such factors are mechanical actions: compression, traction, bending, impact, torsion. In addition to mechanical actions, they can also be thermal, magnetic, etc. These properties are determined, first and foremost, by the bonding forces between the atoms or molecules that make up a solid.

When subjected to a stress, a crystal deforms linearly with respect to this stress, provided the deformation generated is small. When the stress is removed, the material reversibly returns to its standard state. This behavior is observed in all materials and is referred to as "elastic".

In order to understand mechanical stability, we have studied the elastic constants at ambient pressure of cubic phase TiN. The cubic system is characterized by three independent elastic moduli: *C11*, *C12* and *C44*.

For elements with a cubic structure, the criterion for predicting structural stability is as follows:

$C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$

However, the matrix linking deformations and elastic constants is represented by the following relationship:

$$\begin{pmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \sigma_4\\ \sigma_5\\ \sigma_6\end{pmatrix} = \begin{pmatrix}C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16}\\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26}\\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36}\\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46}\\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56}\\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66}\end{pmatrix}\begin{pmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \varepsilon_4\\ \varepsilon_5\\ \varepsilon_6\end{pmatrix}$$

The constant C_{11} is a measure of the resistance to deformation produced by a stress applied to the (100), (010) and (001) planes along the <100> directions (length elasticity).

C_{44} represents the measure of resistance to deformation in the case of shear stress applied to the (100), (010) and (001) planes along the diagonals (shape elasticity).

C_{12} has no simple physical interpretation, but these linear combinations with C_{11} give us the compression modulus *B* and shear modulus *G*.

The elastic constants for the cubic structure of TiN have been calculated and are presented in the Table-2:

Table-2: Elastic constants - comparison with theory and experiment.

Symbols	Our work (Gpa)	Theoretical (Gpa)
C11	602.57615	625
C12	115.48060	165
C44	158.86885	163
C11-C12	487.09555	460

Elastic modules: In this section, we present the corresponding elastic moduli in various Reuss, Hill and Voigt systems.

These moduli reflect the material's rigidity and flexibility against external excitations, and translate the directions of resultant deformation or resultant stress. They are also referred to as elastic coefficients, which are simply the engineer's moduli for nanomaterial properties.

First, we present the mathematical relationships between Young's modulus, compression modulus, Poisson's ratio and shear modulus with elastic constants. i. Compression modulus B is defined as the ratio of hydrostatic pressure to the fractional change in volume produced by this pressure (volume elasticity). ii. The second modulus *G* is the resistance to deformation produced by a shear stress applied to the (110) plane in the [110] direction. iii. The elastic moduli (Bulk modulus B, Shear modulus G and Young's modulus E) are estimated using the Voigt-Reuss-Hill method. Generally speaking, the greater the B, the greater the material's resistance to volume change.

The Table-3 shows all the elastic moduli in different systems of approach for a cubic crystallographic structure.

The results obtained from the expressions of the previous moduli of cubic TiN are presented in the Table-4.

Table-3: Mathematical expressions of elastic moduli for a cubic structure.

$E = \frac{9\mathrm{BG}}{3\mathrm{B}+\mathrm{G}}$	$\nu = \frac{3B-E}{6B}$	$B = \frac{C_{11}+2C_{12}}{3}$
$G_v = \frac{C_{11}-C_{12}+3C_{44}}{5}$	$G_R = \frac{5(C_{11}-C_{12})C_{44}}{4C_{44}+3(C_{11}-C_{12})}$	$G = \frac{G_R+G_V}{2}$
$B_{Hill} = \frac{1}{2}(B_{Reuss}+B_{Voigt})$	$B_R = B_R = \frac{1}{3}(C_{11}+2C_{12})$	$G_{Hill} = \frac{1}{2}(G_{Reuss}+G_{Voigt})$

Table-4: Elastic moduli of cubic TiN.

Size	Symbols	Voigt (Gpa)	Reuss (Gpa)	Hill (Gpa)
Bulk modulus	B	277.84578	277.84578	277.84578
Shear modulus (Mu blade)	G	192.74042	184.53288	188.63665
Lambda blade	λ	149.35217	154.82386	152.08802
Young modulus	E	469.62823	453.25474	461.47435
Fish ratio	ε	0.21829	0.22811	0.22318

The results of the study provide a detailed picture of the mechanical and structural properties of cubic TiN, revealing important insights into its performance and stability:

Crystalline Parameter and Volume: The lattice parameter a = 3003.738 Å and the volume 56.440305 $Å^3$ for cubic TiN are consistent with experimental values, confirming the accuracy of the DFT-GGA (Density Functional Theory with Generalized Gradient Approximation) approach used in the calculations[12,13]. This agreement is crucial as it validates the theoretical model and ensures that subsequent predictions about the material's properties are reliable.

Elastic Constants: The elastic constants C11 = 602.57615 GPa and C12 = 115.48060 GPa reflect TiN's mechanical stability. The high C11 value indicates strong resistance to uniaxial stress along the crystallographic axes, while C12 provides insight into the material's resistance to shear deformation. Together, these constants suggest that TiN is mechanically robust in its cubic phase, capable of maintaining structural integrity under significant mechanical stress[14].

Modulus of Elasticity and Compressibility: The modulus of elasticity (E) of 469.62823 GPa and the modulus of compressibility (B) of 277.84578 GPa provide additional measures of TiN's mechanical properties. The high modulus of elasticity indicates that TiN is very stiff and resists deformation effectively. Meanwhile, the modulus of compressibility reflects the material's ability to withstand compressive forces without significant volume change. Both parameters underscore TiN's exceptional mechanical properties, making it suitable for applications where high strength and durability are required.

Practical Implications: These findings are significant for practical applications of TiN in various industries. TiN's high mechanical stability and resistance to deformation and compression make it ideal for use in cutting tools, wear-resistant coatings, and other high-stress applications. Its robustness under mechanical stress and its ability to maintain structural integrity under high pressure are essential for ensuring long-term performance and reliability in demanding environments.

Future Directions: While the current results affirm TiN's mechanical robustness, further studies could explore its behavior under varying temperatures and different environmental conditions. Additionally, investigations into the effects of alloying or doping TiN could provide insights into tailoring its properties for specialized applications.

In summary, the study confirms that cubic TiN exhibits excellent mechanical properties, supported by accurate DFT-GGA calculations and consistent with experimental data. Its high elasticity and compressibility make it a strong candidate for advanced applications requiring materials with superior mechanical performance[15].

Thermodynamic properties: debye temperature and propagation velocity: The Debye temperature is a key parameter in solid-state physics that represents the temperature at which the heat capacity of a solid reaches its theoretical maximum, based on the Debye model of lattice vibrations. It characterizes the highest frequency of vibrational modes (phonons) within a material and provides insight into its thermal properties. Below this temperature, the material's specific heat capacity follows the Debye T^3 law, while above it, it aligns with the classical Dulong-Petit law. The Debye temperature is crucial for understanding a material's thermal conductivity, thermal expansion, and behavior at low temperatures, influencing its performance in various applications.

A high Debye temperature typically suggests strong lattice vibrations and high thermal stability. Propagation velocity refers to the speed at which sound waves or elastic waves travel through a material. In the context of TiN, this includes longitudinal and transverse sound wave velocities. These velocities are related to the elastic properties of the material, such as Young's modulus, shear modulus, and bulk modulus. High propagation velocities indicate a material's stiffness and mechanical strength, which are important for applications requiring high durability and resistance to deformation.

Both properties are significant for understanding the thermal and mechanical performance of TiN. The Debye temperature provides insights into thermal stability and specific heat behavior, while propagation velocities reveal information about the material's mechanical rigidity and response to dynamic stress.

In this section we present the results for the Debye temperature and wave propagation velocities in the [100], [110] and [111] directions. The results are presented in the Table-5.

Table-5: Debye temperature and propagation velocity.

Physical properties	Values
Bulk modulus (GPa)	277.84578 +/-1.371
Compressibility (1/GPa)	0.00360
Elastic Debye temperature (K)	914.86952
Averaged sound velocity (m/s)	6514.44488

The calculated Debye temperature of approximately 914.87 K for cubic titanium nitride (TiN) reflects the material's robust thermal properties. This high Debye temperature indicates that TiN has strong lattice vibrations, which translates to a high thermal stability. Essentially, TiN can maintain its structural integrity and resist thermal fluctuations effectively even at elevated temperatures.

This characteristic makes TiN particularly valuable for high-temperature applications where thermal resistance and stability are crucial. The high Debye temperature also implies that TiN will exhibit a significant specific heat capacity, which is beneficial for applications requiring materials to handle and dissipate heat efficiently. Overall, the result underscores TiN's suitability for demanding environments where thermal stability and mechanical performance are essential.

Wave propagation velocity: We have calculated the propagation velocities for titanium nitride (TiN), including: i. Longitudinal Wave Velocity Vp : This is the speed at which compressional or longitudinal waves travel through the material. It provides insight into the material's stiffness and elastic properties. A high longitudinal wave velocity indicates that TiN is mechanically rigid and capable of transmitting stress efficiently through its structure. ii. Compression Wave Velocity Vs: This velocity is associated with the propagation of compressive waves and reflects the material's ability to withstand compressive forces. It is closely related to the material's bulk modulus and is important for understanding how TiN will behave under compressive stress. iii. Thermal Wave Velocity Vm: This represents the speed of thermal waves or the rate at which thermal energy propagates through the material. It is influenced by the thermal conductivity and the material's ability to conduct heat.

These propagation velocities are crucial for evaluating TiN's mechanical and thermal performance. The longitudinal wave velocity and compression wave velocity indicate the material's mechanical strength and response to stress, while the thermal wave velocity provides insight into how efficiently heat is distributed through the material. Collectively, these properties highlight TiN's suitability for applications requiring high stiffness, durability under stress, and effective thermal management.The speed relationships are given by the following expressions:

$$v_s = \sqrt{\frac{G_i}{\rho}}\ ; v_p = \sqrt{\frac{B_i + 4G_i/3}{\rho}}\ ;$$

Table-6: Wave propagation speed.

Sizes	System		
	Voight	Hille	Reuss
vs.	4770.13	4350,27	4770,13
vp	7889,24	7553,05	7201,23
vm	5273,514	4830,871	4328,308

We have therefore shown that the direction of longitidunal propagation is much more important than the other two.

Anisotropy : Anisotropy refers to the directional dependence of physical properties in materials, where characteristics such as mechanical strength, thermal conductivity, electrical resistivity, or optical behavior vary depending on the direction of measurement. Unlike isotropic materials, which exhibit uniform properties in all directions, anisotropic materials display different behaviors along different axes. This property is crucial in materials science and engineering, as it influences how materials are designed and utilized in various applications. For instance, in titanium nitride (TiN), anisotropy can affect mechanical properties like hardness and wear resistance, as well as electrical conductivity, depending on the crystallographic orientation. Understanding anisotropy allows for the optimization of material performance and prediction of behavior under diverse conditions.

We have calculated the longitidinal and transverse propagation velocities for the TiN phase in the directions [100], [110] and [111], which we present in the Table-7 with expressions of the velocities relative to the directions.

Table-7: propagation speed and mode.

Management	Propagation mode	Expression	Value/ $\sqrt{1/\rho}$
[100]	Longitudinal	$v_1 = \sqrt{C_{11}/\rho}$	24,54742
[100]	Transversal	$v_2 = \sqrt{C_{44}/\rho}$	12,60431
[110]	Longitudinal	$v_3 = \sqrt{(C_{11} + C_{12} + 2C_{44})}$	22,75735
[110]	Transversal	$v_4 = \sqrt{C_{44}/\rho}$	12,60431
[110]	Transversal	$v_5 = \sqrt{(C_{11} - C_{12})/2\rho}$	15,6060
[111]	Longitudinal	$v_6 = \sqrt{(C_{11} + 2C_{12} + 4C_{44}}$	22,1285
[111]	Transversal	$v_7 = \sqrt{(C_{11} - C_{12} + C_{44})/}$	14,6738

Longitudinal wave propagation in the [100] direction remains the most important, followed by the closely related [110] and [111] directions; while transverse propagations [100] and [110] are equivalent and therefore have the same properties, there is anisotropy.

Electronic structure: In this section we present the results of the electron structure of the TiN cubic phase, the band structure and the density of states were calculated. The values given by theory range from 0.3 to -0.6ev for the gap.

Band structure: Band structure is a fundamental concept in solid-state physics and materials science that describes the relationship between electron energy levels and their wave vectors within a solid. It is crucial for understanding a material's electronic and optical properties. Here's an overview of its significance and importance. Understanding the band structure helps determine whether a material is a conductor, semiconductor, or insulator.

The band structure consists of continuous energy bands where electrons can exist (valence and conduction bands) and forbidden energy gaps where no electronic states are available (band gaps).

Critical points, such as high-symmetry points in the Brillouin zone, are often analyzed to understand the material's electronic properties.

Hybridization of atomic orbitals affects the band structure by altering the energy levels and shapes of the bands. For example, hybridizations can shift the valence or conduction bands, creating distinct features in the band structure.

Band structure is essential for predicting and understanding the electronic properties of materials, including their electrical conductivity, optical response, and behavior as semiconductors in electronic devices.

In summary, band structure is key to understanding a material's electronic properties. It reveals how energy levels vary with the wave vector of electrons, which is fundamental for predicting electronic and optical behaviors of materials.

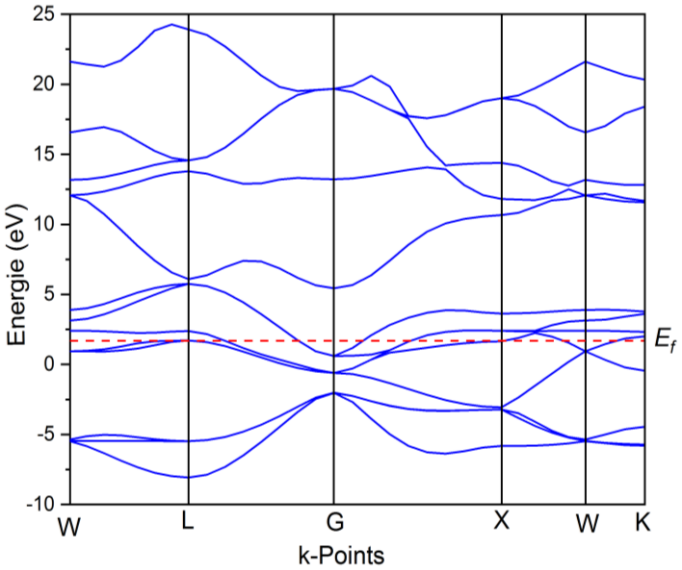

Figure-4: Band structure.

In our band structure analysis of cubic TiN, we have identified a band gap of 0.326 eV, which positions TiN as a semiconductor. The Fermi level, represented by the red dotted line in the Figure-4, is a critical reference point for evaluating the semiconductor properties. At the L point in the Brillouin zone, the energy levels of TiN approach the Fermi level, suggesting that this point is close to where the material's electronic states are likely to be occupied or excited. This proximity indicates that the material has a high density of electronic states near the Fermi level, which is a characteristic feature of semiconductors that can facilitate electronic transitions.

At the G point, which is the Gamma point in the Brillouin zone, TiN reaches its minimum energy value within the band gap. This implies that the conduction band minimum is located at this point, marking the lowest energy state available for electron excitation from the valence band. The relatively small band gap of 0.326 eV indicates that TiN has a small energy barrier between the valence and conduction bands, which can result in significant electronic conductivity at certain temperatures or under specific conditions.

Overall, these observations confirm that cubic TiN behaves as a semiconductor. The close alignment of energy levels to the Fermi level at various points in the Brillouin zone, coupled with the minimal band gap, underscores TiN's potential for applications in electronic and optoelectronic devices where controlled semiconductor properties are essential.

Density of DOS states: The Density of States (DOS) is essential for understanding the electronic properties of materials, representing the number of electronic states available at each energy level. In the context of studying hybridizations, DOS plots reveal how these interactions alter the electronic structure. Significant hybridization points, such as those at -0.0326 eV, -4.1 eV, and 15 eV, Figure-5; often correspond to features in the DOS, such as peaks or dips, indicating changes in the availability of electronic states. By analyzing the DOS around these energy points, we can better understand how hybridizations influence the material's electronic behavior, including its conductivity, reactivity, and mechanical properties.

Here we show the total density of states in cubic TiN, reflecting the electronic contribution of the s, p and d sub layers.

We can restart our study around -10 to 20, the zone in which we observe hybridizations: i. The first hybridization is reached around the point (-0.0326; 3.17eV); ii. The second hybridization is reached around the point (-4.1; 4.18eV); iii. The third hybridization is reached around the point (15; 3.1eV).

The mechanical and electronic properties obtained confirm the robustness of TiN, both in terms of its crystalline structure and its mechanical performance[16]. Calculated elastic constants show that cubic-phase TiN is mechanically stable, with high compressive strength and elasticity.

These properties are in line with tin's known applications in wear- and corrosion-resistant coatings.

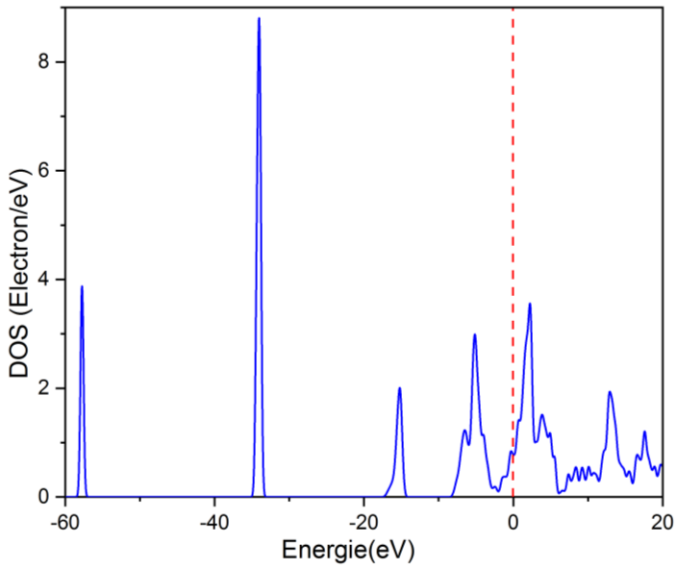

Figure-5: TiN DOS.

The anisotropy observed in the [100] and [110] directions for transverse wave propagation illustrates specific behaviors related to crystal symmetry, which could have implications for industrial applications[17].

In addition, density of states (DOS) analysis reveals an electron gap of 0.642 eV, which is in line with the semi conducting properties of TiN in its cubic phase[18], and is also consistent with its use in electronic applications where low electrical conductivity is required.

This study confirmed the mechanical and electronic properties of cubic TiN using Functional Density theory. The results are consistent with experimental observations, reinforcing the suitability of TiN for applications where mechanical stability and electronic performance are critical[19]. A future study could explore the correlations between the mechanical and electronic properties of TiN, focusing on the effects of crystalline defects and doping on its performance[20].

Conclusion

This study was carried out within the Groupe de Recherche sur les Propriétés Physico-Chimiques des Matériaux (GRPPM) of the Faculté des Sciences et Techniques (FST) of the Université Marien NGOUABI, in order to complete its research on TiN and to understand the origin of the mechanical properties of TiN in the electronic component.

In this work, we studied the mechanical and electronic properties of cubic-phase TiN using Density Functional Theory (DFT) with the Generalized Gradient Approximation (GGA), which was largely sufficient for this study. The results obtained are in line with the experimental data. The pseudo potential Perdew-Burke-Ernzerhof (PBE) was used to calculate crystal parameters; Perdew-Burke-Ernzerhof (PBEsol) for solids was used to evaluate elastic constants. Generalized Gradient Approximation (GGA).

A study of the correlation between mechanical and electronic properties is required. Further studies could include high-temperature simulations to assess thermal stability, as well as investigations into surface properties and interactions with other materials.

References

1. Lütjering, Gerd, and James C. Williams (2007). Titanium matrix composites. *Titanium*. Berlin, Heidelberg: Springer Berlin Heidelberg. 313-328.

2. Trengove, L. (1972). William Gregor (1761–1817) discoverer of titanium. *Annals of Science*, 29(4), 361-395.

3. Dzabana Honguelet, A., et al. (2024). Properties of TiN: A DFT Study. University of Marien NGOUABI.

4. Nsongo, T., et al. (2017). Study on Titanium Thin Films. Journal of Materials Science.

5. Grosso, S. (2017). Architectural Coatings of Ti, TiN and TiOx Grown by Flow Sputtering on Stainless Steel Wires. https://www.theses.fr/2017GREAI083

6. Gockel, B. T., Kolesar, R. S., & Rollett, A. D. (2016). Experimental study of an aerospace titanium alloy under various thermal and tensile loading rate conditions. *Integrating Materials and Manufacturing Innovation*, 5(1), 245-258.

7. Eboungabeka, A. D., Trigo, E. R. M. E., & Nsongo, T. (2021). Reactivity of titanium dental implants in salivary environment in the presence of foods consumed in the Republic of the Congo. *Advances in Materials Physics and Chemistry*, 11(5), 93-99.

8. Mimboui, Y. J. M., Honguelet, A. S. D., & Nsongo, T. (2023). Study of the physical and mechanical properties of titanium in volume by the MEAM method. *Modeling and Numerical Simulation of Material Science*, 14(1), 58-68.

9. Kohn, W., & Sham, L. J. (1965). Self-consistent equations including exchange and correlation effects. *Physical review*, 140(4A), A1133.

10. Perdew, J. P., Burke, K., & Ernzerhof, M. (1996). Generalized gradient approximation made simple. *Physical review letters*, 77(18), 3865.

11. Monkhorst, H. J., & Pack, J. D. (1976). Special points for Brillouin-zone integrations. *Physical review B*, 13(12), 5188.

12. Zunger, A., et al. (1980). Self-Consistent Pseudopotential Method. *Physical Review B*.

13. Hohenberg, P., & Kohn, W. (1964). Inhomogeneous electron gas. *Physical review*, 136(3B), B864.

14. Hill, R. (1952). The elastic behaviour of a crystalline aggregate. *Proceedings of the Physical Society. Section A*, 65(5), 349.

15. Voigt, W. (1928). Lehrbuch der Kristallphysik (BG Teubner Leipzig und Berlin) 980 S. *Reproduced 1966 Spring Fachmedien Wiesbaden GmbH*.

16. Reuss, A. (1929). Berechnung der FlieÃŸgrenze von Mischkristallen. Zeitschrift fÃ¼r Angewandte Mathematik und Mechanik.

17. Born, M., & Huang, K. (1954). Dynamical Theory of Crystal Lattices. Oxford University Press.

18. Grosso, S., et al. (2017). Architectural Coatings of Titanium. *Coatings Journal*.

19. Perdew, J. P. (1997). Generalized gradient approximation made simple. *Phys. Rev. Lett.*, 77, 3868.

20. Williams, J.C, and Thompson, A.W (1980). Structure-Property Relationships in Titanium Alloys. *Annual Review of Materials Science*.