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First-Principles Investigation of Phase Stability, Mechanical Properties, and Electronic Structure of $Ti_xV_{1-x}N$ Solid Solutions

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This study presents a comprehensive first-principles investigation into the phase stability, mechanical properties, and electronic structure of $Ti_xV_{1-x}N$ solid solutions across the entire compositional range ($0 \leq x \leq 1$). Employing density functional theory (DFT) in conjunction with the cluster expansion (CE) method and special quasirandom structures (SQS), we reveal a complex energetic landscape. The system exhibits a thermodynamic tendency towards forming ordered phases at low temperatures, as indicated by the negative mixing enthalpies of the predicted ground-state configurations, while the random solid solution is found to be energetically unfavorable. A significant non-monotonic solid solution strengthening effect is observed, with the Vickers hardness peaking at 22.7 GPa for the ordered structure at x_V=0.5, substantially exceeding the values of the binary end-members. This strengthening is accompanied by a ductile-to-brittle transition, where intermediate compositions ($x_V \approx$ 0.2-0.6) become brittle, as confirmed by Pugh's ratio ($B/G < 1.75$) and negative Cauchy pressures. Analysis of the density of states (DOS), Electron Localization Function (ELF), and Deformation Density (DD) demonstrates that the observed mechanical trends are governed by an enhancement of the covalent character and directionality of the interatomic bonds, resulting from the hybridization of Ti and V d-orbitals. These findings provide fundamental insights into the structure-property relationships in $Ti_xV_{1-x}N$ solid solutions and offer a pathway for designing coatings with an optimized balance of hardness and toughness.

Keywords: Titanium vanadium nitride; density functional theory; cluster expansion; special quasurandom structures; elastic moduli; electronic structure.

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Introduction

Transition metal nitrides (TMNs) are an important class of refractory materials that have found widespread application due to a unique combination of physical and mechanical properties, including high hardness, wear resistance, chemical inertness, high melting points, and high electrical conductivity [1]. These characteristics make them indispensable for creating functional and protective coatings used in metalworking, microelectronics, and the aerospace industry [2], [3]. Among TMNs, titanium nitride (TiN) and vanadium nitride (VN) are some of the most studied representatives. Both compounds crystallize in the face-centered cubic (FCC) B1-type (NaCl) structure. TiN is widely known as a material for wear-resistant coatings that provide hardness in the range of 18–21 GPa [1]. While VN itself has a hardness of ~14 GPa, its alloying into other nitride systems is a known method to substantially enhance their mechanical properties, including both hardness and fracture toughness [4], [5]. Due to their isostructural nature and complete mutual solubility, confirmed both experimentally [6], [7] and by thermodynamic modeling [2], the TiN–VN system is promising for the formation of $Ti_xV_{1-x}N$ substitutional solid solutions. Alloying allows for the targeted control of the material's properties by varying the cation ratio in the metal sublattice. Experimental studies have shown that the lattice parameter of $Ti_xV_{1-x}N$ solid solutions varies nearly linearly with composition, in accordance with Vegard's law. Alloying serves as an effective pathway for simultaneously enhancing hardness, through solid solution strengthening, and improving toughness by reducing brittleness, a critical factor for the material's performance reliability [8], [9]. The high efficiency of first-principles calculations based on density functional theory (DFT) for predicting phase stability, elastic, and electronic properties of TMNs has been well established in [10]. Systematic calculations for a wide range of ternary nitrides have shown that the formation energy (E_{form}), which is a measure of the solid solution's thermodynamic stability, strongly depends on the difference in the atomic radii and electronegativity of the alloying metals [8]. Given their proximity in the periodic table, the solid solution of Ti and V is expected to be stable, which aligns with data from thermodynamic modeling. [2]. However, it should be noted that for systems with a greater parameter mismatch (e.g., TiN-ZrN), *ab initio* calculations predict the existence of a low-temperature miscibility gap [11].

The solid solution strengthening mechanism is generally explained by the interaction of stress fields, created by the solute atoms due to the size difference, with dislocations, which impedes their motion [12]. On the other hand, elastic properties and plasticity are closely related to the nature of the chemical bond. Analysis based on Pugh's [13] (shear modulus to bulk modulus ratio, G/B) and Cauchy pressure criteria for ternary nitride systems shows that an increase in the valence electron concentration (VEC) upon alloying (e.g., when replacing Ti with V) enhances the metallic character of the bond ($p > 0$), which in turn facilitates dislocation slip and increases the material's ductility.

The present investigation entails an *ab initio* modeling of $Ti_xV_{1-x}N$ solid solutions, executed within the density functional theory framework. The methodological approach integrates the Connolly-Williams cluster expansion formalism [14] with the special quasirandom structures (SQS) method [15], [16] to elucidate the most thermodynamically favorable atomic configurations and probable site occupancies within the solid solutions [17]. Subsequently, the full elastic stiffness tensor (C_{ij}) will be computed to derive the macroscopic elastic moduli (bulk modulus B, shear modulus G, and Young's modulus E), as well as hardness and indicators of ductility, such as Pugh's ratio and Cauchy pressure. A key objective is the identification of optimal compositional regimes that yield enhanced mechanical performance for applications in wear-resistant coatings [18] and monolithic ceramics. The nature of the interatomic bonding will be further investigated through an analysis of the total and partial density of states (DOS and pDOS), complemented by a topological analysis of the electron localization function (ELF) and deformation charge density (DD) distributions.

I. Computational details

The theoretical investigation of the $Ti_xV_{1-x}N$ system was conducted using a multi-code, first-principles approach based on density functional theory (DFT).

Initial structural and energetic calculations were executed with the Vienna Ab initio Simulation Package (VASP) [19]. For these calculations, the R^2SCAN meta-GGA functional [20] was employed to accurately capture electronic exchange and correlation effects, while Projector Augmented-Wave (PAW) potentials described the core-valence interactions. A stringent plane-wave kinetic energy cutoff of 520 eV and a dense Monkhorst-Pack k-point grid [21] (KPPRA = 1000) were utilized to ensure robust convergence of total energies and stress tensors.

To model the disordered nature of the $Ti_xV_{1-x}N$ solid solution, two complementary approaches were adopted. The cluster expansion (CE) method, as implemented in the ATAT toolkit [22], was used for an efficient search for low-energy ordered structures. Concurrently, the special quasirandom structures (SQS) methodology was employed to generate supercells that explicitly mimic the atomic correlation functions of a truly random solid solutions. All generated structures underwent full structural relaxation in VASP, optimizing ionic positions, cell volume, and shape. The resulting optimized structures and energies were used to compute the full elastic stiffness tensor (C_{ij}) and derive macroscopic mechanical properties. The output from these elastic calculations was then comprehensively analyzed using the VASPKIT post-processing software [23]. This analysis was used to derive a suite of polycrystalline mechanical and thermodynamic properties, including the macroscopic elastic moduli (B, G, E), theoretical Vickers hardness according to the Tian model [24], the Debye temperature, and key indicators of material ductility such as Pugh's criterion, the Kleinman parameter, and the Cauchy pressure.

The electronic properties of the $Ti_xV_{1-x}N$ solid solutions were investigated using the Quantum Espresso [25] engine as implemented within the Amsterdam Modeling Suite (AMS) software. The interactions between the ionic cores and valence electrons were described using pseudopotentials from the high-accuracy Standard Solid-State Pseudopotentials (SSSP) "Precision" library. The Kohn-Sham wavefunctions were expanded in a plane-wave basis set with a kinetic energy cutoff of 60.0 Ry (~816 eV), while the charge density was expanded with a higher cutoff of 480 Ry (~6530 eV) to ensure high precision. The electronic Brillouin zone was sampled using an automatically generated 5×5×5 Monkhorst-Pack k-point mesh. To handle the metallic nature of the $Ti_xV_{1-x}N$ system, a first-order Methfessel-Paxton smearing scheme was applied with a smearing width of 0.1 eV. Single-point energy calculations were performed on the previously optimized crystal structures. From these calculations, the electronic band structure and the total and partial density of states (DOS and pDOS) were obtained. The density of states was calculated with an energy resolution of 0.05 eV. To further elucidate the nature of the chemical bonding, a topological analysis of the electron density was performed by calculating the Electron Localization Function (ELF) and the Deformation Density (DD) fields.

II. Results and discussion

Pseudobinary energy of mixing for the $Ti_xV_{1–x}N$ solid solutions as a result of energy calculations for 100 clusters is shown on Figure 1. The most prominent feature is the convex hull (light blue line), which defines the minimum energy envelope in energy-composition space and is anchored by ground state structures. The concave shape of this hull, positioned entirely below the zero-energy line, confirms that the $Ti_xV_{1–x}N$ system forms a thermodynamically stable solid solution across the full compositional range, consistent with experimental observations [2].

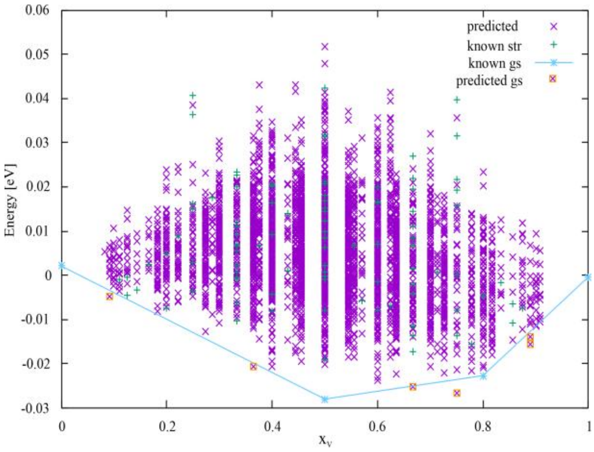


Fig. 1. The pseudobinary energy of mixing plot for the $Ti_xV_{1–x}N$ solid solutions obtained by CE.

The plot distinguishes between known ground states (light blue crosses), such as those observed at compositions of x = 0.5 and x = 0.8 (Figure 2), and newly predicted ground states (orange squares) at specific compositions, such as at approximately x = 0.85 and x = 0.9. These new ground states, confirmed by the ATAT output provide specific targets for experimental synthesis. The numerous data points scattered above the hull (purple 'x' and green '+') represent metastable and unstable configurations. While thermodynamically unstable at 0 K, this detailed energy landscape is critical for understanding non-equilibrium synthesis methods, as these phases can be kinetically stabilized and potentially formed under controlled conditions.

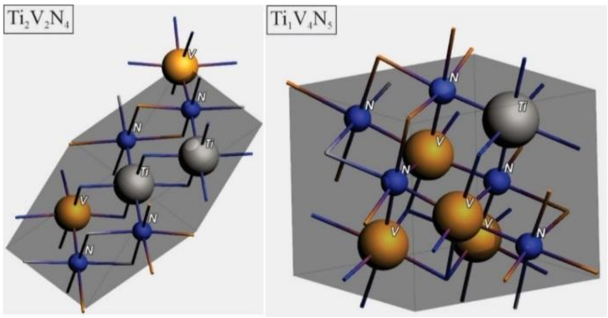
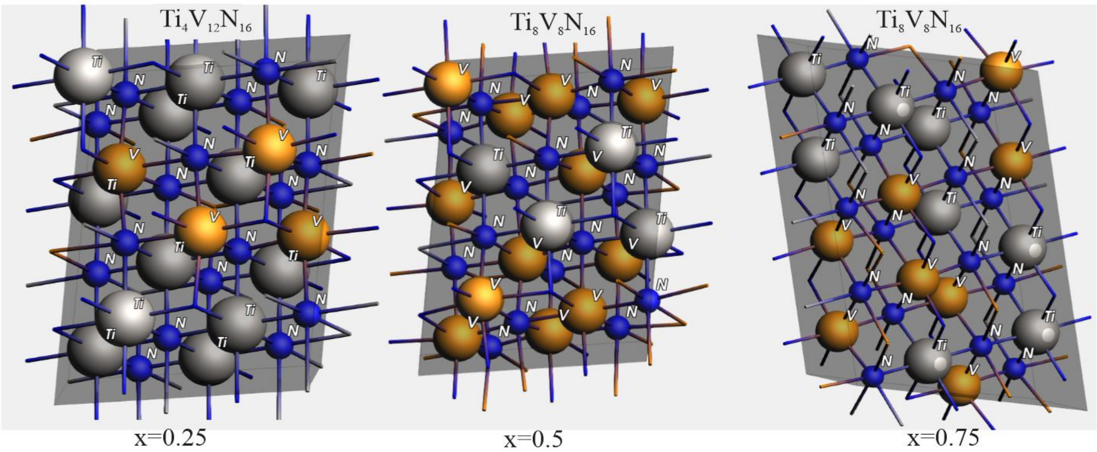


Fig. 2. Ground-state crystal structures of $Ti_xV_{1–x}N$ solid solutions for x = 0.5 and x = 0.8.

The computational results provide a robust theoretical foundation for understanding the $Ti_xV_{1–x}N$ system. The finding that a stable solid solution forms across the entire compositional range is in direct agreement with published experimental literature. The discovery of new ground states, particularly in the V-rich region (e.g., at x = 0.85 and x = 0.9), is of significant practical and theoretical importance. These predicted ordered phases could represent compositions with optimal properties that have not yet been fully explored. The well-known ability to tune material properties in solid solutions (e.g., hardness can be improved by V substitution in TiN) can be refined by targeting these specific, energetically stable compositions. For example, a phase that is only slightly above the convex hull may be easily stabilized in a laboratory setting, while a configuration with a very high energy of mixing would be far more difficult to synthesize.

To complement the cluster expansion analysis, which identifies energetically favorable ordered structures, the disordered state of the $Ti_xV_{1–x}N$ solid solution was modeled directly SQS method. 32-atom supercells were generated for compositions corresponding to x = 0.75, 0.50, and 0.25 (Figure 3). The calculation of the pseudobinary mixing enthalpy for these SQS configurations (Figure 4) revealed positive values across the entire compositional range, with the magnitude increasing with higher vanadium content.

This positive enthalpy of mixing signifies that the formation of a random solid solution is an endothermic process at 0 K, indicating a thermodynamic driving force for phase separation into the constituent binary nitrides, TiN and VN. This result highlights the energetic penalty associated with random atomic mixing, arising from



x=0.25 x=0.5 x=0.75

Fig. 3. SQS crystal structures of $Ti_xV_{1–x}N$ solid solutions.

factors such as lattice strain and unfavorable electronic interactions. This finding for the disordered state contrasts sharply with the predictions from the CE ground-state search, which identified specific ordered configurations on the convex hull with negative mixing enthalpies. Therefore, the combined results suggest a complex stability landscape for the $Ti_xV_{1-x}N$ system: while the random solid solution is unstable with respect to phase segregation, the system exhibits an even stronger energetic preference for forming specific ordered supercells rather than decomposing into its binary end members.

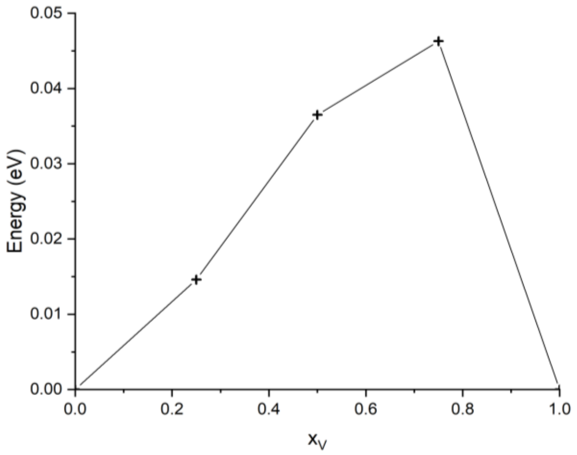


Fig. 4. Pseudobinary energy of mixing SQS crystal structures of $Ti_xV_{1-x}N$ solid solutions.

The concentration dependence of the elastic moduli for the $Ti_xV_{1-x}N$ system, shown in Figure 5, reveals a significant deviation from the linear rule of mixtures, indicating a substantial solid solution strengthening effect. A non-monotonic behavior is observed, particularly for the shear modulus (G) and Young's modulus (E), which reach their maximum values at intermediate concentrations.

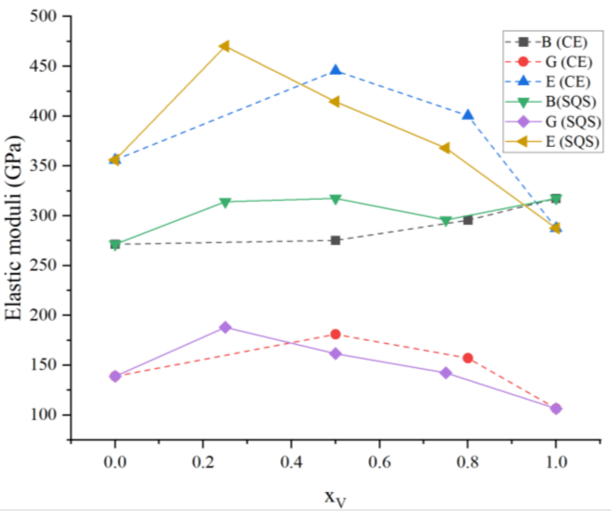


Fig. 5. Elastic moduli versus vanadium content (x_V) for ordered (CE) and disordered (SQS) models of $Ti_xV_{1-x}N$.

For the disordered systems modeled with SQS, the stiffness peaks at the titanium-rich composition ($x_v = 0.25$), where the Young's modulus reaches 470 GPa, significantly exceeding the values for TiN and VN. An even more pronounced strengthening is observed for the ordered configurations obtained by the CE method. At the equiatomic composition ($x = 0.5$), the shear modulus for the ordered structure (181 GPa) is substantially higher than for the corresponding disordered SQS structure (162 GPa). This underscores the significant influence of atomic ordering: the formation of local ordered clusters, identified by the CE method, leads to a considerable increase in shear resistance. Unlike G and E, the bulk modulus (B) exhibits a less pronounced non-linearity, suggesting that the primary strengthening mechanism is associated with resistance to shape change rather than volume change.

To gain a deeper understanding of the relationship between elastic properties and mechanical behavior, the ductility criteria, namely Pugh's ratio (B/G) and the Cauchy pressure ($P_c = C_{12} - C_{44}$, were analyzed. The compositional dependence of these parameters is presented in Figure 6. The analysis of Pugh's ratio (B/G) reveals a distinct ductile-to-brittle transition upon alloying. While the binary compounds TiN (B/G = 1.95) and VN (B/G = 2.98) exhibit ductile behavior (B/G > 1.75), the solid solutions within the approximate compositional range of $x_V = 0.2$ to $x_v = 0.6$ are brittle. The minimum B/G value, corresponding to maximum brittleness, is observed for the ordered structure at $x_V = 0.5$ (B/G = 1.52) and for the disordered SQS structure at $x_V = 0.25$ (B/G = 1.67). This embrittlement region precisely coincides with the domain of maximum strengthening, illustrating the classic trade-off in materials science: an increase in hardness and stiffness is accompanied by a reduction in ductility. Upon further increasing the vanadium content ($x_V > 0.6$), the system reverts to a ductile state, which opens up possibilities for optimizing the composition to achieve a desired balance between hardness and fracture toughness.

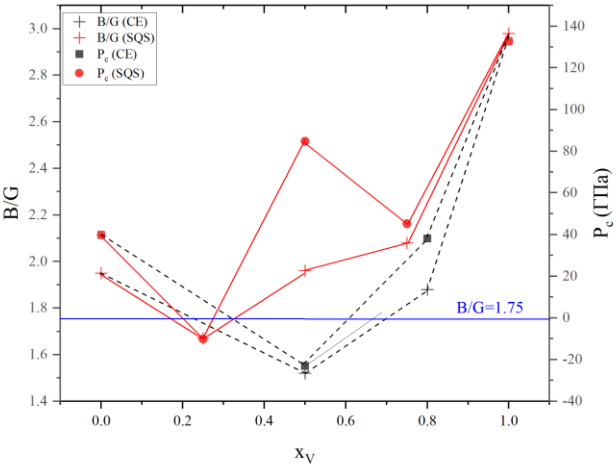


Fig. 6. Pugh's ratio (B/G) and Cauchy pressure (P_c) versus vanadium content (x_V) for ordered (CE) and disordered (SQS) models of $Ti_xV_{1-x}N$, illustrating the ductile-to-brittle transition.

The Cauchy pressure (P_c), an indicator of the chemical bonding character, also demonstrates a strong dependence on composition. The positive P_c values for TiN and VN suggest a predominantly metallic bond character, which promotes ductility. In the intermediate compositional range where embrittlement is observed, the Cauchy pressure becomes negative (e.g., -23.1 GPa for the CE structure at $x_V = 0.5$). This indicates an enhancement of the covalent and directional nature of the bonds, which hinders dislocation glide and leads to brittle failure. The strong correlation between B/G and P_c, visible in the graph, confirms that the mechanical behavior of the $Ti_xV_{1-x}N$ system is directly governed by changes in the electronic structure and the nature of interatomic interactions upon alloying.

Figure 7 presents the compositional dependence of the Vickers hardness (H_V) and the Debye temperature (Θ_D) for the $Ti_xV_{1-x}N$ solid solution. Both parameters exhibit a distinct non-monotonic behavior that correlates well with the trends observed for the elastic moduli.

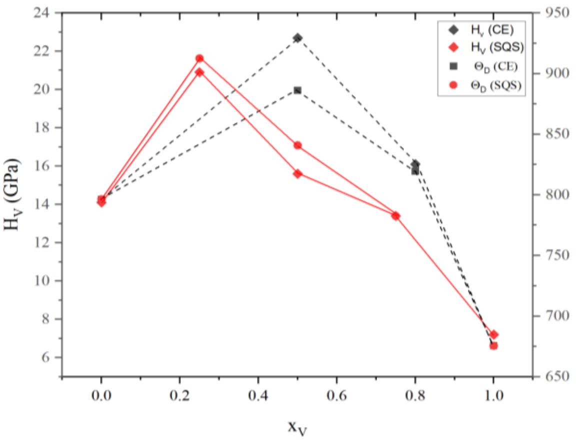


Fig. 7. Compositional dependence of H_V and Θ_D for $Ti_xV_{1-x}N$ solid solutions.

The hardness (H_V) reaches its maximum value in the titanium-rich region, specifically for the disordered SQS structure at $x_V = 0.25$ (20.9 GPa) and for the ordered CE structure at $x_V = 0.5$ (22.7 GPa). This confirms that alloying TiN with vanadium is an effective method for hardness enhancement. It is important to note that the maximum hardness of the ordered (CE) structure exceeds that of the disordered (SQS) structure, which again points to the key role of short-range order in the strengthening of the material. The decrease in hardness at high vanadium concentrations ($x_v > 0.5$) is associated with the reduction in the shear modulus and the increased ductility of the system.

The Θ_D, which is a measure of the crystal lattice stiffness and interatomic bond strength, also reaches its maximum at intermediate concentrations. The highest value of Θ_D (912.5 K) is observed for the SQS structure at $x_V = 0.25$, which coincides with the peak in hardness and elastic moduli. A high Debye temperature indicates stronger interatomic bonds and higher atomic vibrational frequencies, which is a direct consequence of the synergistic effect within the solid solution. The strong correlation between hardness and Debye temperature, visible in the plot, confirms that the strengthening mechanism in the $Ti_xV_{1-x}N$ system is caused by the enhancement of chemical bonds upon solid solution formation.

To clarify the electronic origins of the mechanical property variations, the density of states (DOS) was analyzed. Figure 8 displays the total (TDOS) and partial (pDOS) density of states for the TiN and VN, and for the ordered equiatomic $Ti_{0.5}V_{0.5}N$ structure obtained by (CE).

All three compounds exhibit similar characteristics: the valence band, from -8 to 0 eV, is mainly formed by hybridized N 2p and metal d-states, indicating a strong covalent-ionic Me-N bond. A significant density of states at the Fermi level (E_F) in all cases confirms the metallic nature of these materials. The main difference between TiN and VN arises from their valence electron concentration (VEC), which is 9 for TiN (Ti: d^2s^2; N: s^2p^3) and 10 for VN (V: d^3s^2; N: s^2p^3). The extra electron in VN occupies metallic d-states near E_F, shifting the Fermi level to a region of higher DOS compared to TiN, where E_F lies in a pseudogap. This explains the greater ductility and lower hardness of VN, which aligns with the calculated B/G and P_c values. In the $Ti_{0.5}V_{0.5}N$ solid solution, the electronic structure is effectively averaged. The Fermi level is positioned in a DOS region lower than that of VN but higher than that of TiN. Crucially, the zone of hybridized states broadens, and new bonding states appear due to the interaction of Ti and V d-orbitals. This enhances the covalent character of the bonding, which is corroborated by the calculated negative Cauchy pressure. This enhanced covalency is the cause of the observed solid solution strengthening and the increase in stiffness and hardness at intermediate compositions.

To visualize and analyze the chemical bonding character, Electron Localization Function (ELF) maps were calculated for the (100) plane of the binary compounds TiN, VN, and the ordered $Ti_{0.5}V_{0.5}N$ structure (Figure 9).

In the binary compounds TiN and VN, the ELF distribution is similar. High ELF values (blue areas) are distinctly localized around the nitrogen atoms, indicating a strong ionic component with charge transfer from the metal to nitrogen, as well as the presence of a lone pair on the N atom. Intermediate ELF values in the regions between metal and nitrogen atoms suggest the presence of a covalent Me-N bond. At the same time, significant regions with ELF ≈ 0.5 around the metal atom positions point to the delocalization of d-electrons, confirming the metallic nature of these compounds. The ELF map for the ordered $Ti_{0.5}V_{0.5}N$ structure reveals crucial differences. A notable asymmetry in the electron density distribution is apparent. Electrons become more localized not only around the nitrogen atoms but also in the spaces between Ti and V atoms. The increased localization in the interatomic regions between metals and nitrogen, relative to the binary nitrides, indicates a strengthening of the covalent bond component in the solid solution. This effect is a direct result of the hybridization of Ti and V d-orbitals, as identified in the DOS analysis. This enhancement of covalency and bond directionality in the solid solution is the electronic reason for the observed strengthening. Stiffer, more directional bonds increase the lattice's resistance to shear, which leads to an increase in the G and H_V, and to a decrease in ductility (lower B/G ratio and negative Cauchy pressure).

To further analyze the chemical bonding character and visualize the redistribution of electron density upon its formation, DD maps were calculated for the (100) plane of the TiN, VN, and ordered $Ti_{0.5}V_{0.5}N$ structures (Figure 10).

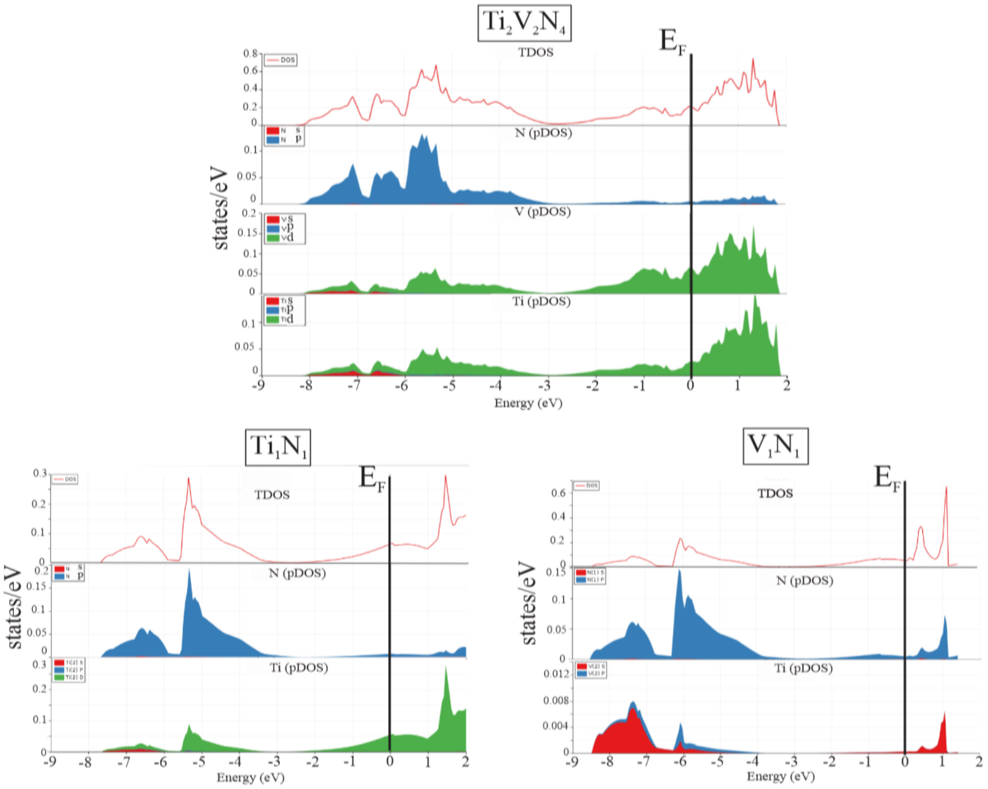


Fig. 8. A comparison of the calculated total and partial density of states (TDOS and pDOS) for the binary end-members TiN and VN, and the equiatomic ordered $Ti_{0.5}V_{0.5}N$ solid solution.

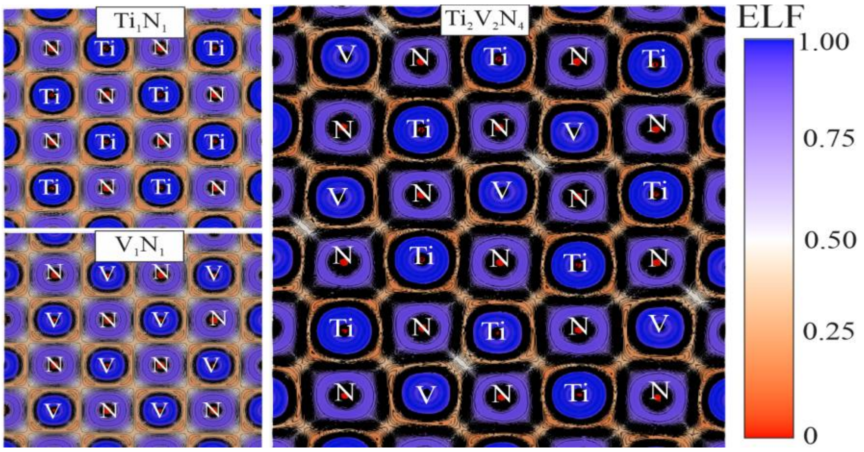


Fig. 9. A comparison of the ELF in the (100) crystal plane for the binary end-members TiN and VN, and the equiatomic ordered $Ti_{0.5}V_{0.5}N$ structure.

In the binary compounds TiN and VN, a classic pattern for iono-covalent nitrides is observed. A significant depletion of electron density (orange regions) is clearly visible around the metal atoms (Ti, V), with its accumulation (blue regions) around the nitrogen atoms. This directly indicates the ionic character of the bond, with charge transfer from the metal cation to the nitrogen anion. Additionally, the accumulation of charge in the regions between Me and N atoms, which has a distinct elongated shape, provides evidence for the formation of strong polar covalent Me-N bonds. The DD map for the ordered $Ti_{0.5}V_{0.5}N$ structure demonstrates a more complex charge redistribution, which confirms the conclusions drawn from the ELF analysis. Not only is Me → N charge transfer observed, but also a noticeable redistribution of density between the metal atoms. Specifically, the charge accumulation regions between the Ti-N and V-N atoms become more pronounced and asymmetric. This suggests that the formation of the solid solution leads to a strengthening of the covalent bond component and its greater directionality. This charge redistribution, resulting in the strengthening of covalent bonds, is the cause of the solid solution strengthening. Stronger and more directional bonds increase the lattice's resistance to shear deformations, which directly leads to an increase in the shear modulus, hardness, and, as a consequence, a reduction in the material's ductility, fully consistent with the analysis of the mechanical properties.

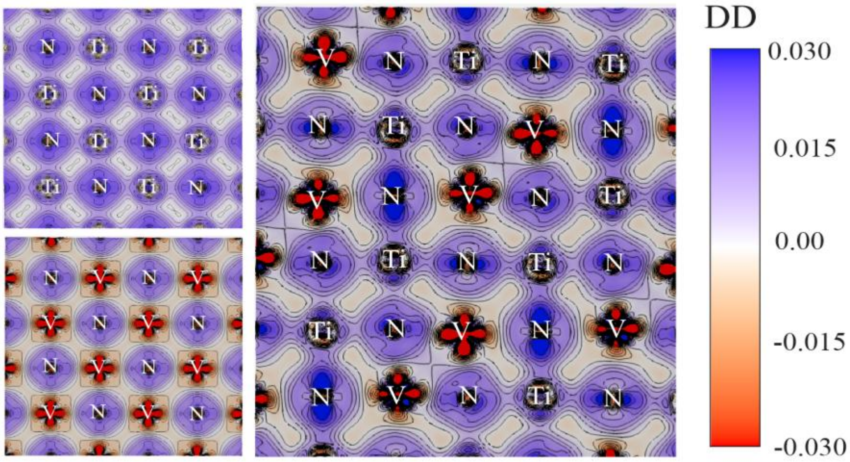


Fig. 10. A comparison of the DD in the (100) crystal plane for the binary end-members TiN and VN, and the equiatomic ordered $Ti_{0.5}V_{0.5}N$ structure.

Conclusion

In this work, the structural, mechanical, and electronic properties of $Ti_xV_{1-x}N$ solid solutions were systematically investigated using a first-principles computational approach. Our analysis revealed a complex energetic landscape where the $Ti_xV_{1-x}N$ system is identified as an ordering system rather than a phase-separating one. While a random solid solution is thermodynamically unstable at 0 K, the existence of ordered ground-state configurations with negative mixing enthalpies makes them the most stable state at low temperatures. A pronounced solid solution strengthening effect was observed, with elastic moduli and Vickers hardness exhibiting a significant non-monotonic dependence on composition. The maximum hardness of 22.7 GPa and peak stiffness were predicted for intermediate compositions ($x_v \approx 0.25$-0.5), demonstrating that alloying is an effective strategy for enhancing the mechanical performance of binary nitrides. Notably, the properties of ordered structures were found to be superior to those of the random solid solution, highlighting the crucial role of short-range order in the strengthening mechanism. This enhancement in hardness is accompanied by a clear ductile-to-brittle transition; while the binary end-members are ductile, the intermediate compositions exhibit brittle behavior, establishing a clear trade-off between hardness and toughness that can be tailored by precise control of the Ti/V ratio. The analysis of the electronic structure (DOS, ELF, and DD) provided a explanation for these mechanical trends, linking the strengthening and embrittlement to an enhanced covalent and directional character of the chemical bonds driven by the hybridization of Ti and V d-orbitals. This study provides a comprehensive theoretical foundation for understanding the structure-property relationships in the $Ti_xV_{1-x}N$ system, offering a predictive framework for designing advanced wear-resistant coatings with a precisely tuned balance of mechanical properties. Future work could focus on the experimental verification of the predicted ordered phases and their influence on the performance of $Ti_xV_{1-x}N$ coatings at operational temperatures.

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Першопринципне дослідження фазової стабільності, механічних властивостей та електронної структури твердих розчинів $Ti_xV_{1-x}N$

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У цьому дослідженні представлено комплексне першопринципне дослідження фазової стабільності, механічних властивостей та електронної структури твердих розчинів $Ti_xV_{1-x}N$ у всьому діапазоні складів ($0 \leq x \leq 1$). Використовуючи теорію функціоналу густини (DFT) у поєднанні з методом кластерного розширення (CE) та спеціальними квазіневпорядкованими структурами (SQS), ми виявили складний енергетичний ландшафт. Система демонструє термодинамічну тенденцію до утворення впорядкованих фаз за низьких температур, на що вказують негативні ентальпії змішування для передбачених основних станів, тоді як невпорядкований твердий розчин є енергетично невигідним. Спостерігається значний немонотонний ефект зміцнення твердого розчину, причому твердість за Віккерсом досягає піку 22.7 ГПа для впорядкованої структури при x_V=0.5, що суттєво перевищує значення для бінарних нітридів. Це зміцнення супроводжується переходом від пластичного до крихкого стану, де проміжні склади ($x_v \approx 0.2$-0.6) стають крихкими, що підтверджується відношенням П'ю ($B/G < 1.75$) та негативним тиском Коші. Аналіз густини станів (DOS), функції локалізації електронів (ELF) та деформаційної густини (DD) демонструє, що спостережувані механічні тренди зумовлені посиленням ковалентного характеру та напрямленості міжатомних зв'язків, що є результатом гібридизації d-орбіталей Ti та V. Ці результати дають фундаментальне уявлення про взаємозв'язки "структура-властивості" у твердих розчинах $Ti_xV_{1-x}N$ та пропонують шлях для розробки покриттів з оптимізованим балансом твердості та в'язкості.

Ключові слова: нітрид титану-ванадію; теорія функціоналу густини; кластерне розширення; спеціальні квазіневпорядковані структури; пружні модулі; електронна структура.