Phase stability and mechanical response of tantalum nitrides to electronic excitation effect

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Abstract

Based on an analysis of electronic structures and phonon spectra calculations as a function of electronic temperature $T_e$ using the density functional theory, we investigated the phase stability and mechanical response to electronic excitation effect on various phases of tantalum nitrides $\text{TaN}_x$ with fully or partially occupied nitrogen sublattices. The results suggest that the cubic phase exhibits lattice instability at room temperature, while the hexagonal phases are dynamically stable. The phase stability increases in the sequence $\text{TaN} (\delta$-type), $\text{TaN}_{0.43}, \text{TaN}_{0.5}, \text{TaN} (\text{AsNi type}), \text{TaN}_{0.83}, \text{TaN} (\epsilon$-type), and $\text{TaN} (\epsilon$-type). The nonmetal vacancies exhibit enhanced lattice stability with hexagonal phases compared to the cubic phase. The electronic excitation effect provides extra stability for cubic $\delta$-$\text{TaN}$ with the increase in electronic temperature, while the excitation results in a lower degree of stability for hexagonal phases. The physical origin of electronic excitation effects on both the cubic and hexagonal phase stability of $\text{TaN}$ can be attributed to the peculiarities of their electronic densities of states near the Fermi level and a combination of three different types of bonding characteristics. The counter-intuitive behavior of lattice stabilities appears or disappears as a response to mechanical properties under electronic excitation.

1. Introduction

Tantalum nitrides ($\text{TaN}$) are of interest because of their unique properties inherent to refractory transition-metal compoundsthat make them important components for making wear-resistant coatings and as diffusion barriers in semiconductor devices as well as optical coatings, cutting tools, magnetic storage devices, generators, maglev trains, and low-temperature electronics [1–3]. Their outstanding properties such as high melting point, good thermal electronic conductivity, superconductivity, heat resistance, chemical stability, and high compressive strength make them potentially useful as industrial materials with characteristics such as load deflection, thermoelastic stress, and fracture toughness [4]. $\text{TaN}$ has three stable phases, i.e., two hexagonal phases ($\epsilon$-type and $\delta$-type structures with the space groups P-62m and P-6m2, respectively) and a cubic NaCl phase ($\delta$-type structure with the space group Fm-3m) [5]. The hexagonal $\epsilon$ phase is the most stable phase under ambient conditions [6]. The hexagonal $\delta$ phase is a low-temperature high-pressure phase [6], which can be synthesized almost from 2 GPa to 10 GPa at temperatures of 1073–1233 K [7], or formed at 2273 K for all the tested pressures [5]. Yan et al predicted a novel hexagonal phase P63/mmc(NiAs), which is the best candidate for $\text{TaN}$ above 87.5 GPa [8]. The cubic $\delta$ phase is a high-temperature high-pressure phase, which was stable at >2073 K [9, 10] and can be synthesized at 3–10 GPa [11] or 2673 K and 2.5 GPa [5]. Moreover, $\delta$-$\text{TaN}$ structures had a superconducting state at 6.5 K or 7.4–9 K at a temperature close to 2073 K [11].

The mechanical properties of various phases were evaluated and compared theoretically. The results suggest that $\text{TaN}$ is ultracompressible and hard owing to its high bulk modulus and large shear modulus comparable to cubic boron nitride, which is expected to lower shearstrain dramatically as many other known hard materials...
TaN from low to high is as follows: $\epsilon < \delta < \theta$ [12]. The hexagonal $\theta$ phase and cubic $\theta$ phase have much higher hardness than hexagonal $\epsilon$ phase [10], while theoretical studies suggest that the $\delta$-type phase has a higher bulk modulus than the $\theta$-type phase [14]. However, other results show that $\delta$ phase has the lowest bulk modulus among the TaN phases [5]. This brief review indicates the discrepancy in the calculation of elastic properties, which prompted our endeavor to evaluate the mechanical response of various TaN phases. The mechanical properties of TaNs function of temperature and pressure were evaluated using first-principles calculations. The results indicate that the elastic properties of TaN depend on the pressure [12]. Moreover, TaN suffers from unavoidable rapid structure transformation, such as ambient pressure $\epsilon$-TaN is transformed to $\theta$-TaN under a high pressure such as at 5 GPa or 3.2 GPa, or to cubic $\delta$-TaN at high temperatures [6, 15–17]. More recently, Chang et al predicted theoretically that $\theta$-TaN is not stable above 53.9 GPa [12]. Interestingly, $\delta$-TaN was suggested as the densest phase at a high pressure and temperature experimentally [5]. However, a first-principles density functional theory (DFT) calculation and experimental results show that the cubic $\delta$-TaN phase exhibits dynamic instabilities characterized by imaginary phonon modes near the X point at room temperature [5, 18–20]. $\delta$-TaN is expected to be dynamically stable at a high temperature and pressure, making them more effective in engineering applications.

The electronic excitation effects can induce a lattice to obtain extra stability. Giret et al calculated phonon dispersions at different electronic temperatures $T_e$ and demonstrated that both fcc and hcp tungsten structures are stabilized by electronic entropy as photoexcited tungsten reaches dynamical stability (PAW pseudopotential and exchange-correlation effects were evaluated in the framework of generalized gradient approximation (GGA)) [5, 8, 12, 13]. An analysis of the calculated results shows that the order of hardness of TaN from low to high is as follows: $\epsilon < \delta < \theta$ [12]. The hexagonal $\theta$ phase and cubic $\theta$ phase have much higher hardness than hexagonal $\epsilon$ phase [10], while theoretical studies suggest that the $\delta$-type phase has a higher bulk modulus than the $\theta$-type phase [14]. However, other results show that $\delta$ phase has the lowest bulk modulus among the TaN phases [5]. This brief review indicates the discrepancy in the calculation of elastic properties, which prompted our endeavor to evaluate the mechanical response of various TaN phases. The mechanical properties of TaNs function of temperature and pressure were evaluated using first-principles calculations. The results indicate that the elastic properties of TaN depend on the pressure [12]. Moreover, TaN suffers from unavoidable rapid structure transformation, such as ambient pressure $\epsilon$-TaN is transformed to $\theta$-TaN under a high pressure such as at 5 GPa or 3.2 GPa, or to cubic $\delta$-TaN at high temperatures [6, 15–17]. More recently, Chang et al predicted theoretically that $\theta$-TaN is not stable above 53.9 GPa [12]. Interestingly, $\delta$-TaN was suggested as the densest phase at a high pressure and temperature experimentally [5]. However, a first-principles density functional theory (DFT) calculation and experimental results show that the cubic $\delta$-TaN phase exhibits dynamic instabilities characterized by imaginary phonon modes near the X point at room temperature [5, 18–20]. $\delta$-TaN is expected to be dynamically stable at a high temperature and pressure, making them more effective in engineering applications.

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In this study, we focused on the structural stability and mechanical response of various TaN phases to electronic excitation effect in the framework of a first-principles approach. We calculated the cubic and hexagonal phase stability at room temperature; the nonmetal vacancies exhibited enhanced lattice stability with hexagonal phases compared to the cubic phase. The evolution of phonon spectra of TaN was computed as a function of electronic temperature $T_e$ using the density functional perturbation theory (DFPT). Cubic $\delta$-TaN afforded extra stability with the increase in electronic temperature, while the acoustic branches of hexagonal phase shifted to lower frequencies. Finally, the physical explanation of electronic excitation effects on the extra stability of cubic and hexagonal structures of TaN can be attributed to the peculiarities of their electronic densities of states (DOS) near the Fermi level. The counterintuitive behavior of lattice stabilities appears or disappears as a response to mechanical properties under electronic excitation.

### 2. Methods and details of calculations

All the electronic structure calculations reported herein are presented within the framework of DFT using the Vienna $ab$ initio simulation package (VASP) code and projector augmented wave (PAW) method [32–34] for two-atom $\theta$-type, four-atom NiAs-type, six-atom $\epsilon$-type, and eight-atom $\delta$-type TaN. The unit cells of cubic and hexagonal structures are shown in figure 1. A cut-off energy of 500 eV was used for plane-wave expansion. The PAW pseudopotential exchange-correlation effects were evaluated in the framework of generalized gradient approximation (GGA) [35–37]. A similar setup was used for basis set and k-point mesh when dealing with different structures. The calculation of phonon spectra in cubic and hexagonal structures used a $3 \times 3 \times 3$ supercell in the framework of DFPT. According to the Monkhorst-Pack scheme [38], a $3 \times 3 \times 3$ regular mesh of k points is sufficient for all supercells. We make a physical equivalent hypothesis based on the fact that electronic excitation plays a key role in metals after irradiation. Namely, different electronic temperatures are used to characterize the strength of the electronic excitation in our study. Under this circumstance, the electronic levels are occupied with a finite fictitious Fermi–Dirac electronic smearing called electronic temperature $T_e$ within DFPT [39]. It was ensured that suitable bands are filled with electrons even at high electronic temperatures. We have re-optimized the structure at $T_e$ and our calculations are made at $V^\text{eq}(T_e)$. The electronic density of states (DOS) was calculated using the tetrahedron method and a (19, 19, 19) mesh. In this study, the bulk modulus and shear modulus are based on Voigt–Reuss–Hill approximation [40, 41]. The elastic
constants of a crystal are defined as the second derivatives of the total energy density with respect to the elements of the infinitesimal strain tensor. In this section, we calculated the total elastic moduli matrix directly with the stress-strain method based on DFT. The mechanical stability of the structure is characterized by the Voigt average shear modulus. For cubic crystals, the Voigt average shear modulus \( G = \frac{(3C_{44} + 2C')}{5} \), where \( C_{44} \) and \( C' = \frac{(C_{11} - C_{12})}{2} \) are the two shear moduli of the cubic crystal. For hexagonal crystals \( G = \frac{(M + 12C_{44} + 12C_{66})}{30} \), where \( M = C_{11} + C_{12} + 2C_{33} - 4C_{13} \) and \( C' = \frac{(C_{11} - C_{12})}{2} \). A common formulation of the stability conditions therefore is \( B > 0; C' > 0; C_{44} > 0 \).

3. Results and discussion

3.1. Lattice dynamics properties

Figure 1 shows a comparison of phonon DOS (PDOS) in acoustic branches as a function of various phases of TaN, with fully or partially occupied nitrogen sublattices. On one hand, the cubic \( \delta \)-type phonon states show prominent imaginary frequencies and exhibit lattice instability, whereas the hexagonal phases with \( \theta \) and \( \varepsilon \) types are dynamically stable. The acoustic phonon frequencies increase in the sequence TaN (\( \delta \)-type), TaN (AsNi type), TaN (\( \theta \)-type), and TaN (\( \varepsilon \)-type). On the other hand, the acoustic phonon frequencies increase in the sequence TaN\(_{0.43}\), TaN\(_{0.5}\), and TaN\(_{0.83}\). Such a sequence indicates that an increase in nonmetal vacancy concentrations induced a prominent shift in the acoustic PDOS to high frequencies. The total acoustic phonon frequencies increase in the sequence TaN (\( \delta \)-type), TaN\(_{0.43}\), TaN\(_{0.5}\), TaN (AsNi type), TaN\(_{0.83}\), TaN (\( \theta \)-type), and TaN (\( \varepsilon \)-type) and suggest the order of phase stability. These results suggest that the nonmetal vacancy concentration has enhanced lattice stability compared to the cubic structure. In particular, the PDOS of TaN\(_{0.83}\) coincides with the results of \( \theta \)-TaN structure, as highlighted in the inset of figure 1. We observed that these data are similar with those obtained for the first-principles study of phase stability of hexagonal and cubic structures of VN and NbN [26, 27]. Compared with the acoustic branch, the optical phonon frequencies change very slightly and can be neglected.

An increase in electronic temperature can also enhance lattice stability. The phonon spectra of fcc Ta as a function of electronic temperature \( T_e \) are shown in figure 3(a), which is dynamically unstable at room temperature. The phonon frequency clearly increases because of an increase in electronic temperature. Interestingly, when the electronic temperature reaches \( T_e = 0.9 \) eV, the phonon frequency of TA mode is completely positive along the \( \Gamma \)-X line. This indicates that the crystal lattice is stabilized under electronic excitation. The dispersion curves for \( \delta \)-TaN as a function of electronic temperature \( T_e \) are shown in figure 3(b).
When $T = 300$ K, the acoustic phonon spectrum showed large imaginary frequencies near the X point, while the acoustic phonon imaginary frequencies along the $\Gamma$-X line decrease rapidly for electronic temperatures up to 3 eV, indicating that the lattice stability has been enhanced. These results suggest the electronic excitation have a positive effect on improving the lattice stability for $\delta$-TaN structure.

In figures 4(a) and (b), we compared the PDOS of both $\delta$-TaN and $\theta$-TaN structures at different $T_e$. The $\delta$-TaN phonon states show prominent imaginary frequencies at $T_e = 0$ eV. An increase in electronic temperature induced a prominent shift in the acoustic PDOS to higher frequencies. The results indicate that $\delta$-TaN structure is stable only at high electronic temperatures. We noted that these data are similar with those obtained by Ivashchenko et al.; they found that the effect of temperature on the phase transition in VN and NbN can be approximated by varying the band-energy smearing parameter $[26, 27]$.

In the case of $\theta$-TaN structure, as shown in figure 4(a), no imaginary frequency was found to induce the destabilization of structure. The acoustic PDOS shifted to lower frequencies as the electronic temperature increased. These results suggest that the excitation results in a lower degree of stability for hexagonal $\theta$-TaN structure. Similar results were obtained in the phase stability calculation of $\varepsilon$-TaN and AsNi type structures. The results indicate that a certain composition may be dynamically stable in $\theta$-TaN, $\varepsilon$-TaN, and TaN (AsNi type) structures at room temperature; nevertheless, its properties within the $\delta$-TaN structure seemed dynamically stable and most promising only at high temperatures. All these results are beneficial for many practical applications of superhard materials under extreme conditions. Figure 4(c) shows the LO–TO splitting degree of $\theta$-TaN as a function of $T_e$. The LO–TO splitting degree at $\Gamma$ point can be used as an important parameter to evaluate the ionic strength of ionic crystals. The results indicate that the ionic character exists in the hexagonal...
phase with $\theta$ types compared to the cubic phase. The ionic strength increases till $T_e = 3$ eV. Moreover, the hexagonal phase structures have higher ionic character than cubic phase structure.

3.2. Electronic properties

To gain more insight into the physical origin of electronic excitation effects on the changes in lattice stability for both $\delta$-TaN and $\theta$-TaN structures, we compared the total DOS versus the energy of these structures. The total DOSs of both cubic $\delta$-TaN and hexagonal $\theta$-TaN are shown in figure 4. Similar to many ionic compounds, the differences in electronegativity and atomic size between Ta and N provide a compound that, on the microscopic level, shows a combination of three different types of bonding characteristics: metallic, ionic, and covalent. The mixed covalent–ionic character of TaN is reflected in the DOS and responsible for the peculiar features of TaN.

An analysis based on the DOS of $\delta$-TaN structure shows that the features obtained from $E = -8$ eV to 4.67 eV were derived from the N 2p orbitals and Ta e.g. ($d_{x^2}$, $d_{y^2}$, $d_{z^2}$) states plus a minor contribution from a small Ta $t_{2g}$ state, whereas the region from 12 eV to 19 eV mainly consists of Ta $t_{2g}$ ($d_{xy}, d_{yz}, d_{zx}$) states. The red and blue curves in figure 5(a) show the corresponding DOS at $T_e = 1$ eV and 3 eV, respectively. The curves show that the band width decreased between the two electronic bands with increasing $T_e$. Compared with the total DOS at $T_e = 0$ eV, the valence and conduction bands shifted to $E_0$ while the width of DOS became significantly smaller to maintain the number of electrons as constant. The excitations of N-Ta hybrids induced to the disappearance of states below Fermi level. The d-p covalent bonding strength drastically increases and plays a role in structural stabilization. In particular, the electrons present in the valence bands are completely shifted above the Fermi level when $T_e = 3$ eV. The conduction band is responsible for the metallicity of TaN and has a net nonlocal Ta ($t_{2g}$) character. The $t_{2g}$ ($d_{xy}, d_{yz}, d_{zx}$) state electrons are directed to the eight nearest-neighbor atoms in the bcc lattice and move to shear-unstable metallic $dd$ bonding states, thus negatively contributing to lattice stability. However, a strong electronic excitation effect causes electron migration and decreases the
electron density direction between neighboring Ta atoms. This breaks the asymmetric occupation of Ta d–t_{2g}
orbitals and reduces the orbital overlap. Thus, the strength of dd bonding rapidly decreased. All these results
positively contribute to the lattice stability of TaN in the rock salt structure.

However, in the case of \( \theta \)-TaN structure, the low-energy band originates from the N 2s state. The d–p band is
mostly derived from the Ta d and N p states. Because of the structural peculiarities of the hexagonal phase, the
d–p band splits into two subbands associated with the (Ta d–N p) \( \sigma \) and (Ta d–N p) \( \pi \) bonds, which lie along the
c axis and in the plane that is perpendicular to the c axis, respectively. The red and blue curves in figure 5(a) show
the corresponding DOS at \( T_e = 1\ \text{eV} \) and 3 eV, respectively. Compared with the total DOS at \( T_e = 0\ \text{eV} \), the
curves show that the DOS has no significant change with increasing \( T_e \) especially near the Fermi level, which are
highlighted in the inset of DOSs, suggesting the slight effect of electronic excitation on lattice stability for \( \theta \)-TaN
structure. In addition, more electrons are transferred from Ta to N as the electron temperature increases,
resulting in a feedback bonding \( \pi \) and decreasing the number of valence electrons of Ta. These results are
beneficial for developing covalent bonding \( \sigma \). Moreover, the development of covalent bonding \( \sigma \) increases the
number of valence electrons of Ta as the electron temperature increases. This is beneficial for developing a
feedback bonding \( \pi \). In summary, \( \sigma \) bonding and \( \pi \) bonding are mutually strengthened, resulting in the
synergistic effect on enhancing the ionic characteristic strength in the hexagonal phase under electronic
excitation.

In summary, a combination of three different types of bonding characteristics on the microscopic level:
metallic, ionic, and covalent, plays a role in changing lattice stability and ionic characteristic strength for both
\( \delta \)-TaN and \( \theta \)-TaN structures under electronic excitation. The phase stability of both cubic and hexagonal
structures of TaN also can be attributed to the peculiarities of their electronic DOS near the Fermi level.

3.3. Mechanical and thermodynamic properties

A striking difference in structures might result in different mechanical properties. It is very necessary to obtain
the relationship between elastic modulus and phase structures. Especially, the elastic constants under electronic
excitation are very important to determine the structural response to external forces, as characterized by the bulk
and shear moduli and can provide a deeper insight into the mechanical behavior and phase stability of materials.
The role of elastic constants on dynamical stabilities was evaluated. The calculated mechanical properties suggest
that both cubic and hexagonal TaN structures are ultraincompressible and hard owing to its high bulk modulus
and large shear modulus. Our calculation shows that the order of bulk modulus of TaN from low to high is as
follows: \( \varepsilon < \delta < \theta \). Both hexagonal \( \theta \) and cubic \( \delta \) phases have much higher hardness than the hexagonal \( \varepsilon \) phase,
while the \( \theta \)-type phase has a higher bulk modulus than the \( \delta \)-type phase. Our results are consistent with the
results obtained by Mashimo and Chang et al [10, 12].

The elastic modulus as a function of electronic temperature \( T_e \) for TaN was thus systematically investigated,
as shown in figure 6. Electronic excitation effects result in the reduction of elastic modulus and elastic constant of
both cubic and hexagonal TaN structures. For \( \varepsilon \)-TaN and \( \theta \)-TaN structures, the high electronic temperature \( T_e \)
induced a very small value of \( C' \) corresponding to a local destabilization of lattice at \( T_e = 3 \\text{eV} \) and 6 eV,
respectively. Therefore, dynamical stability is related to the role of elastic constant within the hexagonal
structures. The elastic constants and the corresponding phonon spectra vary consistently under electronic
excitation.

The fantastic phenomenon shows that phonon instabilities occur when \( \delta \)-TaN structure exhibits cubic elastic stability according to a review of stability criteria. An imaginary frequency of the TA mode is presented
along the \( \Gamma-X \) line above 7 THz, indicating the destabilization of lattice, but exhibited cubic elastic stability
\( (C' > 0 \text{ and } C_{44} > 0) \). Obviously, the values of \( C_{11} \) and \( C_{33} \) are large in both structures, indicating that their
a-axial and c-axial directions are extremely stiff. Moreover, a high electronic temperature led to a higher stability
for δ-TaN structure, whereas the elastic constant and elastic modulus decreased as a function of electronic temperature. These results are counterintuitive (i.e., a higher stability and lower elastic constant). In fact, the appearance of stability as a response to mechanical properties seems counterintuitive. The elastic constants and corresponding phonon spectra vary inconsistently under strong electronic excitation. In spite of decreasing structural stiffness, the previous experimental study indicated that δ-TaN is the densest phase at a high pressure and temperature [5]. The presence of electronic temperature induced a more dense phase to δ-TaN and avoided rapid structural transformation, thus significantly improving the practical applications of superhard materials TaN under extreme conditions.

It is essential to consider the thermodynamic properties aimed at predicting the structural stability of δ-TaN. From figures 7(a) and (b), we can see that both phonon entropy S and phonon heat capacity Cv increase with the lattice temperature. Moreover, the electronic excitation positively affects both quantities, suggesting the larger uncertainty associated with a random variable. An analysis of electronic temperature-dependent phonon dispersion relationships shows that δ-TaN is dynamically stabilized at $T_e = 3$ eV, i.e., higher phonon energies, whereas higher lattice vibrational entropies were found at elevated electronic temperature. These results are counterintuitive (i.e., a higher stability and higher vibrational entropies). Interestingly, phonon entropy S and phonon heat capacity Cv show anomaly at a low lattice temperature $T = 80$ K and 50 K, respectively, as shown in the set, which may arise from the anharmonic vibrations. The thermodynamic contribution was derived from the lattice vibrational entropies at a low temperature. However, δ-TaN is stabilized by electronic entropy as dynamical stability reaches a high $T_e$. Similar to our previous study, electron entropy $S_e$ undergoes a significant modification as a consequence of changes in the DOS, and the increase in $S_e$ affects the electron external pressure $P_e$, eventually improving the stability of cubic system [22].

4. Summary

To evaluate the phase stability and mechanical response to electronic excitation effect on various phases of TaNx with fully or partially occupied nitrogen sublattices, we analyzed the results of electronic structures and phonon spectra as a function of electronic temperature $T_e$ from first-principles calculations. The results indicate that the cubic phase is dynamically unstable, while the hexagonal phase exhibits lattice stability at room temperature. The stability of TaN increases in the sequence TaN (δ-type), TaN0.43, TaN0.5, TaN (AsNi type), TaN0.83, TaN (θ-type), and TaN (ε-type). At room temperature, the small nonmetal vacancies have enhanced lattice stability with hexagonal phases compared to the cubic phase. The cubic δ-TaN obtain extra stability under electronic excitation, while the excitation results in a lower degree of stability for hexagonal phases. The electronic excitation effects influence the lattice stability of both cubic δ-TaN and hexagonal θ-TaN structures because of the peculiarities of their electronic DOS near the Fermi level and a combination of three different types of bonding characteristics. It seems counterintuitive that the lattice stabilities appear or disappear as a response to mechanical properties under electronic excitation (i.e., a higher stability and lower elastic constant).

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