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Mechanical, structural, and thermodynamic properties of TaC-ZrC ultra-high temperature ceramics using first principle methods

Ali Reza Farhadizadeh and Hamid Ghomi

Laser and Plasma Research Institute, Shahid Beheshti University, Evin 1983963113, Tehran, Iran
E-mail: a_farhadizadeh@sbu.ac.ir

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Abstract

In this research, a systematic investigation of the properties of stoichiometric ultra-high temperature ceramics \( \text{Zr}_2 \text{Ta}_8 - x \text{C}_x \) is carried out. The mechanical properties including elastic constants, shear modulus, bulk modulus, Zener ratio, Poisson ratio, Pugh’s index are calculated and then the hardness (H) and \( H^2/E^2 \) based on a semi-empirical approach are estimated. It exhibits that TaC possesses the lowest hardness equal to 22 GPa that increases to maximum hardness 30 GPa when a single Zr atom is substituted with Ta \( (\text{Zr}_1 \text{Ta}_7 \text{C}_8) \). Afterwards, the partial density of states (PDOS) of mentioned ceramics was calculated and plotted. Since the density of states at the Fermi level has some value, it is inferred that they all are electrical conductors. The p-d hybridization, the states at the Fermi level and the Mulliken charges of each atom indicate that the covalent, metallic and ionic nature of bonding exist simultaneously among constituent elements.

1. Introduction

Ultra high temperature ceramics (UHTC) are such promising materials to withstand very high temperature due to their covalent bonding and high melting point temperature reaching 4000 °C [1]. Generally, all borides, oxides, nitrides, and carbides of early transition metals are classified as UHTC. These materials can be used in atmosphere reentry vehicles, hypersonic aircraft that experiences temperature exceeding 2500 °C as well as oxidizing conditions [2]. Among UHTC, TaC and ZrC with very high melting temperature are of great importance in aerospace and with potential applications as thin films in cutting tools and biomedical components [3–5].

Zirconium carbide as thin film was formerly deposited by reactive magnetron sputtering for studying the optical properties [6]. Afterwards, some other features of ZrC coatings including their structural [7] mechanical properties [8], cytocompatibility [9], corrosion resistance [10], tribological properties [5], and ultra-high temperature oxidation [11] were investigated. More recently, the stability of ZrC under high pressure (up to 150 GPa) and high temperature (up to 2000 K) was studied by Lijie Tan et al [12]. The theoretical approach into the properties of ZrC and ZrCN was also carried out using Density Functional Theory (DFT), indicating DFT is such a powerful method to predict the properties of conventional compounds and new designed materials [13–15].

Although TaC is also such a promising ultra-high temperature material [16], it has less studied in comparison to ZrC, and most of research in the field of coatings constitutes the combination of TaC with other materials. For instance, the doped TaC with amorphous carbon as an overcoat has shown good tribological behavior [17]. Deposition of TaC with very thin layer of Ag interlayer has enhanced both the hardness to about 42 GPa and its resistance to wear [18]. It is also shown that TaC is not only wear resistance but it also possesses biocompatible properties appropriate for biomedical applications [3]. The structural, thermodynamic, electronic, and mechanical properties of TaC is also theoretically covered in literature [19–21]. However, to the best of our knowledge, no systematic study on the properties of binary system of TaC-ZrC has been carried out with which it is likely to introduce new materials with better properties.

Density Functional Theory (DFT) has nowadays become very popular due to its ability to predict the properties of a variety of crystalline materials whether they are thermodynamically stable or metastable [22]. The
power of DFT is to design new materials for specific applications and until now, it tremendously succeeded. The current research aims to shed the lights on the properties of the TaC-ZrC system using first principle method in order to grasp the nature of the atomic bonding and their mechanical properties by which the optimized chemical composition for such mechanical applications is revealed. Therefore, the results of this research can provide some insights into novel hard materials as thin films for different application.

2. Computational method

Density functional theory (DFT) with the scheme of pseudo-potential plane wave, implemented in the Cambridge Serial Total Energy Package (CASTEP) [23], was used to do the first principle computations. The evaluation of exchange-correlation energy was carried out through approximation of Perdew Wang (GGA-PW91) [24] and Perdew–Burke–Ernzerhof (GGA-PBE) [25]. As the calculated values using PW91 was different from the experimental results, particularly in Ta-rich compounds, PBE was used by which the amount of error was decreased. At the beginning, the geometry optimization was performed where the convergence thresholds for energy change, maximum force, maximum displacement and maximum stress were $5 \times 10^{-6}$ eV/atom, 0.01 eV/Å, $5 \times 10^{-4}$ Å and 0.02 GPa, respectively. The energy was calculated in the first Brillouin zone employing a $9 \times 9 \times 9$ k-point grid of the Monkhorst-Pack scheme. The cut-off energy was set to 500 eV where the $dE_{\text{tot}}/d\ln E_{\text{cut}}$ approached around $-0.3$ eV, indicating that the convergence was sufficient with respect to energy cut-off and k-point sampling.

The supercell with 16 atoms was built (figure 1) with the formula of $Zr_x Ta_{8-x}C$ where x is an integer varying from 0 to 8. Since the crystallographic structure of stoichiometric TaC and ZrC is NaCl type, in this work, the structure of $Zr_x Ta_{8-x}C$ was modelled in face center cubic (FCC) so that the thermodynamic properties, the mechanical and electronic properties of the different composition were investigated. Since there can be different atomic sites in the supercell, the properties of all different atomic configurations were calculated in each
The obtained properties were almost similar, however, reported results belong to the configuration with the lowest energy. As the Ta, Zr, and C do not possess magnetic behavior, the electron spins in these calculations were considered unpolarized. The Hook’s law was used to compute the elastic constants of the compounds. Afterwards, the Voigt-Reuss-Hill (VRH) approximation was used to obtain bulk modulus (B) and shear modulus (G). Other parameters related to mechanical properties including Poisson’s ratio, anisotropy index, Pugh’s index, and Cauchy pressure were also calculated based on the elastic constants. In the end, the PDOS and analyses of Mulliken charges were employed to analyze the nature character of bonding in each compound.

3. Results and discussion

3.1. Crystal structure of TaC-ZrC system

Since the crystal structure of stoichiometric TaC and ZrC is NaCl type, the presumed structure for solid solution ZrxTa8−xC is also considered face-centered cubic (FCC). The crystal structure is depicted in figure 1 where the big and small spheres represent metal transition (Ta and Zr) and carbon, respectively. As the supercell has two adjacent cubes, consisting of 16 atoms, 8 for carbon, and 8 for Ta and Zr, the crystallographic shape inevitably becomes tetragonal P4/MMC where the lattice constant ‘c’ is nearly as twice as the one ‘a’. Since the final compound is solid solution with FCC structure, the lattice constant for cubic structure is calculated from the volume of supercell. The experimental measurement of TaC and ZrC lattice constant gives the values 4.4547 Å [26] and 4.6930 Å [27], respectively, shown in figure 2. However, no data is available for solid solution TaZrC. Therefore, one way to validate the calculated results is to compare it with the present experimental measurements. The variation of lattice constant with respect to Zr content in ZrxTa8−xC is plotted in figure 2. As shown, when PW91 is used, the lattice constant of ZrC is perfectly matched with the experimental measurement whereas the calculated lattice constant overestimates the dimensions of TaC crystal (around 2.5% error), leading to inaccurate elastic constant calculations. When PBE method is used, the TaC lattice constant is closer to the experimental data even though it is not perfectly the same and possesses around 1% error which is normally considered acceptable error. Though using PBE rather than PW91 method increases the error of ZrC from 0.1% to 1% for Ta-rich compounds, it is more accurate. According to Vegard’s law [28], which is the linear dependency of lattice constant with the amount of constituent elements, the measured lattice constant of TaC and ZrC is interpolated and shown as a dashed line in figure 2. Comparing the results of PBE and PW91 with the interpolation, indicates that it is better to use PW91 in very-rich-Zr compounds while for Zr-rich compounds, it is more accurate. The high accuracy of lattice constant is of importance particularly for further calculation regarding the elastic constants, and subsequent estimation of mechanical properties.

3.2. Thermodynamic stability

The chemical stability of ZrxTa8−xC is investigated through cohesive energy (Ecoh) [29] and formation enthalpy (ΔHf) [30] with the equations stated below:

\[
E_{\text{coh}}(ZrxTa_{8-x}C) = \left(\frac{1}{16}\right)\left[E_{\text{tot}}(\text{supercell}) - xE_{\text{iso}}(Zr)\right] - [(8 - x)E_{\text{iso}}(Ta)] - [8E_{\text{iso}}(C)]
\]

(1)
where $E_{\text{iso}}$ and $E_{\text{bin}}$ are the isolated atom energy and the total energy per atom of pure element in its ground state, respectively, and the number 16 represents the number of atoms in the supercell. Since the cohesive energy is correlated with the binding energy of atoms, it is used to estimate the chemical stability of a structure that the more negative the cohesive energy, the more stable the structure is [31]. As seen in figure 3, the cohesive energy of TaC is $-9.15$ eV that follows an increasing trend when Zr substitutes the Ta in the structure. The cohesive energy reaches the maximum value when the pure stoichiometric ZrC is considered, equal to $-8.75$ eV. The enthalpy of formation has also the same trend in which the $\Delta H_f$ varies from $-0.9$ to $-0.3$ eV for TaC and ZrC, respectively.

Notice that in reactive thin film deposition of ZrTaC by magnetron sputtering (MS), the compound forms from single atoms or ions and, hence, the cohesive energy and the formation enthalpy play a key role in the final composition of deposited films. When atoms are transported into the substrate surface, the one with more negative cohesive energy is more likely to form, leading to non-equality of the number of one species in plasma with the chemical composition. The difference between formation enthalpy of mentioned carbides with metal transition nitrides [32] or oxynitrides [33] is very distinctive. Therefore, the co-deposition of metal nitrides and carbides simultaneously in such methods like physical vapor deposition (PVD) becomes of concern.

### 3.3. Mechanical properties

In this contribution, our main purpose is to trace the mechanical strength variation with chemical composition with corresponding bonding characteristic of atoms. For every material with industrial applications, the mechanical properties are important as it generally defines the resistance of the compound into applied stress. When superhard coatings are the issue, the mechanical properties are of utmost prominence that is addressed here in detail. Firstly, the elastic constants for the cubic solid solution $Zr_xTa_{8-x}C_8$ including $C_{11}$, $C_{44}$, and $C_{12}$ are calculated. Since the number of atoms in simulation is limited, the atomic configuration is also critical for obtaining reliable results. Therefore, different possible atomic arrangements for each compound are taken into account and the elastic constants for those compounds with the lowest energy were used for estimation of mechanical properties listed in table 1. The Zener ratio ($A$) is an index of anisotropy of the crystallographic structure (equation (3)) [34] so that when it is closer to unity, the less anisotropic is the structure. It is stated

![Figure 3. The cohesive energy (a) and the enthalpy formation (b) for $Zr_xTa_{8-x}C_8$ where $X$ varies from 0 to 8.](image)

### Table 1. The mechanical properties of ZrTaC.

| Compound | $C_{11}$ | $C_{44}$ | $C_{12}$ | B | G | E | Zener ratio | $G/B$ | Poisson ratio | Cauchy pressure | $\theta_{12}$ |
|----------|---------|---------|---------|---|---|---|-------------|------|--------------|---------------|------------|
| TaC      | 670     | 173     | 163     | 332| 202| 503| 0.68        | 0.61 | 0.25         | $-10$         | 518        |
| Zr$_x$Ta$_{8-x}$C$_8$ | 773 | 177 | 96 | 322 | 230 | 558 | 0.52 | 0.72 | 0.21 | $-81$ | 568 |
| Zr$_x$Ta$_{8-x}$C$_8$ | 733 | 174 | 96 | 308 | 222 | 537 | 0.55 | 0.72 | 0.21 | $-78$ | 577 |
| Zr$_x$Ta$_{8-x}$C$_8$ | 699 | 174 | 100 | 300 | 217 | 524 | 0.58 | 0.72 | 0.21 | $-74$ | 590 |
| Zr$_x$Ta$_{8-x}$C$_8$ | 600 | 215 | 153 | 302 | 218 | 528 | 0.96 | 0.72 | 0.21 | $-62$ | 616 |
| Zr$_x$Ta$_{8-x}$C$_8$ | 592 | 155 | 128 | 283 | 182 | 450 | 0.67 | 0.64 | 0.23 | $-27$ | 588 |
| Zr$_x$Ta$_{8-x}$C$_8$ | 616 | 168 | 94 | 268 | 201 | 482 | 0.64 | 0.75 | 0.20 | $-74$ | 642 |
| Zr$_x$Ta$_{8-x}$C$_8$ | 560 | 173 | 103 | 255 | 193 | 463 | 0.76 | 0.76 | 0.20 | $-70$ | 662 |
| ZrC      | 530     | 157     | 100     | 243| 178| 430| 0.73         | 0.73 | 0.21         | $-57$         | 671        |
when the anisotropicity of a structure increases, it is more prone to micro crack initiation [35].

\[
A = \frac{2C_{44}}{C_{11} - C_{12}}
\]  \hspace{1cm} (3)

Ductility of a compound is evaluated in terms of three parameters. The first is the Pugh’s index [36] that is defined as the ratio of G/B. When G/B exceeds 0.5, it implies the compound is brittle. The other parameter is Cauchy pressure [37], \( C_{12} - C_{44} \), that also determines the brittleness of a compound. When \( C_{12} \) exceeds \( C_{44} \), i.e., the Cauchy pressure possesses positive value, that is indicative for ductility of the compound. The Poisson ratio, which is the ratio of transverse strain to longitudinal strain, can also be an indicator of brittleness [38]. For metallic compounds, this ratio is roughly between 0.25 and 0.35 whereas for all compounds except for TaC are less than 0.20 to 0.24 (table 1), pointing out that the modelled materials are quite brittle. According to abovementioned parameters to determine the brittleness of such materials, all simulated compounds are brittle; however, the TaC is more ductile than other compounds (table 1).

The Debye temperature (\( \theta_D \)) is another important factor that is closely associated with some physical properties including specific heat, thermal conductivity and melting temperature [39] and it could be obtained from the average sound velocity \( \nu_m \) as follows:

\[
\theta_D = \frac{h}{k_B} \left[ \frac{3n}{4\pi N_a \rho M} \right]^{1/3} \nu_m
\]  \hspace{1cm} (4)

where \( h \) is the Planck’s constant, \( k_B \) is the Boltzmann constant, \( n \) is the number of atoms in the unit cell, \( N_a \) is the Avogadro number, \( \rho \) is the density, \( M \) is the molecular weight, \( n \) is the number of atoms in the unit cell. The average sound velocity \( \nu_m \) can be calculated from the transverse (\( \nu_T^2 \)) and longitudinal (\( \nu_L^2 \)) sound velocities by the following equations:

\[
\nu_m = \left[ \frac{1}{3} \left( \frac{2}{\nu_T^2} + \frac{1}{\nu_L^2} \right) \right]^{-1/3}
\]  \hspace{1cm} (5)

\[
\rho \nu_T^2 = G
\]  \hspace{1cm} (6)

\[
\rho \nu_L^2 = B + 4G/3
\]  \hspace{1cm} (7)

As rendered in table 1, the Debye temperature increases from 518 K for TaC to 641 K for ZrC. It implies that the melting point of ZrC is higher than TaC that is not in agreement with the literature, reporting the melting point of TaC around 3950 °C, exceeding the melting point of ZrC. One reason for this discrepancy could be the non-stoichiometric tantalum carbide like \( \text{TaC}_{0.83} \) is studied, the electronic configuration in p and d orbital varies in a way that the covalent bonding increases at the expense of metallic bonding, strengthening the interatomic bonds and as a consequence the hardness and melting point increase [40].

Hardness of a material is also very important, although it cannot be derived from the pure properties including speciﬁc heat, thermal conductivity and melting temperature. The highest values of hardness and melting point increase when the anisotropicity of a structure increases, that is 0.1 GPa. One should note that the highest hardness is achieved for \( \text{Zr}_n \text{Ta}_m \text{C}_8 \) that is 0.1 GPa. However, the highest \( H^3/E^2 \) belongs to \( \text{Zr}_n \text{Ta}_m \text{C}_8 \) that is 0.1 GPa. One should note that the highest values of hardness and \( H^3/E^2 \) are achieved for \( \text{Zr}_n \text{Ta}_m \text{C}_8 \) and \( \text{Zr}_n \text{Ta}_m \text{C}_8 \), respectively, implying adding a small amount of other metal transition into the carbide structure can enhance the hardness and \( H^3/E^2 \) extensively, that it is unlike the metal transition nitrides, which is shown that adding a metal transition to TiN lowers its hardness [32].

The hardness and \( H^3/E^2 \) are estimated and presented in figure 4, showing the hardness and \( H^3/E^2 \) have similar trend. TaC has the lowest hardness (~22 GPa) that increases to 30 GPa when one Zr atom is replaced with Ta (\( \text{Zr}_n \text{Ta}_m \text{C}_8 \)). However, the highest \( H^3/E^2 \) belongs to \( \text{Zr}_n \text{Ta}_m \text{C}_8 \) that is 0.1 GPa. One should note that the highest values of hardness and \( H^3/E^2 \) are achieved for \( \text{Zr}_n \text{Ta}_m \text{C}_8 \) and \( \text{Zr}_n \text{Ta}_m \text{C}_8 \), respectively, implying adding a small amount of other metal transition into the carbide structure can enhance the hardness and \( H^3/E^2 \) extensively, that is unlike the metal transition nitrides, which is shown that adding a metal transition to TiN lowers its hardness [32].
3.4. Electronic properties

In this part, the electronic properties of ZrTaC are addressed using the PDOS and Mulliken charge analyses. This could help further understand the characteristic of chemical bonding between atoms in the ZrTaC. The PDOS is shown in figure 5 where the Fermi level at $E = 0$ is marked by a horizontal line. As it is well known, the existence of states at $E = 0$ is indicative of electrical conductivity and metallic bonding in which the higher the states, the higher the electrical conductivity and metallic bonding are. The metallic bonding is contributed to formability and ductility of materials, which is a unique feature of metals. The density of states at Fermi level for TaC and ZrC is about 7.5 and 3 states/eV/supercell, respectively, demonstrating the metallic bonding and electrical conductivity are higher in TaC. One reason for lower hardness of TaC than ZrC could be attributed to the higher density of stated for TaC, as stated, indicating more metallic bonding within the structure. The PDOS of zirconium carbide illustrates that the states at Fermi level is attributed to Zr—d and C—p orbitals with small contribution of Zr—p. Although PDOS of TaC is very similar to ZrC, the contribution of Ta—d for TaC is much higher. The Mulliken charges for TaC and ZrC are also presented in table 2, showing that a considerable amount of bonding between Ta (Zr) with C is ionic. If the bonds were mainly covalent or metallic, the charge of atoms should be small.

Therefore, the value of atomic charge represented here can be said is chiefly due to the ionic bonding between carbon and tantalum (zirconium). Additionally, as it just mentioned, there is definitely some metallic bonding in the structure. The covalent bonding is estimated by the hybridization in the valence band that here (figure 5) is between $-6$ and $-2$ eV, which has a peak, named valence peak. For ZrC, the Zr—d, Zr—P, and C—p consists a p—d hybridization where the valence peak is at $-2.5$ eV. It also applies to TaC but the valence peak shifts back to $-4.5$ eV whereas the peak height (density of states) decreases. The lower the energy of the valence peak and the higher the density of states at the peak, results in stronger covalent bonding [43]. The strong p—d hybridization implies that the covalent bonding is also prevalent in these structures [44]. Although the electronic configuration of Zr and Ta are quite similar, when one atom substitutes another one, the net charge on each atom distinguishes (table 2). Let us consider Zr$_7$Ta$_1$C$_8$ where one Zr has replaced one Ta. The atomic charge of Zr tremendously rises to 1.51, which is nearly twice the charge of Zr in ZrC. All carbon atoms charges remain constant $-0.75$ whereas the charge of Ta atoms reduces. In other words, although the addition of Zr into the structure remains the charge of carbon intact, the more electrons of Zr move around the Ta atoms due to the higher electronegativity of Ta, resulting in the high positive charge of Zr equal to 1.63. Note that Zr$_7$Ta$_1$C$_8$ is the hardest
material (\(H = 30\) GPa) that can be attributed to this electronic configuration even though there are many other parameters affecting the hardness. When the number of Zr increases to 2, as seen in table 2, the charge of carbon is unvaried whereas the charge of Ta reduces at the expense of Zr atomic charge. Adding the third Zr atom to the structure (\(Zr_3Ta_5C_8\)) does not change the the charge of carbon but the charge of Zr and Ta follow the same trend. The interesting point is that the charge of carbon in all compounds are almost equal (figure 6) whereas the charges of Ta and Zr tremendously changes.

Figure 5. The partial density of states of \(Zr_xTa_{8-x}C_8\) where X is an integer varying from 0 to 8.
4. Conclusion

The structural, thermodynamical, mechanical, and electronic properties of $\text{Zr}_x\text{Ta}_{8-x}\text{C}_8$ were investigated by DFT method implemented in CASTEP. Firstly, the unit cells of FCC solid solution of mentioned compounds were calculated and showed that they follow the Vegard’s law where by increasing $x$ ($\text{Zr}$) into the structure, the lattice constant linearly extends. Then, the cohesive energy and formation enthalpy of compounds were computed, demonstrating that all of them are thermodynamically stable while the Ta-rich compositions have the more negative value that means they are more stable. Afterwards, the elastic constants were computed and other properties including bulk modulus, shear modulus, Young modulus, Zener ratio, Pugh’s index, Poisson ratio were calculated based on the elastic constants and then the hardness and $H/E$ were estimated. It was shown that the maximum hardness and yield pressure belongs to $\text{Zr}_7\text{Ta}_1\text{C}_6$ and $\text{Zr}_2\text{Ta}_7\text{C}_6$ equal to 30 GPa and 0.1 GPa, respectively. Finally, the electronic properties were examined using PDOS and Mulliken analyses. It was revealed that all compounds have some electrical conductivity and metallic character of bonds. In addition, owing to the net charge of each atom, there possibly are very strong ionic bonds between atoms. However, strong p-d hybridization between metal transition and carbon atoms disclose the covalent bonding. That is to say, there are three types of bonding in studied compounds including metallic, covalent, and ionic, which make them so especial, i.e., they resist high temperature conditions like a ceramic and possess electrical conductivity like a metal. The obtained results will be used to deposit hard coatings by magnetron sputtering with proper mechanical properties.

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ORCID iDs

Ali Reza Farhadizadeh © https://orcid.org/0000-0001-8085-6367
Hamid Ghomi © https://orcid.org/0000-0003-2203-5194

Table 2. The Mulliken charge analyses of $\text{Zr}_x\text{Ta}_{8-x}\text{C}_8$ where $f$ denotes the frequency of that charge.

| Compound  | C charge ($f$) | Ta charge ($f$) | Zr charge ($f$) |
|-----------|---------------|----------------|-----------------|
| TaC       | −0.75 (8)     | 0.75 (8)       |                 |
| $\text{Zr}_1\text{Ta}_7\text{C}_6$ | −0.75 (8) | 0.52, 0.62 (4), 0.68, 0.70 | 1.63 |
| $\text{Zr}_2\text{Ta}_6\text{C}_8$ | −0.75 (8) | 0.48 (6) | 1.56 (2) |
| $\text{Zr}_3\text{Ta}_5\text{C}_8$ | −0.75 (5), −0.76(3) | 0.22, 0.36 (2), 0.44 (2), 1.36, 1.43 (2) |
| $\text{Zr}_4\text{Ta}_4\text{C}_8$ | −0.75 (4), −0.76(4) | 0.20 (4) | 1.31 (4) |
| $\text{Zr}_5\text{Ta}_3\text{C}_8$ | −0.75 (1), −0.76 (4), −0.77 (2), −0.80 (1) | 0.09 (2), 0.18 | 1.08 (2), 1.17 (2), 1.25 |
| $\text{Zr}_6\text{Ta}_2\text{C}_8$ | −0.76 (6), −0.79 (2) | −0.04 (2) | 1.04 (6) |
| $\text{Zr}_7\text{Ta}_1\text{C}_8$ | −0.76 (2), −0.77 (2), −0.78 (4), −0.06 | 0.82 (2), 0.91 (4), 0.97 |
| ZrC       | −0.78 (8)     |                 | 0.78 (8)       |
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