Research Article

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First-principles calculations of mechanical and thermodynamic properties of tungsten-based alloy

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Abstract: The structural, mechanical and thermodynamic properties of tungsten-based alloys, including $W_{0.5}Ti_{0.5}$, $W_{0.67}Zr_{0.33}$, $W_{0.666}Ti_{0.1667}Zr_{0.1667}$, $W_{0.67}Hf_{0.33}$ and $W_{0.666}Ti_{0.1667}Hf_{0.1667}$, have been investigated in this paper by first-principles calculations based on density functional theory (DFT). The calculated elastic constants and mechanical stability criteria of cubic crystals indicated that all of these cubic alloys are mechanical stable. The mechanical properties, including bulk modulus (B), shear modulus (G), Young's modulus(E), ratio B/G, Poisson's ratio, Cauchy pressure and Vickers hardness are derived from the elastic constants C_{ij}. According to calculated elastic modulus and Vickers hardness, the $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ alloy has the greatest mechanical strength. The Vickers hardness of these cubic alloys rank as follows: $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ > $W_{0.67}Zr_{0.33}$ > $W_{0.666}Ti_{0.1667}Zr_{0.1667}$ > $W_{0.5}Ti_{0.5}$ > $W_{0.67}Hf_{0.33}$. Moreover, calculated ratio B/G, Poisson's ratio, Cauchy pressure indicated that the ductility of $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ alloy is the worst among these alloys. The ductility of these cubic alloys rank as follows: $W_{0.67}Hf_{0.33}$ > $W_{0.5}Ti_{0.5}$ > $W_{0.67}Zr_{0.33}$ > $W_{0.666}Ti_{0.1667}Zr_{0.1667}$ > $W_{0.666}Ti_{0.1667}Hf_{0.1667}$. What is noteworthy is that both mechanical strength and ductility of $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ are greater than pure W. Finally, Debye temperature, melting point and thermal conductivity have been predicted through empirical formulas. All these results will provide scientific data for the study on new product development of electrode materials.

Keywords: Density functional theory; Alloy; Mechanical properties; Thermodynamic properties; Electrode materials

1 Introduction

Tungsten and tungsten-based alloys are widely used in aerospace industries and national defense military project due to their high strength, high melting point, good thermal conductivity, hardness, low thermal expansion coefficient etc. [1–4]. And they are also applied in nuclear fusion reactors as the potential first wall materials, and the electrode materials applied in NBI system which is the main method used to heat plasma consisting in a beam of high-energy neutral particles that can enter the magnetic confinement field [2–6]. Recently, in order to improve the low ductility and high ductile-to-brittle transition temperature (DBTT) of tungsten, many experimental and theoretic studies have been reported on the binary W alloy in a wide variety [7]. W-Ti alloy is a typical binary W alloy in those studies. The results indicated that the ductility of W-Ti alloy is improved obviously and metallic bonding is strengthened, but the mechanical strength alloy is lower comparing with pure W. The tungsten - titanium system exhibits a completely solid solution in the β phase at the temperatures between the solidus and the critical temperature of the miscibility gap [8].

There were many researches on binary W alloys, but few on ternary alloys. On the basis of previous studies, binary W alloy, especially ternary W alloy has been consid-

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Table 1: Calculated lattice constants of $W_{0.5}Ti_{0.5}$, $W_{0.67}Zr_{0.33}$, $W_{0.666}Ti_{0.1667}Zr_{0.1667}$, $W_{0.67}Hf_{0.33}$ and $W_{0.666}Ti_{0.1667}Hf_{0.1667}$.

Phase		Space group	k-point mesh	a (Å)	Deviation (%)	Energy cutoff (eV)
$W_{0.5}Ti_{0.5}$	This work	Im-3m	11×11×11	3.177	< 0.22	350
	ref [7]	Im-3m	11×11×11	3.170		350
$W_{0.67}Zr_{0.33}$	This work	Im-3m	8×8×8	3.258	< 2.7	350
	ref [21]	Im-3m	-	3.172		-
$W_{0.666}Ti_{0.1667}Zr_{0.1667}$	This work	Im-3m	8×8×8	3.189	< 0.73	350
	ref [21]	Im-3m	-	3.166		-
$W_{0.67}Hf_{0.33}$	This work	Im-3m	15×15×15	3.186	< 0.03	1000
	ref [21]	Im-3m	-	3.185		-
$W_{0.666}Ti_{0.1667}Hf_{0.1667}$	This work	Im-3m	18×18×18	3.003	< 5.45	1500
	ref [21]	Im-3m	-	3.176		-

ered to be the typical representative for studying in this paper. So far, little work has been reported on W-Hf alloy, W-Zr alloy W-Ti-Hf ternary alloy and W-Ti-Zr ternary alloy. Hafnium (Hf) is a chemical element that has a high melting point, high density of physical properties. A series of alloying compounds made of hafnium, such as HfC, which can be used as an additive to hard alloys due to its hardness and high melting point. Another alloy compound of hafnium, 4TaC·HfC, is known to have the highest melting point [9–11]. Correspondingly, Zirconium is also one of the metals with high melting point. Titanium-zirconium alloy can be used as a kind of biomedical-materials due to its high hardness [12].

In this paper, we investigated the structure, elastic properties, Vicker hardness, Debye temperature, melting point and thermal conductivity of $W_{0.5}Ti_{0.5}$, $W_{0.67}Zr_{0.33}$, $W_{0.666}Ti_{0.1667}Zr_{0.1667}$, $W_{0.67}Hf_{0.33}$, $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ alloys by first-principles calculations based on density functional theory (DFT). This work will be quite helpful to understanding basic physical properties of these alloys, and these calculated results will provide scientific data for the study on new product development of electrode materials.

2 Calculation methods

The simulation method based on density functional theory (DFT) scheme [13] was carried out to research the mechanical properties, Debye temperature, melting point and minimum thermal conductivity of tungsten-base alloys, and the calculations were performed by using the Cambridge Serial Total Energy Package Code (CASTEP) [14, 15]. The interaction between valence electrons and core ion was described by ultra-soft pseudo-potential plane-wave (UPPW) [16]. Exchange-correlation energy was treated by general gradient approximation (GGA) [17] method, including PBE [18] and PBEsol [19]. For the integral in the first Brillouin zone, Monkhorst-pack method [20] was adopted for k-points sampling, as M×M×M for all of tungsten-base alloys. According to the results of the convergence test, M and plane wave cutoff energy were employed as different value with different kinds of structure, this is shown in Table 1. The atomic structure is fully relaxed in the geometry optimization process, until the forces exerting on all atoms are less than 0.01eV/Å. Geometry optimization results are shown in Table 1.

3 Results and discussion

3.1 Structure optimization

The Bravais primitive cell of all the tungsten-base alloys are body-centered cubic, as shown in Figure 1. Before calculated the elastic constant, we tested the convergence. The convergence is good enough when the energy and elastic constants almost no longer change with the increase of cutoff energy and M value. The final determined cutoff energy and M values are shown in Table 1. Compared with the experimental data of references, calculated lattice constants were in good agreement with the former.

3.2 Elastic constants and moduli

Thermodynamic and mechanical properties of crystals, including compressibility, melting point, thermal conductivity and Debye temperature, are related to the elastic

Table 2: The elastic constant (GPa) of $W_{0.5}Ti_{0.5}$, $W_{0.67}Zr_{0.33}$, $W_{0.666}Ti_{0.1667}Zr_{0.1667}$, $W_{0.67}Hf_{0.33}$, $W_{0.666}Ti_{0.1667}Hf_{0.1667}$.

Phase		C_{11}	C_{12}	C_{44}
$W_{0.5}Ti_{0.5}$	This work	238.91	165.68	45.33
	ref [11]	248.78	174.94	39.46
$W_{0.67}Zr_{0.33}$	This work	345.63	176.41	77.29
	ref	-	-	-
$W_{0.666}Ti_{0.1667}Zr_{0.1667}$	This work	363.77	195.10	75.65
	ref	-	-	-
$W_{0.67}Hf_{0.33}$	This work	343.72	203.13	2.32
	ref	-	-	-
$W_{0.666}Ti_{0.1667}Hf_{0.1667}$	This work	572.58	342.58	182.58
	ref	-	-	-

Table 3: Elastic modulus (GPa), ratio B/G and Poisson's ratio (σ) and Cauchy stress (C ', GPa) of W, $W_{0.5}Ti_{0.5}$, $W_{0.67}Zr_{0.33}$, $W_{0.666}Ti_{0.1667}Zr_{0.1667}$, $W_{0.67}Hf_{0.33}$, $W_{0.666}Ti_{0.1667}Hf_{0.1667}$.

Phase		B	G_V	G_R	G_H	B/G	E	σ	C'
Pure W	This work	-	-	-	-	-	-	-	-
	Jiang [7]	317.44	-	-	147.42	2.15	382.96	0.30	35.87
	Söderlind [28]	314.33	-	-	163.40	1.92	417.80	0.28	-
$W_{0.5}Ti_{0.5}$	This work	190.09	41.84	41.39	41.62	4.57	116.37	0.398	60.18
	Jiang [7]	199.56	-	-	38.44	5.19	108.37	0.410	67.74
$W_{0.67}Zr_{0.33}$	This work	232.82	82.22	80.06	80.14	3.32	215.67	0.346	49.56
	ref	-	-	-	-	-	-	-	-
$W_{0.666}Ti_{0.1667}Zr_{0.1667}$	This work	251.32	78.90	78.12	78.01	3.18	212.09	0.358	59.73
	ref	-	-	-	-	-	-	-	-
$W_{0.67}Hf_{0.33}$	This work	249.99	29.51	3.78	16.65	15.01	48.87	0.467	100.41
	ref	-	-	-	-	-	-	-	-
$W_{0.666}Ti_{0.1667}Hf_{0.1667}$	This work	420.24	156.15	148.82	152.48	2.76	408.08	0.338	80.00
	ref	-	-	-	-	-	-	-	-

constant C_{ij} which determine the ability of crystal to resist external forces. The elastic modulus, including bulk modulus (B), shear modulus (G) and Young's modulus (E), and ratio B/G, Poisson's ratio (σ), Cauchy pressure (C'), etc. can be calculated by the elastic constant. Elastic constants C_{ij}could be calculated by generalized Hooke's law. For a body-centered cubic system, there are only three independent elastic constants C_{11}, C_{12}, and C_{44}, as shown in Table 2. The elastic constants of ternary $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ are the greatest. The conditions of mechanical stability of bcc system are [22].

$$C_{44} > 0 \tag{1}$$

$$C_{11} - C_{12} > 0 \tag{2}$$

$$C_{11} + 2C_{12} > 0 \tag{3}$$

All tungsten-base alloys satisfy equations (1)-(3) indicating that they are mechanically stable. Unfortunately, there were few studies on the mechanical properties of $W_{0.67}Zr_{0.33}$, $W_{0.666}Ti_{0.1667}Zr_{0.1667}$, $W_{0.67}Hf_{0.33}$, $W_{0.666}Ti_{0.1667}Hf_{0.1667}$alloys except of $W_{0.5}Ti_{0.5}$. Cauchy pressure (C'), which characterize the ductility of materials, could be represented by [23].

$$C' = \frac{C_{12} - C_{44}}{2} \tag{4}$$

According to Voigt-Reuss-Hill approximation [24–27], the bulk moduli (B) and shear modulus (G) could be calculated, as shown in Table 3. Actually, Young's modulus (E), ratio B/G and Poisson's ratio, including bulk moduli (B) and shear modulus (G), can be calculated from the known elastic constants [28].

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{5}$$

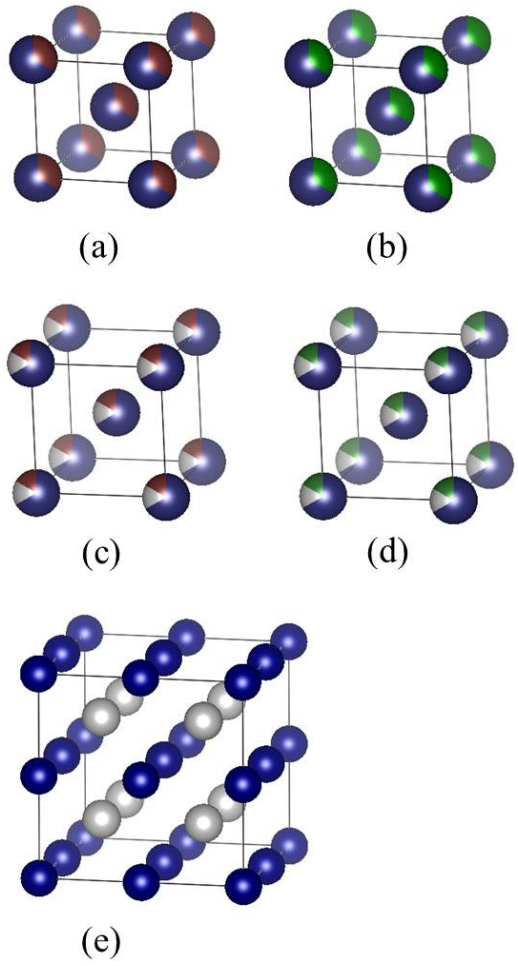

Figure 1: Crystal cell structure of the alloys. (a) $W_{0.67}$ $Hf_{0.33}$; (b) $W_{0.67}$ $Zr_{0.33}$; (c) $W_{0.666}$ $Ti_{0.1667}$ $Hf_{0.1667}$; (d) $W_{0.666}$ $Ti_{0.1667}$ $Zr_{0.1667}$; (e)$W_{0.5}Ti_{0.5}$ (2×2×2 supercell). Blue is W atom, white is Ti atom, red is Hf atom, and green is Zr atom.

$$G_V = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}) \tag{6}$$

$$G_R = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})} \tag{7}$$

$$G_H = \frac{1}{2}(G_V + G_R) \tag{8}$$

$$E = \frac{9BG_H}{3B + G_H} \tag{9}$$

$$\sigma = \frac{3B - 2G_H}{2(3B + G_H)} \tag{10}$$

The tendency of bulk modulus, shear modulus, and Young's modulus to vary with the alloys as shown in Figure 2. It can be seen that the data of $W_{0.5}Ti_{0.5}$ in this work is consistent with the data of Jiang's work.

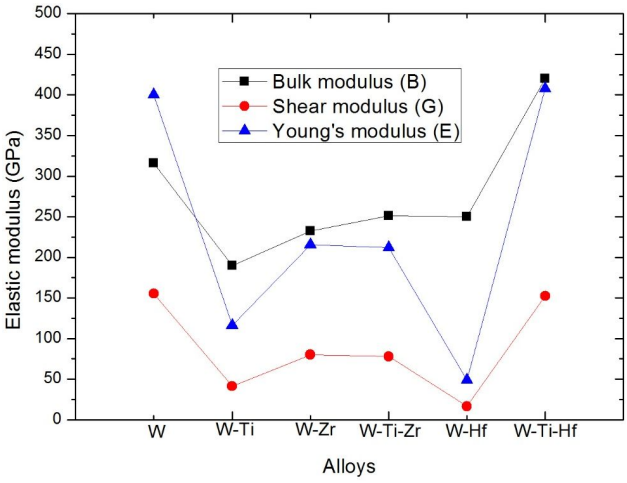

Figure 2: Trends of Bulk modulus (B), Shear modulus (G) and Young's modulus (E) of pure W, $W_{0.5}Ti_{0.5}$, $W_{0.67}Zr_{0.33}$, $W_{0.666}Ti_{0.1667}Zr_{0.1667}$, $W_{0.67}Hf_{0.33}$, $W_{0.666}Ti_{0.1667}Hf_{0.1667}$.

The bulk modulus (B) reflects the strength of the material. As can be seen from Figure 2, the bulk modulus (B) of these materials ranks as follows: $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ > W > $W_{0.666}Ti_{0.1667}Zr_{0.1667}$ > $W_{0.67}Hf_{0.33}$ > $W_{0.67}Zr_{0.33}$ > $W_{0.5}Ti_{0.5}$. The value of bulk modulus (B) of $W_{0.5}Ti_{0.5}$ binary alloy is 190.09 GPa, and the value of bulk modulus (B) of $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ ternary alloy is up to 420.24 GPa. Shear modulus (G) characterizes the material's resistance to shear strain. The shear modulus value of $W_{0.67}Hf_{0.33}$ is the minimum, which is 16.65 GPa, and the value of $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ ternary alloy is still the largest, reached 152.48 GPa. The order is: $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ > W > $W_{0.67}Zr_{0.33}$ > $W_{0.666}Ti_{0.1667}Zr_{0.1667}$ > $W_{0.5}Ti_{0.5}$ > $W_{0.67}Hf_{0.33}$. The larger the Young's modulus (E) is, the stronger the material stiffness is [29]. From Figure 2, it can be seen that the value of Young's modulus of $W_{0.67}Hf_{0.33}$ is the smallest.; the value of Young's modulus of $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ ternary alloy is the largest, which reached 408.08 GPa, the order is: $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ > W > $W_{0.67}Zr_{0.33}$ > $W_{0.666}Ti_{0.1667}Zr_{0.1667}$ > $W_{0.5}Ti_{0.5}$ > $W_{0.67}Hf_{0.33}$. In summary, the values of bulk modulus (B), shear modulus (G) and Young's modulus (E) of $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ ternary alloy are the largest, even larger than pure W. But the mechanical strength of other alloys are lower than pure W.

According to Pugh's theory [3], ratio B/G is closely related to the ductility of metallic materials. When the ratio B/G is greater than 1.75, the materials exhibits ductility; conversely, the materials exhibits brittleness. And the larger the ratio B/G is, the better the ductility of the materials is. As can be seen from Table 3, all tungsten-base alloys are plastic materials and $W_{0.67}Hf_{0.33}$ has the best ductility.

Table 4: Vickers hardness (H_V, GPa) of $W_{0.5}Ti_{0.5}$, $W_{0.67}Zr_{0.33}$, $W_{0.666}Ti_{0.1667}Zr_{0.1667}$, $W_{0.67}Hf_{0.33}$, $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ alloys.

	$W_{0.5}Ti_{0.5}$	$W_{0.67}Zr_{0.33}$	$W_{0.666}Ti_{0.1667}Zr_{0.1667}$	$W_{0.67}Hf_{0.33}$	$W_{0.666}Ti_{0.1667}Hf_{0.1667}$
H_V^G	4.46	11.28	10.90	0.05	24.07
H_V^E	7.07	13.11	12.90	2.97	24.81

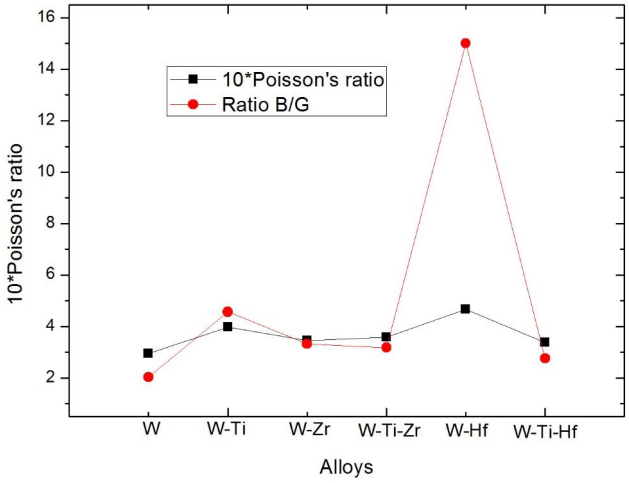

Figure 3: Trends of ratio B/G and Poisson's ratio (σ) of pure W, $W_{0.5}Ti_{0.5}$, $W_{0.67}Zr_{0.33}$, $W_{0.666}Ti_{0.1667}Zr_{0.1667}$, $W_{0.67}Hf_{0.33}$, $W_{0.666}Ti_{0.1667}Hf_{0.1667}$.

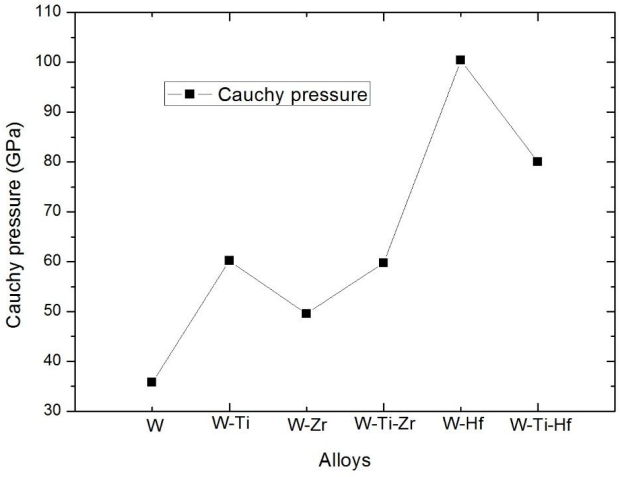

Figure 4: Trend of Cauchy pressure (C') of pure W, $W_{0.5}Ti_{0.5}$, $W_{0.67}Zr_{0.33}$, $W_{0.666}Ti_{0.1667}Zr_{0.1667}$, $W_{0.67}Hf_{0.33}$, $W_{0.666}Ti_{0.1667}Hf_{0.1667}$.

It can be seen from Figure 3 that the ductility of the two ternary alloys are worse than that of the $W_{0.5}Ti_{0.5}$ binary alloy, of which $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ is the worst. Be that as it may, the ductility of all tungsten-base alloys we studied are higher than pure W.

Poisson's ratio (σ) could be used to further analyze the bonding of tungsten-base alloys [31], the greater value of σ is, the better ductility of material is. The conclusions drawn from the ratio B/G could be confirmed by Poisson's ratio (σ). It can be seen from Figure 3 that the trend of the ratio B/G is consistent with Poisson's ratio (σ). Poisson's ratio σ values for different materials range from 0.0 to 0.50. Metallic bonded materials have a big value for σ *i.e.* ~0.33, for covalent materials the critical value is 0.1 and for ionic materials it is 0.25 [31, 32]. It can be seen that metallic bond take the dominant position in all these crystal materials.

When the Cauchy pressure (C') is positive, the metal bond predominates in the crystal cell, thereby exhibiting the ductility of the material [33–35]. and the larger the C' value is, the stronger the metallic bond of the materials and the better the ductility are. Conversely, if the Cauchy pressure is negative, the material exhibits brittleness. The smaller the negative value is, the stronger the covalent bond and the brittler the material are.

3.3 Vickers hardness

In addition to the elastic modulus which can describe the mechanical properties of materials, hardness is also an important parameter. Table 4 lists the Vickers hardness of five tungsten-base alloys. Among them, the value of H_V^G is smaller than H_V^E. As previously analyzed, the alloy material which is of the best mechanical properties is $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ ternary alloy, and its hardness is much bigger than other binary alloys. Vickers hardness (H_V) can be calculated from the elastic modulus. The empirical formula is as follows [36, 37]:

$$H_V^G = 0.1769G - 2.899 \tag{11}$$

$$H_V^E = 0.0608E \tag{12}$$

Table 5: The thermal parameters of $W_{0.5}Ti_{0.5}$, $W_{0.67}Zr_{0.33}$, $W_{0.666}Ti_{0.1667}Zr_{0.1667}$, $W_{0.67}Hf_{0.33}$, $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ alloys.

Phase	v_l	v_t	v_m	θ_D	k_{min}	T_m
$W_{0.5}Ti_{0.5}$	4523.86	1862.34	2017.62	238.15	0.729	1429.10
$W_{0.67}Zr_{0.33}$	4805.34	2348.61	2638.12	303.65	0.840	1909.34
$W_{0.666}Ti_{0.1667}Zr_{0.1667}$	4890.45	2031.75	2590.59	304.64	0.839	1990.97
$W_{0.67}Hf_{0.33}$	3815.18	943.60	1077.44	126.82	0.504	1900.72
$W_{0.666}Ti_{0.1667}Hf_{0.1667}$	5633.17	2785.64	3126.97	390.48	0.990	2930.61

3.4 Thermodynamic property

Thermodynamic property is another important property for materials, such as Debye temperature θ_D (K), minimum thermal conductivity k_{min} (W / (m × K)), and melting point T_m (K). It is known by Solid State Physics that θ_D is mainly related to the dispersion relation of the lattice wave generated by the lattice vibration. Its relationship in solid state physics is [38]:

$$\theta_D = \frac{\hbar\omega_m}{k_B} \tag{13}$$

In the above formula, $\hbar$ is the Planck constant, ω_m is the maximum vibration frequency of the lattice wave, and k_B is the Boltzmann constant. In some references, we found that the Debye temperature can be estimated by the average elastic wave velocity using a semi-empirical formula. The calculation formulas are as follows [38–41]:

$$\theta_D = \frac{h}{k_B}\left[\frac{3n}{4\pi}\left(\frac{N_A\rho}{M}\right)\right]^{\frac{1}{3}} v_m \tag{14}$$

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right)\right]^{-\frac{1}{3}} \tag{15}$$

$$v_l = \left(\frac{B + \frac{4}{3}G}{\rho}\right)^{\frac{1}{2}} \tag{16}$$

$$v_t = \left(\frac{G}{\rho}\right)^{\frac{1}{2}} \tag{17}$$

Where ρ is the density; N_A is the Avogadro constant; M is the weight of a single cell; n is the number of atoms in the unit cell. V_l and V_t represent the longitudinal sound velocity and the lateral sound velocity, respectively, and V_m is the average sound velocity in units of (m/s).

The minimum thermal conductivity k_{min} (W / (m × K)) is an important parameter to characterize the ability of materials to transfer heat. Melting point is an important parameter to characterize the heat resistance of alloy materials. Since the background we assumed is to use these alloys as electrode materials in NBI systems, it must have sufficient high temperature resistance and thermal conductivity. Therefore, the thermal conductivity and melting point of these materials are also estimated in this paper. In the references we found, Cahill and Pohl *et al.* believe that the minimum thermal conductivity and melting point of the material can be roughly obtained by the following empirical formula [41–43]:

$$k_{min} = \frac{k_B}{2.48} n^{\frac{2}{3}} (2v_t + v_l) \tag{18}$$

$$T_m = 354 + 4.5\frac{2C_{11} + C_{33}}{3} \tag{19}$$

Since for body-centered cubic lattice, C_{11} is equal to C_{33}. Therefore, the formula for estimating the melting point used in all alloys in this paper uses the following correction formula:

$$T_m = 354 + 4.5C_{11} \tag{20}$$

It can be seen from Table 5 that the Debye temperature (θ_D) of ternary alloy is greater than binary alloy, and the Debye temperature of these alloys ranks as follows: $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ > $W_{0.666}Ti_{0.1667}Zr_{0.1667}$ > $W_{0.67}Zr_{0.33}$ > $W_{0.5}Ti_{0.5}$ > $W_{0.67}Hf_{0.33}$. It can be seen that the change of Debye temperature is not obvious when Ti is added to the W-Zr unit cell. On the contrary, when Zr is added to the W-Ti unit cell, the Debye temperature is significantly increase. Similarly, there is an obvious increase for Debye temperature when Ti is introduced into W-Hf unit cell or Hf is introduced into W-Ti unit cell.

The minimum thermal conductivity of these alloys ranks as follows: $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ > $W_{0.67}Zr_{0.33}$ > $W_{0.666}Ti_{0.1667}Zr_{0.1667}$ > $W_{0.5}Ti_{0.5}$ > $W_{0.67}Hf_{0.33}$. The addition of Ti to the W-Zr unit cell has no significant change in the minimum thermal conductivity. On the contrary, when Zr is added to the W-Ti unit cell, the minimum thermal conductivity significantly improved. Similarly, there is an obvious increase for minimum thermal conductivity when Ti is introduced into W-Hf unit cell or Hf is introduced into W-Ti unit cell.

The melting point of these alloys ranks as follows: $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ > $W_{0.666}Ti_{0.1667}Zr_{0.1667}$ > $W_{0.67}Zr_{0.33}$ > $W_{0.67}Hf_{0.33}$ > $W_{0.5}Ti_{0.5}$. The addition of Ti to the W-Zr binary alloy has no obvious change for melting

point. The addition of Zr to the W-Ti unit cell has a significantly increase for melting point. There is an obvious increase for melting point when Ti is introduced into W-Hf unit cell or Hf is introduced into W-Ti unit cell.

Unfortunately, there is little previous research on the alloy materials in this paper, so it is difficult to find relevant literature to support our research results.

4 Summary and conclusions

The mechanical properties of tungsten-base alloys, including $W_{0.5}Ti_{0.5}$, $W_{0.67}Zr_{0.33}$, $W_{0.666}Ti_{0.1667}Zr_{0.1667}$, $W_{0.67}Hf_{0.33}$, $W_{0.666}Ti_{0.1667}Hf_{0.1667}$, were simulated by first-principles calculations based on density functional theory (DFT). The elastic constant and the elastic modulus combined with the empirical formula calculated the thermodynamic properties:

1. Comparing with experimental results, the calculated structure parameters are good agreement with it.
2. All tungsten-base alloys are mechanically stable.
3. The bulk modulus (B), shear modulus (G) and Young's modulus (E) of the $W_{0.666}Ti_{0.1667}Hf_{0.1667}$ ternary alloy are the greatest, even higher than pure W.
4. All tungsten-base alloys are ductile materials. The ductility of ternary alloys is lower than that of binary alloys, but higher than that of pure tungsten alloys. Further analysis by Poisson's ratio (σ) and Cauchy pressure (C') shows that metallic bond take the dominant position in all these crystal materials.
5. Debye temperature (θ_D), thermal conductivity and melting point of all alloy materials were predicted and discussed in combination with empirical formulas. These predictions may provide a corresponding reference for the subsequent application of the above alloys.

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