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Mechanical properties of W–Ti alloys from first-principles calculations

D.Y. Jiang[a,b,d], C.Y. Ouyang[c], S.Q. Liu[a,b,*]

[a] Department of Materials Science and Engineering, Nanchang University, Nanchang 330047, China
[b] Department of Physics, Nanchang University, Nanchang 330047, China
[c] Department of Physics, Jiangxi Normal University, Nanchang 330022, China
[d] School of Basic Sciences, Jiangxi University of Technology, Nanchang 330098, China

HIGHLIGHTS

- The mechanical properties of the $W_{1-x}Ti_x$ alloys are calculated from DFT.
- Ti alloying enhances the ductility of W metal substantially.
- The mechanical strength of W-Ti alloys is slightly weaker than W while stronger than Ti.

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ABSTRACT

The effect of Ti concentration on the fundamental mechanical properties of W-Ti alloys has been studied from first principles calculations. The lattice constants, the cell volumes and the formation energies of the $W_{1-x}Ti_x$ (x = 0.0625, 0.125, 0.1875, 0.25, 0.5) alloys were calculated. It is shown that Ti alloying in *bcc* W lattice is thermodynamically favorable when the Ti concentration is lower than 25% and the $W_{0.8125}Ti_{0.1875}$ have the lowest formation energy. With the optimized geometry and lattice, the elastic constants are calculated and then the elastic moduli and other mechanical parameters are derived. Results show that although the mechanical strength of the W-Ti alloys is lower than that of pure W metal, it is much higher than that of pure Ti metal. On the other hand, the B/G ratio and the Poisson's ratio of the W-Ti alloys is much higher than that of pure W, and even higher than that of pure Ti, indicating that Ti alloying can improve the ductility of *bcc* W substantially.

1. Introduction

Tungsten is receiving considerable attention as potential plasma facing material of the divertor and the first wall material in fusion power reactors, due to its high melting point, high strength at high temperatures, high sputtering threshold energy, good thermal conductivity and low thermal expansion coefficient [1–3]. In addition, tungsten is also thought as a shielding material in fusion reactors and other systems involving nuclear reactions [4]. Unfortunately, pure tungsten metal exhibits poor radiation stability and fracture toughness, low ductility associated with a high ductile-to-brittle transition temperature (DBTT). These properties are strongly dependent on the chemical composition and the micro-structural state [5]. Alloying is a good method to improve the physical properties of tungsten. For example, the thermal properties of tungsten are expected to be enhanced by alloying with other elements [6,7].

Among various alloying strategies of W metal, W-Ti alloy is one typical one [8,9]. To our knowledge, most experimental efforts of the binary W-Ti alloys have been devoted to understanding the effect of Ti concentration on the grain growth behaviors [10–14]. However, little attention was paid to the effect of Ti-alloying and the Ti concentration on the fundamental mechanical properties, such as elastic properties and ductile/brittle behaviors. The density-functional theory (DFT) calculation can be used to predict the mechanical performance of materials with relatively low cost and high efficiency, comparing with the experimental evaluations. Since conventional experimental alloy design processes can be very expensive and time-consuming, DFT calculations can be used to study the structure-property relationships and help to design these materials. The computational data may serve as guidance for further optimizing the composition of W-Ti alloys. Computer simulation focus on improving specific alloy properties can narrow down the number of compositions that are needed to be prepared and characterized.

In this paper, we studied the phase stability and mechanical properties of $W_{1-x}Ti_x$ alloys (x = 0.0625, 0.125, 0.1875, 0.25 and 0.5) from first principles calculations. The lattice constants, the cell vol-

* Corresponding author at: Department of Materials Science and Engineering, Nanchang University, Nanchang 330047, China.
E-mail address: sqlgroup@ncu.edu.cn (L. S.Q.).

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Table 1
The elastic constant of *bcc* W.

Method	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
Present work	529.94	211.19	139.44
Experiment [26]	533	205	163
Theory [26,27]	553	207	163

ume, the formation energies and the elastic constants of the $W_{1-x}Ti_x$ alloys are calculated. Based on the mechanical characteristic of B/G ratio, Poisson's ratio (ν) and Cauchy pressure (C'), the ductile/brittle properties of the W-Ti alloys are evaluated.

2. Model and computational details

Computations in the present work were done within the density-functional theory (DFT) and the plane-wave pseudopotential method, which were implemented in the Vienna *ab initio* simulation package (VASP) [15,16]. The core ion and valence electron interaction was described by the projector augmented wave method (PAW) [17], and the exchange-correlation part was described with the generalized gradient approximation (GGA) by Perdew and Wang (PW91) [18]. All models were described by a $2 \times 2 \times 2$ supercell containing 16 atoms in a body centered cubic (*bcc*) structures. Part of W atoms were substituted by the Ti atoms to obtain various alloys with different Ti concentrations, that is pure W, $W_{0.9375}Ti_{0.0625}$, $W_{0.875}Ti_{0.125}$, $W_{0.8125}Ti_{0.1875}$, $W_{0.75}Ti_{0.25}$, $W_{0.5}Ti_{0.5}$ and pure Ti. Except for the case of pure Ti, which was modeled with a hexagonal supercell, all the other systems were modeled with *bcc* supercells. For the Brillouin-zone sampling, we used the $11 \times 11 \times 11$ Monkhorst-Pack mesh [19] for all $W_{1-x}Ti_x$ alloys with *bcc* structures and a $6 \times 6 \times 4$ Monkhorst-Pack mesh for hexagonal close packing (*hcp*) phase titanium metal. A cutoff energy of 350 eV was used for all systems. Gaussian smearing method with a smearing width of 0.05 eV is applied in all calculations in this study.

Within the framework of the continuum elasticity theory [20,21], for the cubic structure, there are three independent elastic constants, i.e. C_{11}, C_{12} and C_{44}. In order to calculate these elastic constants, three sets of specific strains (δ) along different directions are applied to the cubic supercell, and the total energy changes are calculated as a function of the applied strains. Then, the elastic constants can be obtained through fitting the energy changes (ΔE) *vs* the applied strains (δ). For the hexagonal structure, there are five independent elastic constants, i.e. C_{11}, C_{12}, C_{13}, C_{33} and C_{44}. Similarly, five sets of specific strains (δ) along different directions are applied to the hexagonal supercell, and the elastic constants can be obtained through fitting the energy changes (ΔE) *vs* the applied strains (δ). The mechanical properties can be calculated from these single crystal elastic constants, according to the Voigt-Reuss-Hill scheme [22–25].The bulk modulus (B), shear modulus (G), Young's modulus (E), Poisson's ratio (ν) and Cauchy pressure (C') of the cubic W-Ti alloys are calculated with C_{11}, C_{12} and C_{44} and given by the following formula:

$$B = \frac{C_{11} + 2C_{12}}{3}, G = \frac{3C_{44} + C_{11} - C_{12}}{5},$$

Table 2
Bulk modulus (B), shear modulus (G), Young's modulus (E), B/G ratio, Poisson's ratio (ν), Cauchy pressure C' of *bcc* W.

Method	B (GPa)	G (GPa)	E (GPa)	B/G	ν	C' (GPa)
Present work	317.44	147.42	382.96	2.15	0.30	35.87
Experiment [26]	314.33	163.40	417.80	1.92	0.28	21.00
Theory [26,27]	322.33	173.00	440.24	1.86	0.27	22.00

Table 3
The elastic constant for *hcp* Ti.

Method	C_{11} (GPa)	C_{12} (GPa)	C_{13} (GPa)	C_{33} (GPa)	C_{44} (GPa)
Present work	175.61	84.45	81.98	188.34	41.41
Experiment [28]	176.10	86.90	68.30	190.50	50.80
Theory [29]	171.60	86.60	72.60	190.60	41.10

Table 4
Bulk modulus(B), shear modulus (G), Young's modulus (E), B/G ratio,Poisson's ratio (ν), Cauchy pressure C' of *hcp* Ti.

Method	B (GPa)	G (GPa)	E (GPa)	B/G	ν
Present work	115.12	44.94	119.30	2.56	0.327
Experiment [28]	109.96	50.16	130.62	2.19	0.302
Theory [29]	110.81	44.68	118.15	2.48	0.322

$$E = \frac{9BG}{3B + G}, \mathrm{V} = -1\frac{E}{2G}, C' = \frac{C_{12} - C_{44}}{2}$$

Similarly, the mechanic parameters B, G, E and ν of the hexagonal Ti are calculated from elastic constants C_{11}, C_{12}, C_{13}, C_{33} and C_{44}. The specific methods can be found in the literature [22–25].

3. Results and discussion

3.1. The mechanical properties of bcc tungsten (W) and hcp titanium (Ti)

The calculated single crystal elastic constants and mechanical property parameters of W and Ti are listed in Tables 1–4. For comparison purpose, we also list the data from experiments, as well as other theoretical results in the tables. Notice that the elastic constants as well as the mechanical parameters of the *bcc* W and *hcp* Ti metal from our calculations are basically in agreement with the experimental and other theoretical results. This confirms that the model and computational parameters are reasonable in the present work and therefore the following results on the W-Ti alloys are reliable. Furthermore, the elastic constants C_{44} for the *bcc* W is underestimated while the C_{13} for the *hcp* Ti is overestimated comparing with those experimental data. This is due to the GGA pseudopotentials we used in the current study. As GGA always underestimate the lattice constants of metal systems, it transfers this error to the calculation of the elastic constants.

3.2. The energetics and stability of the binary W-Ti alloys

First of all, the atomic positions and W-Ti configuration in the supercell are considered and optimized, and the configuration with the lowest total energy is chosen for further study. The schematic diagrams of the atomic configurations with the lowest total energy of the $W_{1-x}Ti_x$ alloys at different x value are shown in Fig. 1. As it is shown, the W-Ti alloys keep the *bcc* lattice, and the Ti atoms prefer to locate at positions to ensure that the structure is in a highest symmetry. This shows that the solid solution of the W-Ti alloy can be formed at the atomic level. In addition, to obtain the equilibrium lattice constant, we calculated the total energies as a function of the volume and then fit the results using Birch-Murnaghan equation of state. Fig. 2 shows the variation of the equilibrium lattice constants of $W_{1-x}Ti_x$ alloys as a function of the Ti concentration. When Ti concentration is less than 25%, the lattice constant of the $W_{1-x}Ti_x$ alloy decreases almost monotonically with x increases, due to the smaller radius of the Ti atom comparing with that of the W atom. However, when titanium concentration reaches 50%, the lattice starts to expand. The expanded lattice of the $W_{1-x}Ti_x$ alloys when x is high is related with the weakened bonding interaction between the W and Ti atoms, which will be discussed in the