

# First-principles study the phase stability and mechanical properties of binary W-Mo alloys



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## ABSTRACT

Based on the first principles calculations, the effect of Mo alloying on the mechanical properties of W-Mo alloys was investigated. First of all, we calculated the lattice constants, the cell volumes and the formation energies of  $W_{1-x}Mo_x$  ( $x = 0, 0.0625, 0.125, 0.25, 0.5, 0.75, 0.875, 0.9375$  and 1) alloys. Results show that W-Mo alloys remains *bcc* structures, and Mo alloying in *bcc* W lattice is an infinite solid solution. All the structures of W-Mo alloys are thermodynamically stable. Based on the optimized atomic lattices, we calculated the elastic constants of binary W-Mo alloys, and then derived the elastic modulus and other mechanical parameters. Results show that although the mechanical strength of W-Mo alloys is lower than that of pure W metal, it is much higher than that of pure Mo metal. On the other hand, by analyzing the mechanical parameters B/G ratio and Poisson's ratio of W-Mo alloys, Mo alloying can improve the ductility of pure W metal obviously.

## 1. Introduction

Nuclear fusion reactions can provide clean and unlimited use of energy for the future of mankind. However, H/He, high heat flux and neutron irradiation cause a large damage on plasma facing materials (PFMs). Tungsten is considered to be the most promising candidate for PFMs in fusion power reactors, due to its promising properties at higher temperatures [1–3]. However, some properties of tungsten need to be improved for the better survival in the fusion environment. For example, poor radiation stability and fracture toughness at low temperatures, low ductility associated with a high ductile-to-brittle transition temperature (DBTT). Therefore, there is an urgent need to develop tungsten materials. Alloying can improve the physical properties of pure W metal. For example, the thermodynamic properties of tungsten can be improved by alloying with other elements [4,5].

Among all alloying types of W metal, W-Mo alloys can be typical one. According to our survey, W-Mo alloy is a plasma-oriented component that is considered first as an advanced thermonuclear fusion reactor. At lower than DBTT, the W-Mo alloy limiter was operated and found to have a deeper crack throughout the limiter, but the irradiated rupture was lighter than pure W metal. When the temperature continues to rise, the surface of the W material limiter will locally melt under the action of energetic particles. If the W-Mo alloy material is heated prior to irradiation, no similar damage will occur. At the time of irradiation, if the added heat load continues at 20MW/M, W-Mo alloy will melt regardless of whether the cooling system is good or bad [6,7]. Zhang et al. [8]

studied the microstructures of W-Mo functionally graded materials. The relative density is up to 99.2%–99.8%. Martinez et al. [9] studied the microstructure, mechanical and electrical properties of nanocrystalline W-Mo thin films. The W-Mo films deposited under optimum sputtering pressure exhibit superior mechanical characteristics:  $H = 40$  GPa,  $Er = 275$  GPa,  $H/Er = 0.8$ , and  $H^3/Er^2 = 0.145$ , which are higher compared to pure,  $\alpha$ -phase W-films. Turchi et al. [10] applied a parameter-free electronic structure approach study of stability and chemical order in substitutional *bcc*-based Mo-W alloys. The results show that the method is a viable scheme to capture the alloy properties predicted from first-principles electronic structure calculations. Colinet et al. [11] studied the phase equilibrium theory of transition metal Mo-W alloys. Calculations of the enthalpies of formation of binary Mo-W alloys are also presented. The model is also used to calculate the miscibility gaps displayed by the Mo-W system. Zhang et al. [12] calculated the dilute-limit heats of solution and the heats of formation of binary W-Mo alloy with the analytic embedded-atom model for *bcc* pure metals by Johnson and Oh. The dilute-limit heats of solution are generally in agreement with available experimental values, and the calculated heats of formation are in good agreement with the available experimental data, the ab initio calculations, and the thermodynamic calculations. In addition, some transition metal elements, such as Mo, Fe, Cu, Mn, Cr and Ni, are impurities in W. Among them, the concentration of Mo impurity is highest [13]. In particular, the solution energies of Mo element are smaller than zero in the substitutional sites of W lattice, suggesting that Mo element can be easily dissolved in W [14]. So far,

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however, the effect of Mo alloying and the Mo concentration on the mechanical properties of pure W metal have been rarely reported, especially in the theoretical calculations. As we all know that the mechanical properties of binary W-Mo alloys are very important for PFMs. For example, elastic properties and ductile/brittle behavior can be used as a guide to further optimize the composition of binary W-Mo alloys. Since the traditional experimental alloy design process is very expensive and time-consuming, computational materials science can be used to study structure-performance relationships and help design the materials. Computer simulations focused on improving the performance of specific alloys can greatly reduce the number of compositions that need to be prepared and represented [15–19]. The density functional theory (DFT) is an effective approximation method to solve the multi-electron system structure [20], and it will obtain the total energy of the multi-electron system through the energy minimization method. The purpose of this paper is to find the minimum energy structure model as the main condition for calculating mechanical properties.

So, in this paper, first-principles study based on density functional theory, we thus investigated the phase stability and the mechanical properties of binary  $W_{1-x}Mo_x$  alloys ( $x = 0, 0.0625, 0.125, 0.25, 0.5, 0.75, 0.875, 0.9375$  and 1). At the same time, we calculated the cell volume, the lattice constants, the formation energies and the elastic constants of the  $W_{1-x}Mo_x$  binary alloys. According to the mechanical parameters of  $B/G$  ratio, Poisson's ratio ( $\nu$ ) and Cauchy pressure ( $C'$ ), the ductility of binary W-Mo alloys has been evaluated.

## 2. Model and computational details

In the current work, all computations were performed using the Vienna *ab initio* simulation package (VASP) [21,22]. Base on density-functional theory (DFT) and the plane-wave pseudopotential method. The interaction of valence electron and core ion was described by using the projector augmented wave method (PAW) [23]. In the PAW potential, the valence electrons of W and Mo atoms are  $W-6s^25d^4$  and  $Mo-4d^55s^1$ , respectively. The exchange-correlation part was treated using the generalized gradient approximation (GGA) by Perdew and Wang (PW91) [24]. All the models of *bcc* structure using a  $2 \times 2 \times 2$  supercell with 16 atoms. W-Mo alloys with different Mo concentrations are obtained by using Mo atoms instead of W atoms, which are pure W,  $W_{0.9375}Mo_{0.0625}$ ,  $W_{0.875}Mo_{0.125}$ ,  $W_{0.75}Mo_{0.25}$ ,  $W_{0.5}Mo_{0.5}$ ,  $W_{0.25}Mo_{0.75}$ ,  $W_{0.125}Mo_{0.875}$ ,  $W_{0.0625}Mo_{0.9375}$  and pure Mo. For the Brillouin-zone sampling, we used the  $11 \times 11 \times 11$  Monkhorst-Pack mesh [25] for all binary  $W_{1-x}Mo_x$  alloys. A cutoff energy of 400 eV was used for all systems, and further increase the cutoff energy has very little effect on the energy calculation. Gaussian smearing method with a smearing width of 0.05 eV is applied in all calculations to treat metallic systems. In addition, the equilibrium lattice constants of the *bcc* W and Mo were first calculated to be 3.1755 Å and 3.1534 Å, respectively, and the results are in good agreement with other theoretical and experimental values [10,26,27]. Although there are about a 1% discrepancy between the theoretical and experimental values of the lattice constant, the departures from Vegard's law are well reproduced. The results suggest that binary W-Mo alloy formation is favored.

Base on the continuum elasticity theory [28,29], for *bcc* structure, there are three independent elastic constants:  $C_{11}$ ,  $C_{12}$  and  $C_{44}$ . We can through fitting the energy changes ( $\Delta E$ ) vs. the strains ( $\delta$ ) to obtain these elastic constants. As shown in Table 1.

Then we can make use of these elastic constants to obtain the mechanical properties of W-Mo alloys according to the Voigt-Reuss-Hill scheme [30–33]. The bulk modulus ( $B$ ), shear modulus ( $G$ ), Young's modulus ( $E$ ), Poisson's ratio ( $\nu$ ) and Cauchy pressure ( $C'$ ) of binary W-Mo alloys are calculated by the following formula:

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

**Table 1**

The change relationship of strain and total energy of Cubic crystal system.

Strain	The total energy changes
$e = (0,0,0, \delta, \delta, \delta)$	$\frac{\Delta E}{V} = \frac{3}{2}C_{44}\delta^2$
$e = (\delta, \delta, \delta, 0,0,0)$	$\frac{\Delta E}{V} = (C_{11} + C_{12})\delta^2$
$e = (\delta, \delta, \delta, \delta, 0,0,0)$	$\frac{\Delta E}{V} = \frac{3}{2}(C_{11} + 2C_{12})\delta^2$

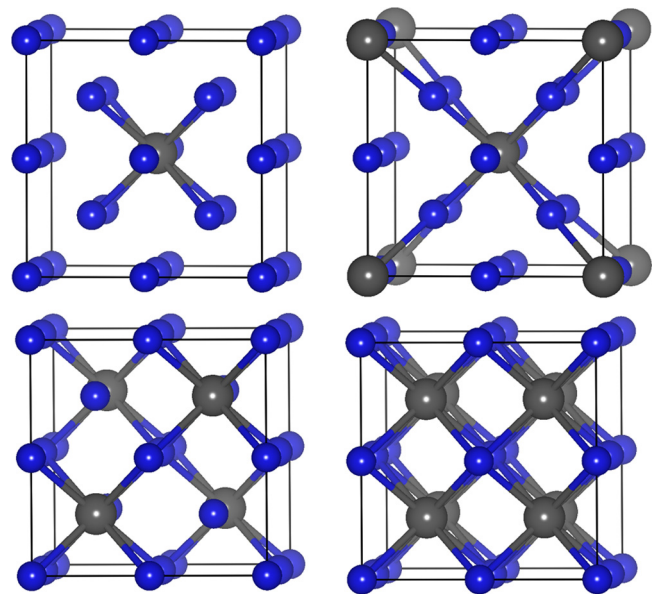
$$E = \frac{9BG}{3B + G}, \quad \nu = -1 + \frac{E}{2G}, \quad C' = \frac{C_{12} - C_{44}}{2}$$

## 3. Results and discussion

### 3.1. The energetics and phase stability of binary W-Mo alloys

First of all, we optimized the configuration and atomic positions of W-Mo alloys with different Mo concentrations in the supercell, and chose the lowest total energy configuration for further study. Fig. 1 shows the part atomic configuration of  $W_{1-x}Mo_x$  alloys with the lowest total energy, and the values of  $x$  are 0.0625, 0.125, 0.25 and 0.5, respectively. Small blue and large grey balls are W and Mo atoms, respectively. As it is shown, the W-Mo alloys remains keep *bcc* structure, and the Mo atoms tend to be in that position to ensure that the structure of W-Mo alloys is of the highest symmetry. It is explained that the solid solution of the W-Mo alloy can be formed at the atomic level.

In addition, we calculated the total energies as a function of the volume to obtain the equilibrium lattice constants of  $W_{1-x}Mo_x$  alloys. All these results were fitted using Birch-Murnaghan equation of state. The variation of the equilibrium lattice constants of  $W_{1-x}Mo_x$  alloys as a function of the Mo concentration are shown in Fig. 2. Because the radius of the Mo atom is smaller than that of the W atom, the lattice constants of W-Mo alloys decrease almost monotonically with Mo



**Fig. 1.** The energetically most favorable atomic arrangements of the *bcc*  $W_{1-x}Mo_x$  ( $x = 0.0625, 0.125, 0.25$  and  $0.5$ ) alloys in a  $2 \times 2 \times 2$  supercell. Small blue and large grey balls are W and Mo atoms, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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