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First-principles study of the phase stability and the mechanical properties of W-Ta and W-Re alloys

Ning Wei,1 Ting Jia,1 Xiaoli Zhang,1 Ting Liu,1 Z. Zeng,1,2,a and XiaoYu Yang3

1Key Laboratory for Materials Physics, Institute of Solid State Physics, Chinese Academy
of Sciences, Hefei, 230031, China
2University of Science and Technology of China, Hefei, 230026, China
3Computer Network Information Center (CNIC), Chinese Academy of Sciences Beijing
100190, P.O. Box 349, China

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The phase stability and mechanical properties of binary $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ alloys were investigated using the full-potential augmented plane-wave method. The special quasirandom structures (SQSs) of these alloys are mechanically stable due to all of the positive elastic constants and negative binding energies. The binding energies of both the $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ alloys also exhibit energy favorable asymmetry toward the W-rich side. In addition, the bulk modulus of the $W_{1-x}Ta_x$ alloys decrease gradually with the increase of the Ta concentration, while those of the $W_{1-x}Re_x$ alloys increase gradually with the increase of the Re concentration. Consequently, the bulk modulus of W metal can be improved by doping with Re, implying that the resistance to deformation is enhanced. Based on the mechanical characteristic $G/B$ and Poisson’s ratio $\nu$, both the $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ alloys are regarded as being ductile materials, the ductility of which improves with the increase of Ta or Re. © 2014 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution 3.0 Unported License. [http://dx.doi.org/10.1063/1.4875024]

I. INTRODUCTION

Tungsten has attractive engineering properties, including its high melting temperature, significant high-temperature strength and low sputtering rate, and it is of interest as a shielding material in fusion reactors and other systems involving nuclear reactions.1 Recently, tungsten is receiving attention as a candidate material for use in fusion power-plant technology, for example plasma-facing armor or shielding components, as well as for structural applications.2,3 However, tungsten has the problems of low-temperature brittleness and poor radiation stability. Alloying is a good method for improving the properties of tungsten. The thermal properties of tungsten are expected to be enhanced by alloying with other elements (Ni, Cu).4,5 Because Re and Ta are adjacent to W in the periodic table, efforts have been made from both experimental and theoretical aspects that focus on understanding the mechanical properties of $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ structures.6–9 It has been indicated that W and Ta form a continuous series of body-centered cubic (bcc) solid solutions according to the phase diagram of the W-Ta system. However, uncertainty exists in the phase diagram. For example, Turchi’s first-principles study within the tight-binding linear muffin-tin orbital formulation of the coherent pontential approximation (TB-LMTO-CPA)7 predicted three ordered phases: the B2 (CsCl structure) phase for $W_{0.5}Ta_{0.5}$ and the DO3 (Fe3Al structure) phase for $W_{0.75}Ta_{0.25}$ and $W_{0.25}Re_{0.75}$; meanwhile, Muzyk’s cluster expansion (CE) approach10 found new ordered structures for $W_{0.5}Ta_{0.5}$ and $W_{0.25}Ta_{0.75}$. There is a controversy regarding the ordered phases of $W_{1-x}Ta_x$ alloys. In fact, alloys generally represent randomness, and the existence

aElectronic mail: zzeng@theory.isp.ac.cn

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of intermediate phases has not been identified. Hence, we will focus our attention on the random phase of $W_{1-x}Ta_x$ alloys. However, experimentally, tungsten may transmute to rhenium under neutron irradiation, and its alloying with rhenium can go into a bcc solid solution under the equilibrium phase. Moreover, tungsten alloying with rhenium can reduce the ductile transition temperature (BDTT)\textsuperscript{11} and improve mechanical properties, such as increasing the ductility and the hardness, which, however, still lacks a theoretical explanation. Hence, in this work, we will focus on the random phase of $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ alloys and seek insight into the mechanical mechanism.

Elastic constants are important mechanical parameters, which provide helpful information about the comprehensive properties of materials. Generally, the elastic constants of pure phases can be calculated using electronic structure methods because they usually rely on periodic boundary conditions. However, the prediction of the elastic properties of random alloys is less straightforward. The most direct approach is the supercell method, in which the supercell must be sufficiently large to describe a random feature. This approach, therefore, requires more computation time, as well as more powerful computational tools. The special quasirandom structure (SQS)\textsuperscript{12} approach provides an effective means to solve this problem. In the SQS approach, instead of occupying the mixed-atom sites of a huge unit cell randomly to gain statistical significance, a relatively smaller unit cell is used. The small SQS cell is designed in such a way that the most physically relevant structural correlation functions of the small SQS cell best match the random alloy. Because the physical properties of an alloy are uniquely determined by its atomic structure, the SQS that mimics the atomic correlation function of a random alloy should also have physical properties similar to the random alloy. The structure can be completely relaxed by using density functional theory (DFT) codes and can be applied to any other system by changing the atoms because they are structural templates.\textsuperscript{13}

In this paper, we construct cells of 16-atom SQSs of $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ alloys at $x = 0.25, 0.50$ and $0.75$ to investigate their phase stability and their mechanical properties. The lattice constants of $W_{1-x}Ta_x$ increase gradually with increasing Ta concentration, while those of $W_{1-x}Re_x$ alloys decrease gradually with increasing Re. This behavior is caused by the difference in the atomic radius between the Ta and Re atoms. In addition, our equilibrium lattice constants of $W_{1-x}Ta_x$ alloys are in good agreement with the experimental values. Furthermore, our SQSs are mechanically stable, with positive elastic constants $C_{44}, C_{11}, C_{12}$ and $C_{11}/C_{12}$ and negative binding energies. The obtained value of Poisson’s ratio $\nu$, which is a critical value to indicate the ductility and its increase with doping of Ta or Re, of each of the SQSs is close to 0.3, and the obtained $B/G$, which is another criteria to distinguish the ductility and brittleness, of each of the SQSs is less than 0.57 and decreases with doping of Ta or Re, which imply that both $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ alloys are ductile materials and that the ductility of tungsten has been improved by alloying.

II. COMPUTATIONAL METHODS

The elastic constant, binding energy and electronic structure calculations were performed using the standard full-potential linearized augmented plane-wave code WIEN2K\textsuperscript{14} within density functional theory. The generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof form was used. The plane-wave cutoff parameters of $R_{MT}K_{\text{max}}$ and $G_{\text{max}}$ were chosen as 7.0 and 12.0, respectively. We used 1000 k points for the integration over the Brillouin zone.

The concept of SQS was first developed by Zunger \textit{et al.}\textsuperscript{12} to mimic random solutions without generating a large supercell or using many configurations. The SQS characterized the structure of the alloy by multisite correlation functions. For binary systems, any given arrangement of $A$ and $B$ atoms on a lattice is discretized into its component figures $f = (k, m)$, which is defined by the number $k$ of atoms located on its vertices ($k = 1, 2, 3$ are, for instance, sites, pairs and triplets) and the order $m$ of the neighbor distances separating them ($m = 1, 2, 3$ are, for instance, first, second and third-nearest neighbors). The correlation functions $\prod_{k,m}$ are the average of the products of the site occupations of figure $k$ at a distance $m$ and are used to describe the atomic distribution.\textsuperscript{15,16} For a perfectly random $A_{1-x}B_x$ structure, the many-body correlation functions are $(\prod_{k,m})_R = (2x-1)^k$, where $x$ is the composition. Consequently, the optimum SQS for a given composition is the one that
TABLE I. Pair and triple correlation functions of binary bcc SQSs at different compositions, where $x = 0.25, 0.50, 0.75$.

|                | Random | $x = 0.25$ | Random | $x = 0.50$ | Random | $x = 0.75$ |
|----------------|--------|------------|--------|------------|--------|------------|
| $\prod_{21}$   | 0.25   | 0.25       | 0      | 0          | 0.25   | 0.25       |
| $\prod_{22}$   | 0.25   | 0.1667     | 0      | 0          | 0.25   | 0.1667     |
| $\prod_{23}$   | 0.25   | 0.1667     | 0      | $-0.333$   | 0.25   | 0.1667     |
| $\prod_{24}$   | 0.25   | 0.25       | 0      | 0          | 0.25   | 0.25       |
| $\prod_{25}$   | 0.25   | 0          | 0      | 0          | 0.25   | 0.00       |
| $\prod_{31}$   | $-0.125$ | $-0.0833$ | 0      | 0          | 0.125  | $-0.083$   |
| $\prod_{32}$   | $-0.125$ | $-0.0833$ | 0      | 0          | 0.125  | $-0.083$   |
| $\prod_{33}$   | $-0.125$ | 0          | 0      | $-0.1667$  | 0.125  | 0          |
| $\prod_{34}$   | $-0.125$ | 0          | 0      | 0          | 0.125  | 0          |

The performance of the SQS method has already been successfully applied to investigate the thermodynamic and mechanical properties of binary solid solution phases for fcc, bcc and hcp phases.\textsuperscript{8, 17, 18} In this work, we constructed the SQSs of $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ alloys using $2 \times 2 \times 2$ bcc supercells at three compositions of $x = 0.25, 0.50$ and 0.75. The correlation functions of the generated SQSs are given in Table I. The selected SQSs at three different compositions match the requirement of later elastic constant calculations, because they are adequate with respect to their size and correlation functions.

Our generated SQSs are still cubic. By applying the cubic crystal symmetry operation, there are only three independent elastic constants: $C_{11}$, $C_{12}$ and $C_{44}$.

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

The elastic constants are defined by means of a Taylor expansion of the total energy $E(V, \delta)$ of the system, with respect to a small strain ($\delta$) of the lattice. The energy of the strained system by means of a Taylor expansion in the distortion parameters is

$$E(V, \delta) = E(V_0, 0) + V_0 \left( \sum_{i=1}^{6} \tau_i \delta_i + \frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} C_{ij} \delta_i \delta_j + O(\delta^3) \right)$$

where $\delta_i$ are related to the strain on the crystal, $C_{ij}$ are elastic constants, and $V_0$ is the volume of unstrained cubic system. The elastic constants are obtained by applying small strains to the unstrained lattice. For the cubic crystal, we require three different strains to determine three independent constants, as adopted in the WIEN2K\textsuperscript{14} package:

$$D_1 = \begin{pmatrix} 1 + \delta & 0 & 0 \\ 0 & 1 - \delta & 0 \\ 0 & 0 & \frac{1}{1 - \delta^2} \end{pmatrix}$$
\[ D_2 = \begin{pmatrix} 1 + \delta & 0 & 0 \\ 0 & 1 + \delta & 0 \\ 0 & 0 & 1 + \delta \end{pmatrix} \] (5)

\[ D_3 = \begin{pmatrix} 1 & \delta & 0 \\ \delta & 1 & 0 \\ 0 & 0 & \frac{1}{1-\delta^2} \end{pmatrix} \] (6)

where \( D_1 \) is the volume-conserving orthorhombic distortion, \( D_2 \) represents the change of the lattice parameter in the \( a \)-lattice direction and \( D_3 \) is the volume-conserving monoclinic distortion, respectively. \( \delta \) corresponds to the magnitude of the strain, which is varied from -0.04 to 0.04 in our work.

The energy change corresponding to these distortions is given by

\[ E_1(V, \delta) = E_1(V_0, 0) + V_0 \left((C_{11} - C_{12})\delta^2 + O(\delta^4)\right) \] (7)

\[ E_2(V, \delta) = E_2(V_0, 0) + V_0\delta(\tau_1 + \tau_2 + \tau_3) + V_0 \left(\frac{3}{2}(C_{11} + 2C_{12})\delta^2 + O(\delta^4)\right) \] (8)

\[ E_3(V, \delta) = E_3(V_0, 0) + V_0\left(2C_{44}\delta^2 + O(\delta^4)\right) \] (9)

By fitting the calculated energy-strain relationship using the third-order Birch-Murnaghan\textsuperscript{19, 20} equation and polynomial, \( C_{44} \) could be directly determined from Eq. (8). \( C_{11} \) and \( C_{12} \) are determined by combining the coefficient obtained from the \((C_{11} - C_{12})\) in Eq. (6) with the those obtained from the \((C_{11} + 2C_{12})\) in Eq. (7). Next, we can obtain the bulk modulus \( (B) \) and the shear modulus \( (G) \) as

\[ B = \frac{(C_{11} + 2C_{12})}{3} \] (10)

\[ G = \frac{(C_{11} - C_{12})}{2} \] (11)

The stability of the given structures and the values of other physical constants, such as Poisson’s ratio and Young’s modulus, could be derived through the use of the elastic constants.

### III. RESULTS AND DISCUSSION

#### A. Structure parameters

The schematic diagrams of the created SQSs with 16 atoms at different compositions are shown in Fig. 1. To obtain the equilibrium structural parameters, we calculated the total energies as a function of the volume and then fit the calculation results to Murnaghan’s equation of states. In Fig. 2(a), we show the variation of the equilibrium lattice parameters of \( W_{1-x}Ta_x \) alloys together with the TB-LMTO-CPA and the experiment result. The experimentally assessed lattice parameter-composition relation is represented by

\[ a = 3.164 + 0.1054c_{Ta} + 0.03226c_{Ta}^2, \]

where \( a \) is the lattice parameter, and \( c_{Ta} \) is the composition of \( Ta \).\textsuperscript{21} We can see that the generated SQSs are closer to the experiment than the TB-LMTO-CPA result. The lattice parameters of \( W_{1-x}Ta_x \) alloys increase slowly with an increase in the proportion of \( Ta \), while that of \( W_{1-x}Re_x \) alloys decrease slowly with an increase in the proportion of \( Re \) (Fig. 2(b)), due to either the smaller radius of \( Re \) or the larger radius of \( Ta \) in comparison to the radius of \( W \).

#### B. Phase stability and mechanical properties

Both \( W \) and \( Ta \) belong to the bcc phase, while \( Re \) belong to the hcp phase. Hence, \( Ta \) and \( W \) have three elastic constants: \( C_{11}, C_{12} \) and \( C_{44} \). In addition, \( Re \) has five independent elastic constants: \( C_{11}, C_{12}, C_{13}, C_{33} \) and \( C_{44} \). The calculated elastic constants of \( W, Ta \) and \( Re \) are listed in Tables II and III; for comparison, we also list the data from experiments, as well as other theoretical results. Notice that the bcc \( W \) and \( Ta \) metal calculated results are in good agreement with the experimental
FIG. 1. Atomic arrangements of the $A_{1-x}B_x$ binary bcc SQS in their ideal, unrelaxed forms, A is W and B is Ta or Re; (a) $x = 0.25$; (b) $x = 0.50$; (c) $x = 0.75$. 

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results for all the elastic constants as well as the bulk modulus and the shear modulus. For hcp phase Re, our calculated elastic constants ($C_{11}$, $C_{12}$, $C_{13}$, $C_{33}$ and $C_{44}$) are much closer to the experimental results comparing with the results of FP-LMTO-LDA. Overall, our results are satisfactory, which illustrates that our method is suitable for use in studying the elastic properties of the three metals considered.

Our primary concern is determining whether our generated SQSs are stable. The elastic constants and binding energy of W$_{1-x}$Ta$_{x}$ and W$_{1-x}$Re$_{x}$ summarized in Table IV is defined as:

$$E_b = E(eq) - (1-x)E_A - xE_B$$  

(12)
TABLE II. The elastic constants for bcc W and Ta.

| Method        | B  | G (Gpa) | C_{11} (Gpa) | C_{12} (Gpa) | C_{44} (Gpa) |
|---------------|----|---------|--------------|--------------|--------------|
| W Experiment  | 310.40 | 164.00 | 533.00 | 205.00 | 163.00 |
| Present work  | 299.86 | 165.90 | 521.09 | 186.25 | 150.54 |
| Theory        | 322.33 | 173.00 | 553.00 | 207.00 | 163.00 |
| Ta Experiment | 196.10 | 54.00  | 266.00 | 158.00 | 87.00  |
| Present work  | 204.04 | 60.60  | 284.82 | 163.65 | 65.51  |
| Theory        | 205.00 | 64.50  | 291.00 | 162.00 | 87.00  |

TABLE III. The elastic constants for hcp Re.

| Method        | B  | C_{11} (Gpa) | C_{12} (Gpa) | C_{33} (Gpa) | C_{44} (Gpa) |
|---------------|----|--------------|--------------|--------------|--------------|
| Experiment    | 360.00 | 273.00 | 206.00 | 683.00 | 161.00 |
| Present work  | 376.00 | 298.61 | 240.65 | 740.77 | 177.17 |
| Theory        | 447.00 | 323.00 | 278.93 | 822.01 | 222.00 |

TABLE IV. The elastic constants and \( E_b \) for binary \( W_{1-x}Ta_x \) and \( W_{1-x}Re_x \) alloys generated by SQS.

| Composition   | B  | G (Gpa) | C_{11} (Gpa) | C_{12} (Gpa) | C_{44} (Gpa) | \( E_b \) (eV) | G/B  | \( \nu \) |
|---------------|----|---------|--------------|--------------|--------------|--------------|------|-------|
| \( W_{0.25}Ta_{0.75} \) | 217.53 | 56.89  | 293.38 | 179.60 | 67.29 | – 7.752 | 0.25 | 0.38 |
| \( W_{0.50}Ta_{0.50} \) | 242.77 | 97.76  | 373.12 | 177.59 | 78.68 | – 9.384 | 0.40 | 0.32 |
| \( W_{0.75}Ta_{0.25} \) | 273.12 | 136.56 | 453.84 | 182.76 | 92.00 | – 10.88  | 0.50 | 0.29 |
| \( W \) | 299.86 | 165.90 | 521.09 | 189.25 | 150.54  | 0.00 | 0.55  | 0.27 |
| \( W_{0.75}Re_{0.25} \) | 312.32 | 156.55 | 521.06 | 207.95 | 148.94 | – 11.696 | 0.50 | 0.29 |
| \( W_{0.50}Re_{0.50} \) | 328.60 | 74.50  | 427.95 | 278.93 | 222.01 | – 9.928  | 0.23  | 0.39 |
| \( W_{0.25}Re_{0.75} \) | 344.43 | 106.13 | 485.94 | 273.67 | 299.00 | – 8.704  | 0.33  | 0.35 |

where \( x \) is the composition, \( E_A \) \( (E_B) \) is the energy of \( A(B) \), and \( E(eq) \) is the total energy of the alloy. The fact that the eigenvalues of the elastic constant matrices are positive and that all the binding energies are negative illustrates that our generated \( W_{1-x}Ta_x \) and \( W_{1-x}Re_x \) alloys are mechanically stable. The variation of the binding energy in Fig. 3(a) exhibits a strong energy favorable asymmetry towards the W-rich side. This binding energy characteristic was also determined by other theoretical approaches, such as US-PP, TB-LMTO CPA, CALPHAD, which provides validation to our use of SQSs. In addition, our SQSs have even lower binding energy than the first-principles or coherent potential approximations (CPA) predicted structures at the same concentrations. From Fig. 3(b), we also see a similar binding energy trend for the \( W_{1-x}Re_x \) alloys. This phenomenon is observed because tungsten has the highest cohesive energy among all of the transition metals in the Periodic Table. The alloys with high W concentration will have stronger binding. Therefore, our results, which exhibit a binding energy with a minimum value towards the W-rich side for both \( W_{1-x}Ta_x \) and \( W_{1-x}Re_x \) binaries, are reasonable.

Finally, we analyze the mechanical properties of the generated SQSs. The bulk modulus values listed in Table IV decrease with increasing Ta for the \( W_{1-x}Ta_x \) alloys, while the bulk modulus \( (B) \) increases gradually with the increase of the Re concentration for \( W_{1-x}Re_x \) alloys. The alloys doped with Re will improve the bulk modulus in comparison with that of pure tungsten. Hence, the resistance to deformation of tungsten will be raised by doping Re. In addition, the value of \( G \) versus \( B \) \( (G/B) \) and the value of Poisson’s ratio \( \nu \) are important mechanical characterizations. In fact, the value of \( G/B \) is used to distinguish the ductility and brittleness, i.e., the material exhibits ductility when the value of \( G/B \) is less than 0.57. The smaller the value of \( G/B \) is, the more ductile is the material. From the Table IV, we see all the values of \( G/B \) are less than 0.57, implying that both the \( W_{1-x}Ta_x \) and \( W_{1-x}Re_x \) alloys are ductile materials. In addition, the ductility of alloys with the increasing Ta or Re concentration are gradually improved. Regarding Poisson’s ratio \( \nu \), the value

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is also correlated with the ductility. Poisson’s ratio can be expressed in terms of the bulk modulus and the shear modulus: $\nu = (\frac{3B}{G} - 2)(\frac{6B}{G} + 2)$. This equation defines the numerical limits for Poisson’s ratio, $-1 \leq \nu \leq 0.5$, where the Poisson’s ratio of a ductile material is close to 0.3. The higher the value of Poisson’s ratio is, the more ductile is the material. As seen from Table IV, our values of Poisson’s ratio approach 0.3 exhibiting ductility and being enhanced by doping with Ta or Re. This behavior supports the $G/B$ result that both $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ alloys belong to the ductile material.

C. Electronic structure

The total electronic density of states (DOS) for $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ alloys at different compositions are shown in Fig. 4. The major contribution near the Fermi level from $-5$ eV to $2$ eV...
FIG. 4. The density of states (DOS) of bcc-based chemically random $W_{1-x}Ta_x$ and $W_{1-x}Re_x$. (a) $W_{1-x}Ta_x$ when $x = 1$; (b) $W_{0.25}Ta_{0.75}$; (c) $W_{0.5}Ta_{0.5}$; (d) $W_{0.75}Ta_{0.25}$; (e) $W_{1-x}Re_x$ when $x = 0$; (f) $W_{0.75}Re_{0.25}$; (g) $W_{0.5}Re_{0.5}$; (h) $W_{0.25}Re_{0.75}$. The energy is with respect to the Fermi level.

is from the 5d orbital of W, Ta, or Re. There is no significant change among all the DOS because all three elements are neighbors in the periodic table, with little difference in their electronic orbital features. In principle, the Fermi level of W metal spans a deep minimum of the DOS, which clearly separates the bonding and antibonding states in the alloy electronic structure. As the concentration of Ta increases, the Fermi level moves away from the minimum of the DOS and towards the left peak, which is primarily derived from the 5d electrons of the alloy atom. In addition, bonding in the alloys becomes more metallic. For the $W_{1-x}Re_x$ alloys, the Fermi level shifts gradually away from the bottom of the DOS to the right side as the concentration of Re increases. This variation of the electronic structure properties is entirely determined by the variation of the total number of valence electrons of the $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ alloys.

IV. CONCLUSIONS

We have created periodic SQSs with 16 atoms for the $A_{1-x}B_x$ binary bcc substitutional alloys at three different compositions where $x = 25, 50,$ and $75$ percent and performed detailed calculations.
on their phase stability, mechanical properties and electronic structure using the DFT method. All of the elastic constants of the generated SQSs are positive, which indicates that our structures possess mechanical stability. The results exhibit a binding energy with a strong energy favorable asymmetry toward the W-rich side for both $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ binaries from the obtained binding energy of the SQSs. The bulk modulus indicates that W doped with Re is good for the improvement of the resistance to deformation. By analyzing the value of Poisson’s ratio $\nu$ and the value of $B/G$, we demonstrate that both $W_{1-x}Ta_x$ and $W_{1-x}Re_x$ alloys are ductile materials. In addition, increasing the Ta or Re doping concentration in tungsten is helpful to improve the ductility.

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