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Comparative study of metastable phase formation in the immiscible Cu–W system by *ab initio* calculation and *n*-body potential

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Abstract

The lattice constants and cohesive energies of some possible metastable Cu–W compounds are obtained by *ab initio* calculation and the formation of a metastable phase at Cu₇₅W₂₅ is predicted for the equilibrium immiscible Cu–W system. The prediction is in agreement with the fact that a metastable hcp phase was indeed observed in the Cu₇₅W₂₅ multilayer films upon ion beam mixing. Furthermore, some of the *ab initio* calculated properties are used in deriving an *n*-body Cu–W potential under the embedded atom method. The constructed Cu–W potential is then used to predict the phase stability of the metastable Cu–W phases over the entire composition and the prediction is also supported by some experimental observations.

1. Introduction

With the development of various highly nonequilibrium materials processing techniques, such as ion beam mixing (IBM), vapour deposition, mechanical alloying, etc, a variety of metastable alloys in the immiscible binary metal systems have been obtained during the past decades [1, 2]. It is of interest that a number of similar nonequilibrium crystalline phases have been obtained by IBM. For instance, in the equilibrium immiscible Cu–W system with a positive heat of formation (ΔH_f) of +33 kJ mol⁻¹ [3, 4], some metastable Cu–W phases have been synthesized during the last two decades [5–9]. To understand the formation of such nonequilibrium phases is a challenging issue for theoretical investigation. Some researchers have studied the thermodynamic stabilities of nonequilibrium solid phases [5]. To reveal the

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physical origins of formation and stabilities of nonequilibrium phases at the atomic scale level and the electronic structure level, it is necessary to perform first-principles calculations and construct the n -body potential which, however, has scarcely been studied hitherto. For the immiscible Cu–W system, there does not exist any equilibrium compound that could provide useful physical data for deriving the cross potential. For such a case, there has been some literature [10–13] showing that the first-principles calculations could be of significant help in acquiring some useful physical properties for deriving the potentials.

In the present study, we combine *ab initio* calculation and n -body potential calculation to predict the metastable phase formation in the Cu–W system. First, *ab initio* calculation is conducted to predict the lattice constants and cohesive energies of some possible compounds with the compositions of $\text{Cu}_{75}\text{W}_{25}$ and $\text{Cu}_{50}\text{W}_{50}$ respectively and some possible metastable states have been predicted for $\text{Cu}_{75}\text{W}_{25}$ alloy. Second, through fitting the *ab initio* calculated properties of the metastable Cu–W compounds, an n -body potential is derived under the framework of an embedded-atom method (EAM) [14]. Third, applying the newly constructed EAM potential, the metastable phase selection is predicted over entire composition range in the Cu–W system. Finally, the calculated results drawn from *ab initio* calculation and n -body potential will be compared with some typical experiments.

2. Calculation methods

2.1. Method of first-principles calculation

The first-principles calculation is based on the well established Vienna *ab initio* simulation package (VASP) [15]. In the package, the calculations are conducted in a plane-wave basis, using fully nonlocal Vanderbilt-type ultrasoft pseudopotentials to describe the electron–ion interaction [16], which allows the use of a moderate cut-off for the construction of the plane-wave basis for the transition metals. In the calculation, the exchange and correlation items are described by the generalized-gradient approximation (GGA) proposed by Perdew and Wang [17]. The integration in the Brillouin zone is done on special k points determined according to the Monkhorst–Pack scheme [18].

It is known that for an A–B metal system, there are about 20 most common structures for the A_3B or AB_3 phases, i.e., A15, Ae, D0₂, D0₃, D0₉, D0₁₁, D0₁₈, D0₁₉, D0₂₀, D0₂₁, D0₂₂, D0₂₃, D0₂₄, D0_a, D0_b, D0_c, D0_d, L1₂, L1_a, and L₆₀. The choosing of the possible structures in our *ab initio* calculation is based on the following considerations: firstly, we exclude those complicated structures, such as D0₂, D0₂₁ and L1_a, that have more than 16 atoms per unit cell according to Pearson notation [19]. Generally, for a complicated structure, its unit cell containing more atoms frequently corresponds to a larger size than the one composing fewer atoms, and therefore it probably requires a relatively large critical radius for nucleation and growth. It follows that the above-mentioned phases of complicated structures probably require a long time for atoms to organize themselves into an ordered configuration. In other words, if kinetic conditions are restricted, it is difficult for these structures to form. Secondly, the nonequilibrium crystalline phases obtained so far by IBM are usually of simple structures, such as hcp and fcc structures, but never of any possible complicated structures due to the restricted kinetic conditions available in the material preparation processes [20]. Therefore, six structures, i.e., A15, D0₂₂, D0₁₉, L₆₀, D0₉, and L1₂, are calculated to find out whether the respective nonequilibrium phases of A_3B type might be relatively stable and obtained by IBM or other methods. Besides, the $\text{Cu}_{75}\text{W}_{25}$ compound with L1₂ structure and the $\text{Cu}_{50}\text{W}_{50}$ compound with B2 structure are selected and calculated for providing some useful physical properties for deriving the n -body potentials.

2.2. Construction of n -body Cu–W potential

In the present study, an n -body Cu–W potential is constructed under the framework of a well known embedded atom method [14]. The EAM is based on the density-functional theory (DFT), and is one of the most efficient methods for constructing the realistic n -body potentials. In the EAM, the total energy E_{tot} , which can be written as a unique function of the electron density ρ_i , is mainly the energy to embed the atom into the electron density of the neighbouring atoms, supplemented by a short-range doubly screened pair interaction that accounts for the core–core repulsions [21]. That is,

$$E_{\text{tot}} = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{\substack{i,j \\ (i \neq j)}} \phi_{ij}(r_{ij}) \quad (1)$$

$$F(\rho_i) = -F_0 \left[1 - \ln \left(\frac{\rho_i}{\rho_e} \right)^n \right] \left(\frac{\rho_i}{\rho_e} \right)^n + F_1 \left(\frac{\rho_i}{\rho_e} \right) \quad (2)$$

$$\rho_i = \sum_{j \neq i} f_j(r_{ij}) \quad (3)$$

where $F(\rho_i)$ is the energy required to embed atom i into the background electron density ρ_i , $\phi_{ij}(r_{ij})$ and r_{ij} are respectively the short-range pair potential and the separated distance between atom i and atom j , and $f_j(r_{ij})$ is the electron density at the site of atom i contributed by atom j . The atomic electron density $f(r)$ takes the form of function $f(r) = f_e \exp[-\chi(r/r_e - 1)]$, where f_e is a scaling factor determined by the cohesive energy E_c and the atomic volume Ω . $F_0 = E_c - E_v^f$, where E_v^f is the vacancy formation energy. F_1 is an adjustable parameter for pure Cu with an fcc structure while it is set to be zero for pure W with a bcc structure [22]. ρ_e is the host electron density in an equilibrium state. Since the embedding function is universal, not depending on the source of the background electron density, the same embedding function can be used to calculate the energy of an atom in an alloy as is used in the pure metal [23].

In the present study, the pair potential $\phi(r)$ adopts the expression proposed by Cai and Ye [24] for pure Cu, and the one suggested by Johnson and Oh [22] for pure W. Accordingly, they are expressed as

$$\phi_{\text{Cu}}(r) = -\alpha[1 + \beta(r/r_a - 1)] \exp[-\beta(r/r_a - 1)] \quad (4)$$

$$\phi_{\text{W}}(r) = \begin{cases} \Phi(r) = k_0 + k_1(r/r_e - 1) + k_2(r/r_e - 1)^2 + k_3(r/r_e - 1)^3, & r_e \leq r \leq r_s \\ \Phi_a(r) = \Phi(r) + k_a[\Phi(r) - \Phi(r_e)](r/r_e - 1)^2, & r < r_e \end{cases} \quad (5)$$

where r is the interatomic distance, r_e is an equilibrium first-neighbour distance, k_a is a constant in the form of $k_a = 4.5[1 + 4/(A_r - 0.1)]$ depending on an anisotropy ratio A_r , and the cut-off distance (from r_s to r_e) is set to be between the second- and third-neighbour distances [25]. In the function forms of the potentials, there are five parameters (χ , α , β , r_a , F_1) to be fitted for the Cu–Cu potential and another five parameters (χ , k_0 , k_1 , k_2 , k_3) to be fitted for the W–W potential. The Cu–W cross potential takes a combination of the Cu–Cu and W–W potentials, which was proposed recently by Gong [12],

$$\phi_{\text{CuW}}(r) = A[\phi_{\text{Cu}}(r + B) + \phi_{\text{W}}(r + C)] \quad (6)$$

where A , B , and C are three potential parameters to be fitted. It should be pointed out that some experimental data of Cu and W are used in fitting the Cu–Cu and W–W potentials, and the *ab initio* calculated cohesive energies and lattice constants of the possible $\text{Cu}_{75}\text{W}_{25}$ compound with $L1_2$ structure and $\text{Cu}_{50}\text{W}_{50}$ compound with $B2$ structure are used in fitting the Cu–W cross potential.

With the constructed n -body potential, the total energy for fcc (or bcc) solid solution can be calculated by the following equation, which was proposed recently by Fang [26]:

$$E_{\text{fcc (bcc)}} = X_{\text{Cu}} \left[\frac{1}{2} \phi_{\text{Cu}} + F_{\text{Cu}}(\rho) + E_c^{\text{Cu}} \right] + X_{\text{W}} \left[\frac{1}{2} \phi_{\text{W}} + F_{\text{W}}(\rho) + E_c^{\text{W}} \right] \quad (7)$$

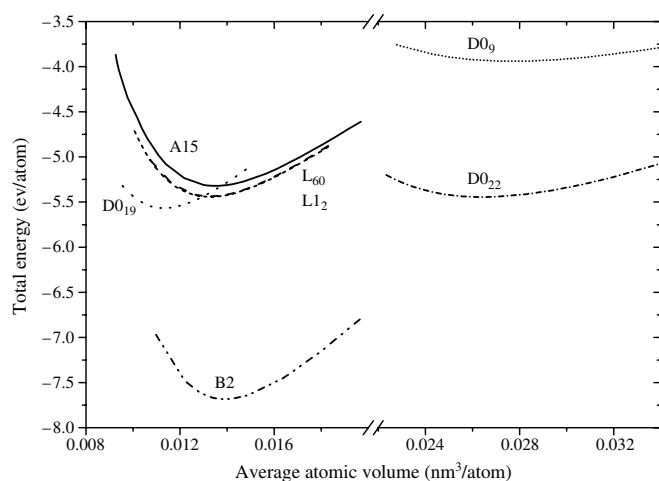


Figure 1. The *ab initio* calculated total energy versus average atomic volume for $\text{Cu}_{50}\text{W}_{50}$ compounds with B2 structure and $\text{Cu}_{75}\text{W}_{25}$ compounds with D0₉, D0₁₉, D0₂₂, A15, L₆₀, and L1₂ structures respectively.

where X_{Cu} and X_{W} are the compositions for Cu and W in fcc (or bcc) solid solution respectively. ϕ_{Cu} and ϕ_{W} are the pair potentials for atoms Cu and W in fcc (or bcc) solid solution respectively. $F_{\text{Cu}}(\rho)$ and $F_{\text{W}}(\rho)$ are the embedding energy for atoms Cu and W in the fcc (or bcc) solid solution respectively. E_{c}^{Cu} and E_{c}^{W} are the cohesive energy for metals Cu and W respectively. As for any compositions, the total energy for fcc (or bcc) solid solution can be calculated by minimizing the average energy $E_{\text{fcc (bcc)}}$ of fcc (or bcc) solid solution per atom with respect to lattice parameter.

3. Results and discussion

3.1. *Ab initio* calculation results

In this section, the calculation results for the possible $\text{Cu}_{75}\text{W}_{25}$ compounds are presented. The correlations between the total energy and average atomic volume for the $\text{Cu}_{75}\text{W}_{25}$ and $\text{Cu}_{50}\text{W}_{50}$ compounds with different simple structures, i.e., D0₉, D0₁₉, D0₂₂, A15, L₆₀, and L1₂ structures for the $\text{Cu}_{75}\text{W}_{25}$ compounds and B2 structure for the $\text{Cu}_{50}\text{W}_{50}$ compound, are calculated and shown in figure 1. Figure 1 shows that the increasing order of relative structural stability for the possible $\text{Cu}_{75}\text{W}_{25}$ compounds is D0₉, A15, L₆₀, L1₂, D0₂₂, and D0₁₉. The D0₁₉ structure has the lowest minimum total energy among the above six structures. It is commonly known that an energetic reference state at a specific alloy composition is referred to a corresponding mechanical mixture of the constituent metals. For the Cu–W system, a mechanical mixture of pure Cu and pure W with a chemical stoichiometry of 3:1 is set as a reference state and its cohesive energy is calculated to be 6.0206 eV/atom. Based on this reference state, the formation energy of an alloy phase is defined as the difference between the metastable and the reference states. Some characteristics, such as lattice constants, cohesive energies, etc., of D0₉, D0₁₉, D0₂₂, A15, L₆₀, and L1₂ structures for the $\text{Cu}_{75}\text{W}_{25}$ compounds and pure fcc Cu and bcc W are calculated and listed in table 1. Based on these data, the formation energies of $\text{Cu}_{75}\text{W}_{25}$ compounds in the six structures are calculated and also listed in table 1. From the table, it can be seen that the formation energies of $\text{Cu}_{75}\text{W}_{25}$ compounds are higher than that of the reference state, suggesting that the equilibrium $\text{Cu}_{75}\text{W}_{25}$ compounds are energetically impossible and cannot be formed by equilibrium experimental conditions. With respect to energy, if some extra energy can be provided to overcome the energy gap by employing some powerful nonequilibrium or even far-from-equilibrium method, such as ion beam mixing of

Table 1. The calculated formation energy of Cu₇₅W₂₅ compounds in D0₉, A15, L1₂, L₆₀, D0₂₂, and D0₁₉ structures and the characteristics of pure Cu and W.

Pure metal			Cu ₇₅ W ₂₅			
Pure metal	<i>a</i> (Å)	<i>E_c</i> (eV/atom)	Structure	<i>a</i> (Å)	<i>E_c</i> (eV/atom)	ΔH (eV/atom)
Fcc Cu	3.641	3.724	D0 ₉	4.811	3.939	2.0816
Bcc W	3.173	12.911	A15	4.758	5.319	0.7016
Cu ₇₅ W ₂₅ ^a		6.0206	L1 ₂	3.759	5.436	0.5846
			L ₆₀	3.962	5.441	0.5796
			D0 ₂₂	3.618	5.444	0.5793
			D0 ₁₉	2.645	5.566	0.4546

^a The mechanical mixture of pure Cu and W with a chemical stoichiometry of 3:1.

multilayers, the metastable D0₁₉ Cu₇₅W₂₅ compounds with the lowest energy among the six structures might be obtained.

3.2. *n*-body potential calculation results

With the calculated total energy and equilibrium lattice constants for the metastable L1₂ Cu₇₅W₂₅ and B2 Cu₅₀W₅₀ compounds, the *n*-body potential can be fitted for the Cu–W systems. The selection of L1₂ structure for the Cu₇₅W₂₅ compound and the B2 structure for the Cu₅₀W₅₀ compound is arbitrary and only from the point of simplification for fitting the potential. In order to fit the Cu–W cross potential, the Cu–Cu and W–W potentials should be fitted first. However, the cohesive energies fitted for the Cu–Cu and W–W potentials are not from *ab initio* calculation but from experimental data. Consequently, the cohesive energies for L1₂ Cu₇₅W₂₅ and B2 Cu₅₀W₅₀ compounds obtained by *ab initio* calculation cannot directly be used for fitting the Cu–W cross potential and should be corrected by the cohesive energy adopted for fitting the Cu–Cu and W–W potentials. To make such a correction, the formation enthalpy should be obtained from the *ab initio* calculation by

$$\Delta H = \frac{E_{\text{CuW-ab}} - X_{\text{Cu}}E_{\text{Cu-ab}} - X_{\text{W}}E_{\text{W-ab}}}{(X_{\text{Cu}} + X_{\text{W}})} \quad (8)$$

where $E_{\text{CuW-ab}}$, $E_{\text{Cu-ab}}$ and $E_{\text{W-ab}}$ are the cohesive energies obtained by *ab initio* calculation for the CuW compound, the pure metal Cu and pure metal W, respectively. X_{Cu} and X_{W} are the atom concentrations of Cu and W, respectively. And then, according to the calculated formation enthalpy, the realistic cohesive energies can be corrected by the following formula:

$$E_{\text{c}} = \frac{X_{\text{Cu}}E_{\text{Cu-exp}} + X_{\text{W}}E_{\text{W-exp}}}{(X_{\text{Cu}} + X_{\text{W}})} + \Delta H \quad (9)$$

where E_{c} , $E_{\text{Cu-exp}}$, and $E_{\text{W-exp}}$ are the corrected cohesive energy for the CuW compounds and the cohesive energies adopted for fitting the Cu–Cu and W–W potentials, respectively.

After the fitting procedure and optimization, the potential parameters of the Cu–W system are obtained and listed in table 2. Accordingly, table 3 lists the fitted results of the Cu–Cu and W–W potentials and one can observe that the Cu–Cu and W–W potentials could reproduce the exact values of some physical properties of the pure Cu and W metals [27–29]. Applying the constructed potential for the pure metal, the cohesive energies, and the lattice constants for the Cu₅₀W₅₀ compound in B2 and the Cu₇₅W₂₅ compound in L1₂ structure, the Cu–W cross potential is derived, and the fitted parameters are also listed in table 3. With the constructed potentials, the physical properties of the possible Cu₇₅W₂₅ compound in L1₂ structure and the possible Cu₅₀W₅₀ compound in B2 structure can be calculated and compared with the results

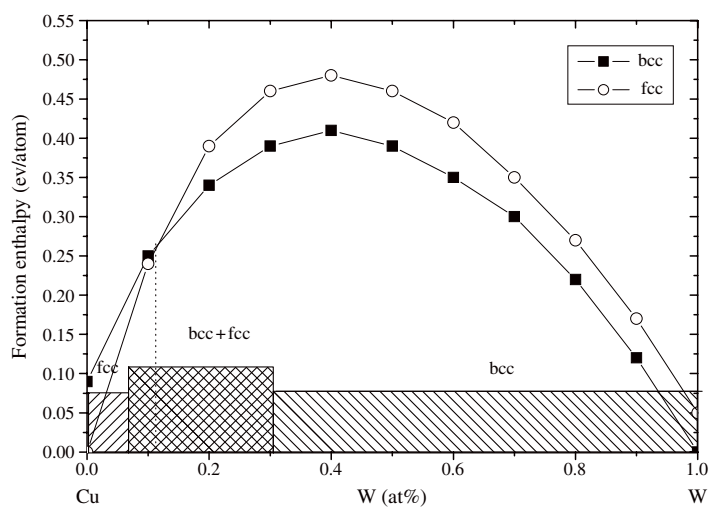


Figure 2. Calculated formation enthalpy (ΔH_f) by n -body potential versus the W compositions for the metastable fcc and bcc Cu-W phases, respectively.

Table 2. Fitted parameters for the Cu-Cu, W-W, and Cu-W potentials.

	Cu-Cu		W-W		Cu-W	
χ	11.134 11	χ	6.180 475	A	0.566 522	
α (eV)	0.728 40	k_0 (eV)	-0.581 958	B (Å)	0.495 555	
β	3.450 96	k_1 (eV)	-2.175 059	C (Å)	0.083 299	
r_a (Å)	1.626 84	k_2 (eV)	17.053 662			
F_1 (eV)	0.676 48	k_3 (eV)	-8.215 139			
r_s (Å)	3.696	r_s (Å)	3.236			
r_c (Å)	4.102	r_c (Å)	3.592			
n	0.333 333	n	0.44			

Table 3. The values of cohesive energy E_c (eV), lattice constant a (Å), elastic constants (Mbar), and vacancy formation energy E_v^f (eV) of Cu and W between calculated and experimental data [27–29].

	Cu		W	
	Experimental	Fitted	Experimental	Fitted
E_c (eV)	3.54	3.54	8.66	8.66
a (Å)	3.615	3.615	3.16	3.16
C_{11} (Mbar)	1.70	1.70	5.326	5.326
C_{12} (Mbar)	1.225	1.225	2.05	2.05
C_{44} (Mbar)	0.758	0.758	1.63	1.63
E_v^f (eV)	1.30	1.30	3.95	3.95

obtained from *ab initio* calculation. All of the calculated results are listed in table 4. From the table, it is readily found that the agreement for the $\text{Cu}_{75}\text{W}_{25}$ compound with $L1_2$ structure is within an error of 0.8%, and for the $\text{Cu}_{50}\text{W}_{50}$ compound with B2 structure it is within an error of 0.74%. The results obtained by the fitted interatomic potentials are therefore in good agreement with those obtained from *ab initio* calculation.

With the constructed potential, the metastable phase selection for fcc and bcc solid solutions over the entire composition range is calculated by minimizing the average energy

Table 4. Total energy E_t and lattice constant a of the $\text{Cu}_{75}\text{W}_{25}$ compound in L1_2 structure and the $\text{Cu}_{50}\text{W}_{50}$ compound in B2 structure obtained by *ab initio* calculations as well as derived by the fitted potential.

Phase	Structure	By <i>ab initio</i> calculation		From the fitted potential	
		E_t (eV/atom)	a (Å)	E_t (eV/atom)	a (Å)
$\text{Cu}_{50}\text{W}_{50}$	B2	−5.5707	3.034	−5.6116	3.099
$\text{Cu}_{75}\text{W}_{25}$	L1_2	−4.2699	3.759	−4.2846	3.820

per atom with respect to lattice parameter. After that, some physical properties of the fcc (or bcc) solid solution are calculated and the calculated ΔH_f of the $\text{Cu}_{100-x}\text{W}_x$ solid solutions versus the W compositions are shown in figure 2. It can be observed from the figure that when $11 < x \leq 100$, the bcc $\text{Cu}_{100-x}\text{W}_x$ phase has lower ΔH_f and is more stable than the fcc one, and when $0 \leq x \leq 11$, the fcc $\text{Cu}_{100-x}\text{W}_x$ phase becomes energetically favoured.

3.3. Comparison with experimental results

We now turn to compare the *ab initio* calculation results concerning the metastable compounds (MC) with those obtained by ion beam mixing of the $\text{Cu}_{75}\text{W}_{25}$ multilayered sample [5]. It was shown that before the critical irradiation dose of $1 \times 10^{15} \text{Xe}^+ \text{cm}^{-2}$ a crystalline solid phase was observed and identified by selected-area diffraction to be of Cu-rich MC hcp phase. The lattice parameters of the hcp phase were determined to be $a_{\text{hcp}} = 2.71 \text{Å}$ and $c_{\text{hcp}} = 4.34 \text{Å}$ within an error of 4%. Note that the lattice constant of the D0_{19} structure from *ab initio* calculation and from n -body potential is $a_{\text{hcp}} = 2.645 \text{Å}$ and $a_{\text{hcp}} = 2.69 \text{Å}$, respectively. Apparently, the experimental and calculated lattice constants of the MC $\text{Cu}_{75}\text{W}_{25}$ hcp phase are in good agreement within an error of 2.4%. It should be pointed out that the above diffraction analysis only confirms the existence of a $\text{Cu}_{75}\text{W}_{25}$ hcp structure, but not exactly an ordered $\text{Cu}_{75}\text{W}_{25}$ hcp structure. Nonetheless, the reported ion beam mixing results do confirm the existence of such a metastable state located near $\text{Cu}_{75}\text{W}_{25}$ with an hcp structure in the Cu–W system. In this sense, the experimental and first principles calculation results are considered to be compatible.

As for the metastable phase selection over the entire composition in the immiscible Cu–W system, there are many experimental results that are in support of the above prediction by the constructed n -body potential. The selected experimental results [5–9] are also marked with differently filled pattern in figure 2. From the figure, it can clearly be seen that in experiments the fcc solid solution was obtained in the composition range when $0 < x \leq 5$ and the bcc solid solution was obtained when $33 < x \leq 100$, while until now only the bcc + fcc mixture was obtained when $5 < x \leq 33$. It should be pointed out that there is a significant stretch of coexisting bcc and fcc phase (from 5 to 33 at.% W), which is absent in the theoretical calculation. Such a case cannot be fully interpreted only from the point of view of energy, but may be determined by some kinetic factors in specific experiments. Therefore, the coexistence of bcc and fcc phases cannot be interpreted by the present study and requires further studies. Nonetheless, some other experimental observations are also in support of the above prediction drawn from the n -body potential, i.e., when $33 < x \leq 100$, the bcc $\text{Cu}_{100-x}\text{W}_x$ phase has lower ΔH_f and is more stable than the fcc one, and when $0 \leq x \leq 5$, the fcc $\text{Cu}_{100-x}\text{W}_x$ phase becomes energetically favoured.

4. Concluding remarks

- (1) Using the well established Vienna *ab initio* simulation package, the lattice constants and cohesive energies of some possible metastable $\text{Cu}_{75}\text{W}_{25}$ compounds are calculated for

the highly immiscible Cu–W system. The results reveal that the calculations are quite relevant in correctly predicting the existence of a metastable Cu₇₅W₂₅ hcp phase, which has indeed been observed experimentally.

- (2) An *n*-body EAM potential is constructed for the Cu–W system by fitting some of the *ab initio* calculated results together with some experimental data, and applying the constructed potential the total energies for the L1₂ and B2 structures are calculated and are in reasonable agreement with the results obtained from *ab initio* calculation.
- (3) Based on the constructed *n*-body EAM potential, the metastable phase selection of the Cu–W system over the entire composition range is predicted and the results show that the metastable Cu_{100–x}W_x phase in an fcc structure is more stable than in the bcc structure when $0 \leq x \leq 11$, whereas the bcc structure becomes energetically favoured when $11 < x \leq 100$ in the Cu–W system, which is indeed supported by some of the selected experimental results.

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