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Atomistic Calculations of Interface Properties for Co-Al-W Alloys

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Abstract

With an increasing need for large-scale atomistic simulations on Co-Al-W systems, one needs an interatomic potential model that can describe all the constituent elements and their alloy systems simultaneously using a common mathematical formalism. The Second-Nearest-Neighbor Modified Embedded-Atom Method (2NN MEAM)-a semi-empirical inter-atomic potential formalism, has been applied to obtain interatomic potentials for ternary Co-Al-W system based on the previously evaluated potentials for pure Co, Al and W and binary systems- Co-Al, Co-W an Al-W. The values of fundamental physical properties for the ternary Co-Al-W system generated by using the new potentials are relatively accurate. The enthalpy of formation, the thermal stability and the elastic constants match well with experimental and the first-principles results. The formation energy of $L1_2$-$Co_3Al_{0.05}W_{0.05}$ structure is smaller than that of the DO_{19}-$Co_3Al_{0.05}W_{0.05}$ structure. The potentials can be easily combined with already-developed MEAM potentials to describe Co-Al-W multicomponent systems and can be utilized for an atomistic computation to the elaborate alloy design of advanced Co-Al-W superalloys through the investigation of the interfacial properties (the interfacial energy and the work of separation). Results showed that Al additions increase the interfacial energy and lower the work of separation while W additions lower the interfacial energy and increase the work of separation.

Keywords: Modified embedded-atom method, Atomistic simulation, Co-Al-W, Interatomic potential, Interface properties.

Introduction

For the demand to increase the operating temperature of gas turbines serving in power plants and aircraft engines,recently, Soto, et al. [1] found a new Co-based superalloy with outstanding high-temperature strength better than traditional Ni-based superalloys. Similar to Ni-based superalloys, the regularly aligned coherent cuboidal γ'-$Co_3(Al, W)$ ($L1_2$ structure) phase precipitates in a γ-Co (disordered fcc structure) solid-solution phase matrix. Lately the study of the Co-based superalloys with two coherent phase γ/γ' has attracted great attention. Many researchers have investigated the microstructures [2,3], mechanical properties [4-7], phase equilibria [8], structural stability and elastic properties [9,10], properties variation with alloying elements [11-13] of these new Co-basedsuperalloys. Additionally, studies have been performed on the effects of replacement of W by other elements such as Mo (or Ta), precipitation of γ'-Co_3(Al, Mo) (or Co_3(Al, Ta) [14,15]. But there is still a lack of other properties such as interface properties, so studies need to be performed to evaluate the interface properties of γ-Co/γ'-$L1_2$.

It should be emphasized here that the microstructural evolution in an alloy is strongly affected by the interfacial properties/interactions during the various processing steps (e.g., annealing, hot rolling, extrusion, forging, super plastic deformation, recrystallization and grain growth). Therefore, information on the γ/γ' interfaces in Co-based superalloys, particularly their structure, energy, solute segregation and dynamics behavior, is required to gain a better understanding of the strengthening effect an mechanisms in these alloys. Among these fundamental properties, interfacial energy and the work of separation strongly affect the size of the critical nucleus and the nucleation rate with respect to the host. Furthermore, the calculation of the interfacial properties is a pre-requisite to the calculation of the energies of γ/γ' interface and solute segregation which may significantly influence coarsening, as well as precipitate-dislocation interactions. This would help in modification of mechanical properties by employing the approach of adding micro-alloying elements to lower the interfacial energy between γ/γ' in order to increase the volume fraction of γ'. The discussion of these approaches will be deferred for future work. However, the interfacial properties mentioned above are quantities hard to measure experimentally. In addition, due to the size (or number of atoms) limit, it is often not possible to investigate precipitation behavior using only first-principles calculations. Another approach is to use (semi-) empirical interatomic potentials, which can deal with more than a million atoms and can calculate the interfacial energies and solute segregation much easily.

With an increasing need for large-scale atomistic simulations on Co-Al-W systems, one needs an interatomic potential model that

can describe all the constituent elements and their alloy systems simultaneously using a common mathematical formalism. However, most of interatomic potential models are mainly for a single type or similar types of elements. From this point of view, the second nearest-neighbor modified embedded-atom method (2NN MEAM) formalism which was proposed by Lee et al [21,22] by generalizing the MEAM [23] is more widely applicable, because it can describe a wide range of elements (body-centered cubic (bcc), face-centered cubic (fcc), hexagonal close-packed (hcp), diamond-structure and even gaseous elements), binary systems and ternary systems. It is currently being used widely to calculate many properties [19] in various alloy systems. The 2NN MEAM has already been applied to successfully calculate inter-atomic potentials for pure Co [20], Al [21], W [18] and Mo [18] as well as forhcp elements like Ti and Zr [22], and for binary systems such as Co-Al[20], Co-W[24] and Al-W[24]. It has also been successfully used for exploring many aspects of solid interfacial properties, especially the interfacial energy and the work of separation [20,23,25]. Therefore, it can be said that the 2NN MEAM can be a suitable potential formalism to investigate the Co-based superalloys. This article presents a brief description of the 2NN MEAM formalism and the procedure for the determination of Co-Al-W ternary system potential parameters. The reliability of the calculated potential is then examined by comparing calculated values of the physical properties with available experimental or other calculations data. The calculated potentials are then used to calculate the interfacial properties of Co-Al-W-based alloys.

Atomistic Modeling

In the 2NN MEAM, a potential for a Co-Al-W ternary system can be obtained without further effort once the potentials for constituent binary systems and constituent elements are available. The potential parameters for all the necessary pure elements Co [20], Al [21], W [17] and binary alloys and Co-Al [20], Co-W [24],Al-W [24] are listed in Tables 1and 2, respectively.

Potential formalism

In the MEAM, the total energy of a system is given by

$$E = [\Sigma_i Fi(\bar{\rho}i) + \frac{1}{2}\Sigma_{j(\neq i)} Sij\phi ij\ (Rij)], \quad (1)$$

where F_i is the embedding function for atom i embedded in background electron density $\bar{\rho}_i$, S_{ij} and $\phi_{ij}(R_{ij})$ are the screening function and the pair interaction, respectively, between atoms i and j separated by distance R_{ij}. For energy calculations, the functional forms for F_i and ϕ_{ij} should be given. The background electron density at each atomic site is computed considering the directionality of bonding, i.e. by combining several partial electron density terms for different angular contributions with weight factors $t^{(h)}(h$ = 1-3). Each partial electron density is a function of atomic configuration and atomic electron density. The atomic electron densities $\rho^{a(h)}$ (h= 0-4) are given as

$$\rho^{a(h)}(R) = \rho_0 \exp[-\beta^{(h)}\ (R/r_e - 1)], \quad (2)$$

where ρ_0(the atomic electron density scaling factor) and $\beta^{(h)}$(the decay lengths) are adjustable parameters, and r_e is the nearest-neighbor distance in the equilibrium reference structure. A specific form is given to the embedding function F_i, but not to the pair interaction ϕ_{ij}. Instead, a reference structure where individual atoms are on the exact lattice points is defined, and the total energy per atom of the reference structure is estimated from the zero-temperature universal equation of state of Roseet al [26]. Then, the value of the pair interaction is evaluated from the known values of the total energy per atom and the embedding energy as a function of the nearest-neighbor distance. In the original MEAM [18], only first-nearest-neighbor interactions are considered. Neglecting second- and more distant nearest-neighbor interactions is accomplished by the use of a strong, many-body screening function [27]. The second-nearest-neighbor interactions in the modified formalism are considered by adjusting the screening parameters, C_{min}, so that the many-body screening becomes less severe. In addition, a radial cutoff function [27] is applied to reduce the calculation time. Details of the (2NN) MEAM formalism have been published in the literature [16-18,21,27] and will not be repeated here.

Determination of ternary potential parameters for Co-Al-W

The MEAM potential parameter set for a ternary system is obtained by combining all sub-unary and binary parameters. All necessary unary and binary parameters for the Co-Al-W system are presented in Tables 1 and 2. In addition, three more ternary parameters for each of $C_{min}(i–k–j)$ and $C_{max}(i–k–j)$ are required.

As shown in Table 1, each element has its own value of C_{min} and C_{max}. $C_{min}(i\text{-}k\text{-}j)$ and $C_{max}(i\text{-}k\text{-}j)$ determine the extent of the screening of an atom (k) to the interaction between two neighboring atoms (i and j). For pure elements, the three atoms are all the same type (i-k-j = A-A-A or B-B-B). For binary alloys, one of the interacting atoms and/or the screening atoms can be different types (there are four cases: i-k-j = A-B-A, B-A-B, A-A-B, and A-B-B). Different C_{min} and C_{max} values may have to be given in each case. In the case of ternary alloys, because the value of C_{min} and C_{max} for each Co, Al and W is different, the degree of screening by a Co atom to the interaction between Al and W atoms [C_{min} and C_{max}(Al-Co-W)] was assumed to be the average between those by a Co atom to the Al-Al [C_{min} and C_{max}(Al-Co-Al], by a Co atom to the W-W [C_{min} and C_{max}(W-Co-W)], by a Co atom to the Co-W [C_{min} and C_{max}(Co-Co-W)], by a Co atom to the Co-Al [C_{min} and C_{max}(Co-Co-Al)], by an Al atom to the Al-W [C_{min} and C_{max}(Al-Al-W)] and by a W atom to the W-Al [C_{min} and C_{max}(W-W-Al)] interactions. Similarly, the degree of

Table 1: 2NN MEAM potential parameters for pure Co, Al and W (Reference structures are HCP Co, FCC Al and BCC W)

	E_c/eV	R_e/Å	B/GPa	A	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	$\beta^{(3)}$	$t^{(1)}$	$t^{(2)}$	$t^{(3)}$	C_{min}	C_{max}	d
Co[1)]	4.41	2.50	194.8	0.9	3.50	0.0	0.0	4.0	3.00	5.00	-1.0	0.49	2.00	0.00
Al[2)]	3.36	2.86	79.4	1.16	3.20	2.60	6.00	2.60	3.05	0.51	7.75	0.49	2.80	0.05
W[3)]	8.66	2.740	314	0.40	6.54	1.00	1.00	1.00	-0.6	0.3	-8.7	0.49	2.80	0.00

[1)] Ref. [20], [2)] Ref. [21], [3)] Ref. [17]

Table 2: 2NN MEAM potential parameters for the Co-Al, Co-W and Al-W system (Reference structures are B2-CoAl, $L1_2$-Co_3W and B1-AlW)

	Co-Al[1)]	Co-W[2)]	Al-W[2)]
Reference State	B2_CoAl	$L1_2$_Co_3W	B1_AlW
E_c/eV	$0.5E_c^{Co}+0.5E_c^{Al}-0.565$	$0.75E_c^{Co}+0.25E_c^{W}-0.05$	$0.5E_c^{Al}+0.5E_c^{W}+0.45$
r_e/Å	2.4768	2.5872	2.4916
B/GPa	162	$0.75B^{Co}+0.25B^{W}$	$0.5B^{Al}+0.5B^{W}$
d	$0.5d^{Co}+0.5d^{Al}$	$0.75d^{Co}+0.25d^{W}$	$0.5d^{Al}+0.5d^{W}$
$\rho_0^A:\rho_0^B$	1:1	1:1	1:1
$C_{min}(A\text{-}B\text{-}A)$	$0.49(=C_{min}^{Co})$	$0.49(=C_{min}^{Co})$	0.81
$C_{min}(B\text{-}A\text{-}B)$	1.10	$0.49(=C_{min}^{W})$	0.36
$C_{min}(A\text{-}A\text{-}B)$	$[0.5\,(C_{min}^{Co}C_{min}^{Co})^{1/2}+0.5(C_{min}^{Co}C_{min}^{Al})^{1/2}]^2$	1.21	2.0
$C_{min}(A\text{-}B\text{-}B)$	$[0.5\,(C_{min}^{Co}C_{min}^{Co})^{1/2}+0.5(C_{min}^{Co}C_{min}^{Al})^{1/2}]^2$	1.21	2.0
$C_{max}(A\text{-}B\text{-}A)$	$2.0(=C_{max}^{Co})$	1.44	$2.80(=C_{max}^{Al})$
$C_{max}(B\text{-}A\text{-}B)$	$2.8(=C_{max}^{Al})$	1.44	$2.80(=C_{max}^{W})$
$C_{max}(A\text{-}A\text{-}B)$	2.8	2.8	$[0.5(C_{max}^{Al})^{1/2}+0.5(C_{max}^{W})^{1/2}]^2$
$C_{max}(A\text{-}B\text{-}B)$	2.8	2.8	$[0.5(C_{max}^{Al})^{1/2}+0.5(C_{max}^{W})^{1/2}]^2$

[1)] Ref. [20], [2)] Ref. [24]

screening by an Al atom to the interaction between Co and W atoms [C_{min} and C_{max}(Co-Al-W)] was assumed to the the average between those by an Al atom to the Co-Co [C_{min} and C_{max}(Co-Al-Co], by an Al atom to the W-W [C_{min} and C_{max}(W-Al-W)], by an Al atom to the Al-W [C_{min} and C_{max}(Al-Al-W)], by an Al atom to the Co-Al [C_{min} and C_{max}(Co-Al-Al)], by a W atom to the W-Co [C_{min} and C_{max}(W-W-Co)] and by a Co atom to the Co-W [C_{min} and C_{max}(Co-Co-W)] interactions. Similarly, the degree of screening by a W atom to the interaction between Al and Co atoms [C_{min} and C_{max}(Al -W-Co)] was assumed to the the average between those by a W atom to the Al-Al [C_{min} and C_{max}(Al-W-Al], by an W atom to the Co-Co [C_{min} and C_{max}(Co-W-Co)], by a W atom to the W-Al [C_{min} and C_{max}(W-W-Al)], by a W atom to the W-Co [C_{min} and C_{max}(W-W-Co)], by a Co atom to the Co-Al [C_{min} and C_{max}(Co-Co-Al)] and by an Al atom to the Al-Co [C_{min} and C_{max}(Al-Al-Co)] interactions. Originally, these assumptions were introduced in the 2NN MEAM potential study of the Fe-Ti-C, Fe-Ti-N and Ni-Al-V systems [25,28] for the case where one had to determine ternary potential parameter values without sufficient ternary information. Using these assumptions, the ternary parameters are automatically determined from potential parameters for the constituent binary systems, as shown in Table 3.

Calculation of physical properties

In this section, the fundamental physical properties of Co-Al-W ternary alloys are calculated using the present 2NN MEAM potentials and are compared with experimental data or other calculations in order to evaluate the reliability of the potential parameters. The 2NN MEAM formalism includes up to second-nearest-neighbor interactions. Therefore, the radial cutoff distance during atomistic simulations should be larger than the second-nearest-neighbor distance in structures under consideration. In the present study, a value of 4.5Å, which is larger than the second-nearest-neighbor distance of aluminum, has beenchosen as the radial cut-off distance. Moreover, if not designated, all 2NN MEAM values presented here are those calculated at 0 K. The calculations have been performed using a homemade molecular dynamics (and statics) code, KISSMD, which is available online [19].

The calculated lattice parameter, the enthalpy of formation and the elastic constants of the Co-Al-W compound ($Co_3Al_{0.5}W_{0.5}$ ($L1_2$)) are compared with experimental data [1,10] or first-principles calculations [6,9,29-31] in Tables 4-6, respectively. It is shown that the calculated lattice parameter matches well with reference data although the values obtained from the present calculation is slightly larger than those from the experimental data and first-principles results [1,9,29-31]. That is due to the concentration difference from the experimental values leading to a difference in the resulting values. Additionally, the enthalpy of formation and the elastic constants of the $Co_3Al_{0.5}W_{0.5}$ calculated using our 2NN MEAM parametersagree reasonably with the reported values [9,10,28,31].

In order to further confirm the reliability of the potential values calculated here, we also calculated the formation energy at various concentrations (site fraction of W on Al sublattice) with different structures ($L1_2$ and DO_{19} structures) of $Co_3Al_{1-x}W_x$ compounds presented in Figure 1. The results are compared with available literature data [29]. It is shown that the results of the formation energy of $Co_3Al_{1-x}W_x$ compounds are excellently reproduced by the method presented here, especially using the middle fraction. The formation energy of $L1_2$-$Co_3Al_{0.05}W_{0.05}$ structure (-0.1483eV/atom) is calculated to be smaller than that of the DO_{19}-$Co_3Al_{0.05}W_{0.05}$ structure (-0.1397eV/atom), so the $L1_2$-$Co_3Al_{0.05}W_{0.05}$ structure is expected to be more stable than the DO_{19}-$Co_3Al_{0.05}W_{0.05}$ structure when site fraction of W is at 0.5 which matches the factual report. Also, the thermal stability of $L1_2$-$Co_3Al_{0.05}W_{0.05}$ structure is very high since it stabilizes uniformly at 1800K very closely to the literature data [32].

The agreement between the calculation and experimental data for the fundamental physical properties of Co-Al-W ternary intermetallic compounds over a wide range of composition indicates the validity of the present formalism for further atomistic investigation of interfacial properties of Co-Al-W alloys.

Table 3: Parameter sets of C_{min} and C_{max} determined from the constituent binary parameters for the Co-Al-W ternary system

		Co-Al-W	Assumption[1)]
C_{min}	C(Al-Co-W)	0.84	$\left\{\frac{1}{6}\left[\left(C^{\text{Al-Co-Al}}\right)^{1/2}+\left(C^{\text{W-Co-W}}\right)^{1/2}+\left(C^{\text{Al-Al-W}}\right)^{1/2}+\left(C^{\text{Co-Co-W}}\right)^{1/2}+\left(C^{\text{W-W-Al}}\right)^{1/2}+\left(C^{\text{Co-Co-Al}}\right)^{1/2}\right]\right\}^2$
	C(Co-Al-W)	0.88	$\left\{\frac{1}{6}\left[\left(C^{\text{Co-Al-Co}}\right)^{1/2}+\left(C^{\text{W-Al-W}}\right)^{1/2}+\left(C^{\text{Co-Co-W}}\right)^{1/2}+\left(C^{\text{Al-Al-W}}\right)^{1/2}+\left(C^{\text{W-W-Co}}\right)^{1/2}+\left(C^{\text{Al-Al-Co}}\right)^{1/2}\right]\right\}^2$
	C(Al-W-Co)	1.13	$\left\{\frac{1}{6}\left[\left(C^{\text{Al-W-Al}}\right)^{1/2}+\left(C^{\text{Co-W-Co}}\right)^{1/2}+\left(C^{\text{W-W-Co}}\right)^{1/2}+\left(C^{\text{Al-Al-Co}}\right)^{1/2}+\left(C^{\text{W-W-Al}}\right)^{1/2}+\left(C^{\text{Co-Co-Al}}\right)^{1/2}\right]\right\}^2$
C_{max}	C(Al-Co-W)	2.54	$\left\{\frac{1}{6}\left[\left(C^{\text{Al-Co-Al}}\right)^{1/2}+\left(C^{\text{W-Co-W}}\right)^{1/2}+\left(C^{\text{Al-Al-W}}\right)^{1/2}+\left(C^{\text{Co-Co-W}}\right)^{1/2}+\left(C^{\text{W-W-Al}}\right)^{1/2}+\left(C^{\text{Co-Co-Al}}\right)^{1/2}\right]\right\}^2$
	C(Co-Al-W)	2.66	$\left\{\frac{1}{6}\left[\left(C^{\text{Co-Al-Co}}\right)^{1/2}+\left(C^{\text{W-Al-W}}\right)^{1/2}+\left(C^{\text{Co-Co-W}}\right)^{1/2}+\left(C^{\text{Al-Al-W}}\right)^{1/2}+\left(C^{\text{W-W-Co}}\right)^{1/2}+\left(C^{\text{Al-Al-Co}}\right)^{1/2}\right]\right\}^2$
	C(Al-W-Co)	2.54	$\left\{\frac{1}{6}\left[\left(C^{\text{Al-W-Al}}\right)^{1/2}+\left(C^{\text{Co-W-Co}}\right)^{1/2}+\left(C^{\text{W-W-Co}}\right)^{1/2}+\left(C^{\text{Al-Al-Co}}\right)^{1/2}+\left(C^{\text{W-W-Al}}\right)^{1/2}+\left(C^{\text{Co-Co-Al}}\right)^{1/2}\right]\right\}^2$

Table 4: The calculated lattice parameters of Co-Al-W intermetallic phases in comparison with experimental data and other calculations (unit: Å)

Phase	Lattice parameter, a	
$Co_3Al_{0.5}W_{0.5}$	3.648	Present work
$Co_{0.818}Al_{0.092}W_{0.09}$	3.599	Expt. [1)]
$Co_3Al_{0.5}W_{0.5}$	3.562	FP calc. [2)]
	3.571	FP calc. [3)]
	3.582	FP calc. [4)]
	3.572	FP calc. [5)]
	3.565	FP calc. [6)]

[1)] Ref. [1], [2)] Ref. [6], [3)] Ref. [9], [4)] Ref. [29], [5)] Ref. [30], [6)] Ref. [31]

Calculation of interface properties

In order to obtain the desirable high temperature properties of the superalloys mentioned earlier, it is important to understand the microstructural evolution in these alloys as well as be able predict the microstructural features. Knowledge of interfacial

Table 5: The calculated enthalpy of formation of Co-Al-W intermetallic phases in comparison with literature data (unit: kJ/(g·atom))

Phase	ΔH	
$Co_3Al_{0.5}W_{0.5}$	-14.31	Present work
	-14.47	FP calc.[1)]
	-15.99	FP calc.[2)]

[1)] Ref. [29], [2)] Ref. [9]

Table 6: The calculated elastic constants C_{11}, C_{12}, C_{44} for Co-Al-W intermetallic phases in comparison with literature data (unit: GPa)

Phase	C_{11}	C_{12}	C_{44}	B	
$Co_3Al_{0.5}W_{0.5}$	328	147	147	207	Present work
$Co_{0.79}Al_{0.1}W_{0.11}$	271	172	162	205	Expt. [1)]
$Co_3Al_{0.5}W_{0.5}$	363	190	212	248	FP calc. [2)]
	264	162	153	196	FP calc. [3)]
	301	169	172	213	FP calc. [4)]

[1)] Ref. [10], [2)] Ref. [9], [3)] Ref. [29], [4)] Ref. [31]

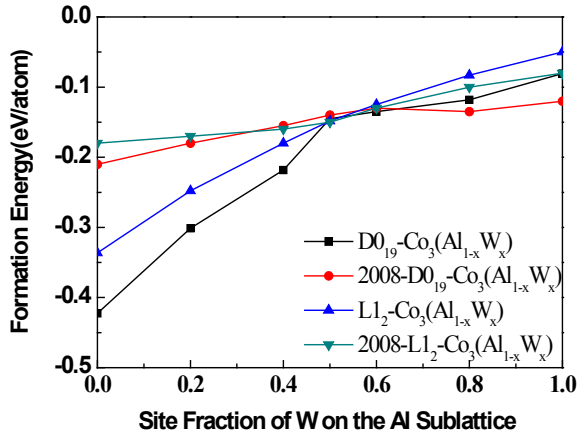

Figure 1: The formation energy various concentrations (site fraction of W on Al sublattice) with different structures ($L1_2$ and DO_{19} structures) of $Co_3Al_{1-x}W_x$ compounds. Literature data is from Ref. [29]

energies plays an important role in evaluating phase nucleation and morphology. However bulk thermodynamic and diffusion data are insufficient in this field. Now that the agreement between the potential values calculated and presented in the last section and quantitative or qualitative experimental information of properties has been shown, we will further demonstrate the applicability of the present atomistic simulation approach to the investigation of the microstructure and properties of Co-based alloys. The following section demonstrates how to use the 2NN MEAM potentials to calculate the interfacial properties of the coherent (001) interfacial properties at 0K between γ-Co and γ'-Co_3(Al, W).

For the calculation of interfacial properties, supercells composed of equal amounts of γ-Co and γ'- $Co_3Al_{0.5}W_{0.5}$ and involving an interface between the two phases at a given orientation were prepared. In the present work, three types of (001) interfaces were considered: random Al in γ-Co, random W in γ-Co and random Al+W in γ-Co which contains cubic γ'-$Co_3Al_{0.5}W_{0.5}$ unit cells and cubic γ-Co cells. When the γ-Co is not pure Co, in order to minimize the statistical error, large size of supercells 20 × 40 ×20 are used for these interfaces and the individual calculated values used are average values of ten calculations using differently random solutions.

The interfacial properties (the interfacial energy and the work of separation) are calculated by the same method as the previous works [20,23,25]. Similarly in the present research, the composition and temperature dependence of Al/W/Al+W in γ-Co of the (001) interfaces was also discovered (see Table 7 and 8). From the results, we can see that the addition of the alloying element Al will increase the interfacial energy (from -28.76 mJ/$m^2$to -16.15 mJ/m^2) and lower the work of separation (from 4.34 J/m^2 to 4.33 J/m^2). On the contrary, the addition of the alloying element W will lower the interfacial energy (from -28.76 mJ/$m^2$to -42.24 mJ/m^2) and increase the work of separation (from 4.34 J/m^2 to 4.39 J/m^2). With increasing alloying element concentration in Co-20 at.%, both the Al and W will increase the interfacial energy (from -28.76 mJ/m^2 to 7.89 or -11.86 mJ/m^2) and lower the work of separation (from 4.34 J/m^2 to 4.28 or 4.33 J/m^2). Thermal stability of the γ' phase is crucial to improve the high temperature strength for the γ/γ' Co-based superalloys[1].

Table 7: The calculated coherent interfacial energy at 0 K between γ-Co and $Co_3Al_{0.5}W_{0.5}$ at various Al, W or Al+W contents in γ-Co (unit: mJ/m^2)

(001) interface	Interfacial energy		
	c_{Al} in γ-Co	c_W in γ-Co	c_{Al+W} in γ-Co
0	-28.76	-28.76	-28.76
0.05	-16.15	-42.24	-17.20
0.1	-9.21	-40.34	-14.89
0.15	-3.23	-31.80	-4.19
0.2	7.89	-11.86	5.27

Table 8: The calculated work of separation at 0 K between γ-Co and $Co_3Al_{0.5}W_{0.5}$ at various Al, W or Al+W contents in γ-Co (unit: J/m^2)

(001) interface	Work of separation		
	c_{Al} in γ-Co	c_W in γ-Co	c_{Al+W} in γ-Co
0	4.34	4.34	4.34
0.05	4.33	4.39	4.33
0.1	4.31	4.38	4.33
0.15	4.30	4.36	4.32
0.2	4.28	4.33	4.30

Interfacial properties are an important aspect of this understanding but have so far been neglected in the studies. One can now predict that the metastable γ'-Co_3Al is stabilized by alloying with W because the addition of the alloying element W can lower the interfacial energy and increase the work of separation.In other words, an increasing W content stabilizes this phase and by increasing the W content it is possible to generate γ'-Co_3(Al, W) phase. The results agree well with the experimental analysis of previous literatures, and may do some help in the Co-based alloy design andprocess design [33]. In this article,results showed that the γ'solvus temperature and γ' volume fraction increases with increasing W content. Actually, not only W additions but also Ta additions affect the high-temperature propertities in Co-based superalloys [13,34], which demonstrated the γ'solvus temperature increases obviously with increasing Ta content.

It is generally known that both Al and W disperse randomly in the γ-Co near the γ/γ'-Co_3(Al,W) interface in the real Co-Al-W-based superalloy. The Al+W content of γ-Co in equilibrium with γ'-Co_3(Al,W) at 1300 K (the solvus temperature γ'-Co_3(Al,W)) is about 20 at.%. Therefore, if the temperature dependence of the interfacial enthalpy can be assumed to be small, then the calculated value for the Co-20 at.% (Al+W) can be regarded to be close to the interfacial enthalpy between γ-Co andγ'-Co_3(Al,W) at 1300 K. That means, the approximate value of interfacial energy and the work of separation of γ/γ'-Co_3(Al,W) interface is 5.27 mJ/m^2 and 4.30 J/m^2, respectively. The negative value calculated for the interfacial energy is another way of expressing thatat these concentrations, the interfaces are unstable and a solid solution would be formed to lower the energy than a two-phase mixture.

In addition to the interfacial properties, the understanding of alloying with other elements that can increase the γ' solvus temperature and reduce the stacking fault energy of the γ' phase at elevated temperatures is required to improve the high-temperature strength. The γ/γ' misfit strain is also an important parameter that controls the interface between γ/γ' and especially

its high temperature stability. It is difficult to predict which element would reduce misfit strains that can decrease the coherency strains between γ and γ'. All of these complications have been the reason for lack of any formal theories in the field of commercial alloy development even today. The strongest advantage of the present MEAM approach is that all the above-mentioned properties can be investigated for practical evaluation of Co_3(Al, W) multicomponent alloys since the Co, Al, W, Mo, Ti, Zr, Co-Al, Al-W and Co-W potentials are already available, and can be easily combined into the ternary or quaternary potential.

Conclusions

a. We have introduced an interatomic potential that can be used to calculate various fundamental physical properties of Co-Al-W ternary system in good agreement with other reported values.The enthalpy of formation, the thermal stability and the elastic constants match well with experimental and the first-principles results. However, the lattice parameters are a little bigger than the values obtained from experimental data and those from first-principles calculations for different concentrations. This newly developed potential, in turn, is employed to investigate interfacial properties (interfacial energy and work of separation) between γ-Co and γ'-Co_3(Al, W)interfaces in these alloys.

b. The results of calculations indicate that the formation energy of $L1_2$-$Co_3Al_{0.05}W_{0.05}$ structure is smaller than that of the DO_{19}-$Co_3Al_{0.05}W_{0.05}$ structure,which mens $L1_2$-$Co_3Al_{0.05}W_{0.05}$ will be formed and stable in the 75%Co-12.5%Al-12.5%W alloy. This matches well with the experimental results.

c. It was also found that the addition of alloying element Al increases the interfacialenergy and lowers the work of separation while alloying with W increases the work of separation and lowers the interfacialenergy. With further research, this potential can be further applied for atomistic simulations of advanced Co-based superalloys.Further study of this alloy, including mechanical properties and alloying other additions to affect the solvustemperature regulation of Co-based superalloys, is in progress.

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