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THERMODYNAMIC DESCRIPTION OF THE Al-Cu-Yb TERNARY SYSTEM SUPPORTED BY FIRST-PRINCIPLES CALCULATIONS

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Abstract

Phase relationships of the ternary Al-Cu-Yb system have been assessed using a combination of CALPHAD method and first-principles calculations. A self-consistent thermodynamic parameter was established based on the experimental and theoretical information. Most of the binary intermetallic phases, except Al_3Yb, Al_2Yb, Cu_2Yb and Cu_5Yb, were assumed to be zero solubility in the ternary system. Based on the experimental data, eight ternary intermetallic compounds were taken into consideration in this system. Among them, three were treated as line compounds with large homogeneity ranges for Al and Cu. The others were treated as stoichiometric compounds. The calculated phase diagrams were in agreement with available experimental and theoretical data.

Keywords: *Al-Cu-Yb; Thermodynamic calculation; Phase diagram; CALPHAD*

1. Introduction

Interest in aluminum alloys is increasing continuously, especially for their potential applications in the automotive and aerospace industries. Microalloying has been used to improve the high temperature strength of selected age hardening aluminum alloys (such as Al-Cu-Mg-Zn and Al-Cu-Mg-Ag alloys) [1-6]. It has been demonstrated that rare earth elements are benefit to casting process in conventional aluminum alloys [7,8] owing to their capability of improving tensile strength, heat resistance and corrosion resistance, etc for many years [7]. For example, when Sc was added into Al alloys, a thermo-stable $L1_2$-type ($AuCu_3$) Al_3Sc phase would form in the Al solid solution, which was able to inhibit the re-crystallization and the grain growth and then significantly improve the high temperature properties of the alloys [8]. A similar to the addition of Sc, a $L1_2$-type ($AuCu_3$) phase Al_3Yb formed when Yb was added into Al alloys [11,12] and such process could significantly refine the grains and improve the mechanical properties of the alloy. Additionally, it could accelerate the aging process and improve the effect of aging strengthening [13-16]. Subsequently, it was found that after partial replacement of expensive Sc by Yb, the mechanical properties were improved, such as the shorter incubation time and the higher peak hardness of Al alloys [17]. Zhang et al. [18] reported that the introduction of Yb into Al alloys could increase not only the tensile and yield strength but also the fracture toughness of Al-Zn-Mg-Cu-Zr alloys.

Knowledge of thermodynamics and phase diagrams is vital in the field of materials research and process control in preparation and manufacture, which holds the balance for new alloy development. The aim of this work is to evaluate the Al–Cu-Yb ternary system and develop a self-consistent thermodynamic description by means of calculation of phase diagram (CALPHAD) technique [19].

2. Experimental

2.1 Binary systems

In addition to solution phases including Liquid, Fcc, and Bcc, there are 15 intermetallic phases existing in the three binary systems [20-22].

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Experimental data on the ternary solubility for most of the binary compounds are not available. The Al-Cu system was thermodynamically studied by Saunders [23]. Recently, Witusiewicz et al. [20] reassessed the liquid and $\gamma D8_3$ phases of the Al-Cu system on the ground of new experimental thermodynamic data of the $\gamma D8_3$ phase. In this work, the thermodynamic parameters by Witusiewicz et al. [20] were adopted. The Al-Yb system was thermodynamically assessed by Meng et al. [21]. The thermodynamic description available for the Cu-Yb system was performed by Zhang et al. [22].

2.2 Ternary compounds

As summarized by Riani et al. [24], there are seven ternary intermetallic compounds in the Al-Cu-Yb ternary system [25]. Their structures are listed in Table 1.

In the Al-rich corner, a ternary compounds taking on $ThMn_{12}$ type structure (denoted as Al_4Cu_8Yb) was reported in the Al-Cu-Yb ternary systems [26,27], which was identified as the same structure of the Al_6Cu_6Yb alloy [28]. Recently, Stel'makhovych et al. [29] reinvestigated the Al-Cu-Yb system and found that τ_1 phase had a homogeneity range, which is named as $(Al,Cu)_{12}Yb$ in this work.

Another five new ternary compounds in the Al-Cu-Yb ternary system were reported by Stel'makhovych et al. [29]. These compounds are $(Al_{0.47}Cu_{0.53})_{17}Yb_2$ with Th_2Zn_{17} type structure, $Al_{49}Cu_{17}Yb_8$, Al_4Cu_2Yb with Al_4Mo_2Yb type structure, $Al_{2.1}Cu_{0.9}Yb$ with Ni_3Pu type structure, and $Al_6Cu_{17}Yb_6$ with $Mn_{23}Th_6$ type structure. The $(Al_{0.47}Cu_{0.53})_{17}Yb_2$ phase is found to have a homogeneity range and the others are stoichiometric compounds. These compounds are denoted as τ_2-τ_6, respectively.

The AlCuYb compound with ZrNiAl type structure (τ_7) was discovered by Dwight et al. [30] and confirmed by Stel'makhovych et al. [29].

2.3 Phase equilibria in the ternary system

The only set of experimental data available for Al-Cu-Yb ternary phase diagram is at 870 K reported by

Table 1. *Crystallographic data of intermetallic phases*

Phase	Lattice parameters			Structure Type,Pearson Symbol,Space Group
	a (nm)	b (nm)	c (nm)	
θ	0.6067		0.4877	$CuAl_2$,*tI*12,*I4/mcm*
η	1.2066	0.4105	0.6913	CuAl,*mC*20,*C2/m*
ζ	0.40972	0.71313	0.99793	$Cu_{11.5}Al_9$,*oI*24,*Imm2*
ε	0.4146		0.5063	Ni_2In,*hP*6,*P63/mmc*
γ D83	0.87023			Cu_9Al_4,*cP*52,$P\bar{4}3m$
γ				Cu_5Zn_8,*cI*52,$I\bar{4}3m$
β	0.2946			W,*cI*2,$Im\bar{3}m$
Al_3Yb	0.4202			$AuCu_3$,*cP*4, $Pm,\bar{3}m$
Al_2Yb	0.7877			$MgCu_2$,*cF*24,$Fd\bar{3}m$
Cu_5Yb	0.5044		0.4146	$CaCu_5$,*hP*6, *P6/mmm*
Cu_9Yb_2	4.8961	4.8994	4.5643	Cu_9Yb_2, *mC*7448
Cu_7Yb_2				?
Cu_2Yb	0.4286	0.6894	0.7382	$CeCu_2$,*oI*12,*Imma*
CuYb	0.7568	0.4267	0.5776	FeB,*oP*8, *Pnma*
τ_1-$(Al,Cu)_{12}Yb$	0.8724		0.5118	$Mn_{12}Th$,*tI*26,*I4/mmm*
τ_2-$(Al,Cu)_{17}Yb_2$	0.8877		1.2734	Th_2Zn_{17},*hR*57,$\bar{3}R$
τ_3-$Al_{49}Cu_{17}Yb_8$	0.8565		1.6255	$Al_{49}Cu_{17}Yb_8$,*tI**,*I4/mmm*
τ_4-Al_4Cu_2Yb	0.6386		0.4926	Al_4Mo_2Yb,*tI*14,*I4/mmm*
τ_5-$Al_{2.1}Cu_{0.9}Yb$	0.5471		2.5358	$PuNi_3$,*hR*36,$R\bar{3}m$
τ_6-$Al_6Cu_{17}Yb_6$	1.2234			$Mn_{23}Th_6$,*cF*116, $Fm\bar{3}m$
τ_7-AlCuYb	0.6925		0.399	ZrNiAl,*hP*9,*P62m*

Stel’makhovych et al. [29]. The reported experimental isothermal section is shown in Fig. 1. Riani et al.[24] and Cacciamani and Riani [25] had assessed the experimental phase diagram. There were seven ternary compounds: τ_1 to τ_7, as shown in Fig. 1. Among them, τ_3-$Al_{49}Cu_{17}Yb_8$, τ_4-Al_4Cu_2Yb, and τ_5-$Al_{2.1}Cu_{0.9}Yb$, τ_6-$Al_6Cu_{17}Yb_6$, τ_7-AlCuYb are stoichiometric compounds whereas Al and Cu can partially substitute in τ_1-$(Al,Cu)_{12}Yb$, τ_2-$(Al,Cu)_{17}Yb_2$ which were named semi-stoichiometric phases in this work. At 870 K, Al_3Yb could dissolve up to 5 at.% Cu, Al_2Yb up to 15 at.% Cu and Cu_5Yb up to 35 at.% Al, respectively [29].

3. Thermodynamic Model

3.1 Solution phases

The lattice stabilities for element Al, Cu and Yb are cited from Dinsdale [31]. An ordinary substitutional solution model is employed to describe Liquid, Fcc, Bcc and Hcp terminal solution. The mole Gibbs energy of a solution phase Φ (Φ = Liquid, Fcc, Bcc) can be represented as a sum of weighted Gibbs energy for the pure components with the ideal entropy term describing a random mixing of the components and the excess Gibbs energy describing the degree of deviation from ideal mixing, i.e.

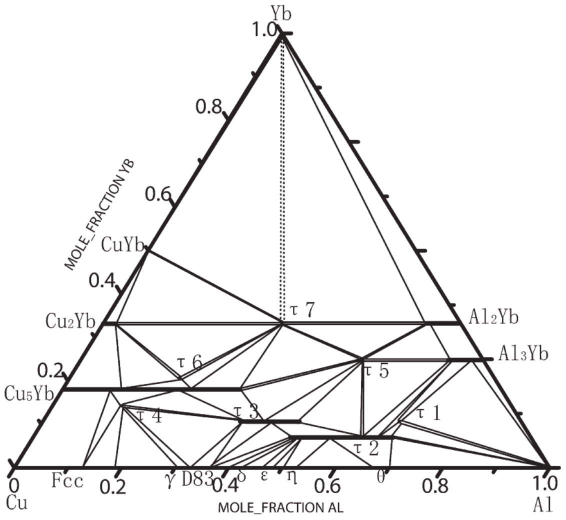

Figure 1. *The measured 870 K isothermal section of Al-Cu-Yb system [29]*

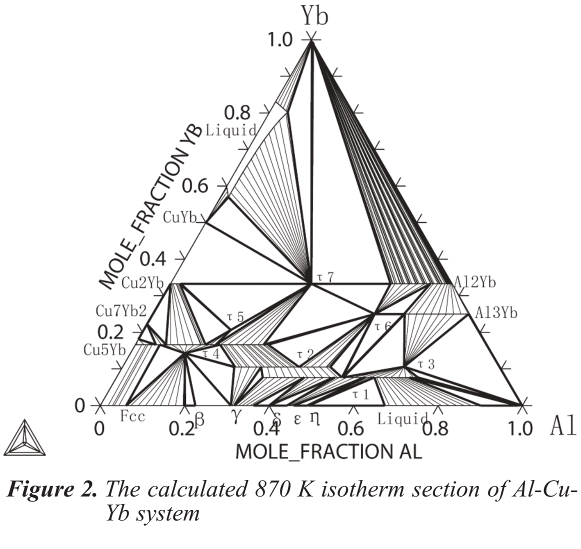

Figure 2. *The calculated 870 K isotherm section of Al-Cu-Yb system*

$$G^{\varphi} = \sum_{i=Al,Cu,Yb} x_i\, {}^{0}G_i^{\varphi} + RT \sum_{i=Al,Cu,Yb} x_i \ln(x_i) + {}^{ex}G^{\varphi} \qquad (1)$$

where

$$\begin{aligned} {}^{ex}G^{\varphi} = {} & x_{Al}x_{Cu} \sum_{j=0,1...}^{N} (x_{Al}-x_{Cu})^{j}\, {}^{(j)}L^{\varphi}_{Al,Cu} \\ & + x_{Al}x_{Yb} \sum_{j=0,1...}^{N} (x_{Al}-x_{Yb})^{j}\, {}^{(j)}L^{\varphi}_{Al,Yb} \\ & + x_{Cu}x_{Yb} \sum_{j=0,1...}^{N} (x_{Cu}-x_{Yb})^{j}\, {}^{(j)}L^{\varphi}_{Cu,Yb} \\ & + x_{Al}x_{Cu}x_{Yb} L^{\varphi}_{Al,Cu,Yb} \end{aligned} \qquad (2)$$

where ϕ denotes the solution phases, x_i (i = Al, Cu and Yb) denotes the mole fraction of the component i and ${}^{0}G_i^{\varphi}$ is the molar Gibbs energy of the pure element in the structural state of ϕ .

${}^{(j)}L^{\varphi}_{Al,Cu}$ is taken from Witusiewicz et al. [20], ${}^{(j)}L^{\varphi}_{Al,Yb}$ is taken from Meng et al. [21] and ${}^{(j)}L^{\varphi}_{Cu,Yb}$ is taken from Zhang et al. [22]:

$L^{\varphi}_{Al,Cu,Yb}$ is a ternary interaction parameter. Due to the lack of experiment data, it is set to be zero.

3.2 Binary intermetallic phases

According to Stel’makhovych et al. [26], the Al_3Yb, Al_2Yb, Cu_2Yb and Cu_5Yb phases exhibit the homogeneity regions in Al-Cu-Yb ternary system. The Gibbs energy expression of these phases are formalized as:

$$\begin{aligned} G^{(Al,Cu)_x Yb_y} = {} & Y^I_{Al} G_{Al:Yb} + Y^I_{Cu} G_{Cu:Yb} \\ & + \frac{x}{x+y} RT (Y^I_{Al} \ln Y^I_{Al} + Y^I_{Cu} \ln Y^I_{Cu}) \\ & + Y^I_{Al} Y^I_{Cu} L_{Al,Cu:Yb} \end{aligned} \qquad (3)$$

where x and y are the stoichiometry ratios. The superscript I denotes the first sublattice Y^I_{Al} and Y^I_{Cu} stand for the site fractions of Al, Cu in the first sublattice, respectively. The term $L_{Al,Cu:Yb}$ represents the interaction between the Al and Cu in the first sublattice, expressed by the Redlich-Kister polynomials. The parameter $G_{Cu:Yb}$ in the Cu_5Yb and Cu_2Yb phases and $G_{Al:Yb}$ in the Al_3Yb and Al_2Yb phases can be taken from the binary systems. $G_{Al:Yb}$ in the Al_3Yb and Al_2Yb phases and $G_{Cu:Yb}$ in the Cu_5Yb and Cu_2Yb phases are expressed as

$$G_{MM:Yb}=\frac{x}{x+y}{}^{0}G_{MM}^{Fcc}+\frac{y}{x+y}{}^{0}G_{Yb}^{Fcc}+A+BT \tag{4}$$

The expressions above presume that the Gibbs energy of the assumed Al_5Yb and Al_2Yb compounds have Cu_5Yb and Cu_2Yb structures and the assumed Cu_2Yb and Cu_3Yb compounds have Al_2Yb and Al_3Yb structures.

A and *B* are the adjustable parameters to be optimized in this work.

3.3 Ternary intermetallic compounds

In the ternary system, τ_3-$Al_{49}Cu_{17}Yb_8$, τ_4-Al_4Cu_2Yb, and τ_5-$Al_{2.1}Cu_{0.9}Yb$, τ_6-$Al_6Cu_{17}Yb_6$ and τ_7-AlCuYb are modeled as stoichiometric phases ($Al_xCu_yYb_z$), i.e. Al，Cu, and Yb cannot substitute each other in any sublattice. τ_1-$(Al,Cu)_{12}Yb$ and τ_2-$(Al,Cu)_{17}Yb_2$ are treated as semi-stoichiometric phases ($(Al,Cu)_xYb_y$), i.e. Al and Cu can partially substitute each other in the first sublattice, but Al and Cu cannot substitute Yb atoms in the second sublattice. The Gibbs energy expression for each of these stoichiometric compounds is written as:

$$G_{Al_xCu_yYb_z}=\frac{x}{x+y+z}{}^{0}G_{Al}^{Fcc}+\frac{y}{x+y+z}{}^{0}G_{Cu}^{Fcc} \\ +\frac{z}{x+y+z}{}^{0}G_{Yb}^{Fcc}+A+BT \tag{5}$$

where *x*, *y* and *z* are the stoichiometry ratios of the sublattices. For the semi-stoichometric compounds, it becomes

$$G^{(Al,Cu)_xYb_y}=Y_{Al}^{I}G_{Al:Yb}+Y_{Cu}^{I}G_{Cu:Yb} \\ +\frac{x}{x+y}RT(Y_{Al}^{I}\ln Y_{Al}^{I}+Y_{Cu}^{I}\ln Y_{Cu}^{I}) \\ +Y_{Al}^{I}Y_{Cu}^{I}L_{Al,Cu:Yb} \tag{6}$$

$$G_{Al:Yb}=\frac{x}{x+y}{}^{0}G_{Al}^{Fcc}+\frac{y}{x+y}{}^{0}G_{Yb}^{Fcc}+A+BT \tag{7}$$

$$G_{Cu:Yb}=\frac{x}{x+y}{}^{0}G_{Cu}^{Fcc}+\frac{y}{x+y}{}^{0}G_{Yb}^{Fcc}+A+BT \tag{8}$$

where $L_{Al,Cu:Yb}$ represents the interaction between Al and Cu in the first sublattice, expressed by the Redlich-Kister polynomials. *A* and *B* are the adjustable parameters to be optimized in the present work.

4. Results and discussion

The first-principles calculations were employed to calculate the enthalpies of formation of some compounds in this ternary system. First-principles calculations were performed by using the scalar relativistic all-electron Blöchl's projector augmented-wave (PAW) method [32,33] within the generalized gradient approximation (GGA), as implemented in the highly-efficient Vienna ab initio simulation package (VASP) [34,35]. For the GGA exchange-correlation function, the Perdew-Bucke-Ernzerhof parameterization (PBE) [36,37] was employed. A plane-wave energy cutoff of 350 eV was held constant for the study of the different $Al_xCu_yYb_z$ compounds. Brillouin zone integrations were performed using Monkhorst-Pack K-point meshes [38], and the Methfessel-Paxton technique [39] with a smearing parameter of 0.2 eV. The reciprocal space (k-point) meshes were increased to achieve convergence to a precision of 1meV/atom. The total energy was converged numerically to less than 1×10^{-6} eV/unit with respect to electronic, ionic and unit cell degrees of freedom and the two latter were relaxed using calculated forces with a preconditioned conjugated gradient algorithm. The calculated formation enthalpies from first-principles calculations are shown in Table 2.

Table 2. *Comparison of the optimized standard enthalpies of formation with results from first-principles calculations*

Phase	Structure	First-principles calculations (kJ/mol)	CALPHAD
			(kJ/mol)
Al_2Yb	$CeCu_2$,*oI*12	-32.4892	-32.792
Cu_2Yb	Cu_2Mg,*cF*24	-13.251	-13.92
Al_5Yb	$CaCu_5$,*hP*6	-14.6986	-14.639
τ_1-$Al_{12}Yb$	$Mn_{12}Th$,*tI*26	-5.073	-5.209
τ_1- $Cu_{12}Yb$	$Mn_{12}Th$,*tI*26	-4.472	-4.739
τ_2-$Al_{17}Yb_2$	Th_2Zn_{17},*hR*57	-8.963	-8.539
τ_2-$Cu_{17}Yb_2$	Th_2Zn_{17},*hR*57	-12.321	-12.437
τ_4-Al_4Cu_2Yb	Al_4Mo_2Yb,*tI*14	-31.886	-29.05
τ_7-AlCuYb	ZrNiAl,*hP*9	-32.897	-34.8

On the basis of lattice stabilities cited from Dinsdale [31], the optimization of the Al-Yb system was carried out using the Parrot module in the Thermo_Calc program [40,41] The parameters for the liquid phase were first optimized using the vertical sections information from experiments. The thermodynamic parameters of the ternary compounds were assessed next by using phase diagram data and the standard enthalpies of formation which were calculated from first-principles calculations. The other compounds were optimized accordingly. All the parameters were finally evaluated together to give a reasonable description of this system. Since the thermochemical and liquid projection information for the Al-Cu-Yb ternary system was not available, the ternary interaction parameters of liquid were then set to be zero. Seven ternary compounds were assessed based on the phase relations by Stel'makhovych et al. [29]. All the evaluated parameters are listed in Table 3.

***Table 3.** Thermodynamic parameters of Al-Cu-Yb system*

Phase	Thermodynamic Parameters	Ref
Al_2Yb Model: $(Al,Cu)_{0.667}(Yb)_{0.333}$	$G^{Al2Yb}_{Al:Yb} = -35350.36 + 2.53935T + 0.667GHSERAL + 0.333GHSERYB$	[22]
	$G^{Al2Yb}_{Cu:Yb} = -13920.02 + 4.83054T + 0.667GHSERCU + 0.333GHSERYB$	This work
	${}^{0}L^{Al2Yb}_{Al,Cu:Yb} = -21000$	This work
Cu_5Yb Model: $(Cu)_{0.8333}(Yb)_{0.1667}$	$G^{Cu5Yb}_{Cu:Yb} = -15339.485 + 2.2025T + 0.8333GHSERCU + 0.1667GHSERYB$	[32]
	$G^{Cu5Yb}_{Al:Yb} = +10339.5 - 0.20T + 0.8333GHSERAL + 0.1667GHSERYB$	This work
	${}^{0}L^{Cu5Yb}_{Al,Cu:Yb} = -94939.485$	This work
Cu_2Yb Model: $(Al,Cu)_{0.6667}(Yb)_{0.3333}$	$G^{Cu2Yb}_{Cu:Yb} = -17792.41 + 0.577T + 0.6667GHSERCU + 0.3333GHSERYB$	[32]
	$G^{Cu2Yb}_{Al:Yb} = -17792 + 0.58T + 0.6667GHSERAl + 0.3333GHSERYB$	This work
	${}^{0}L^{Cu2Yb}_{Al,Cu:Yb} = -16001.2$	This work
CuYb Model: $(Cu)_{0.5}(Yb)_{0.5}$	$G^{CuEr}_{Al:Yb} = -14796.22 - 1.4309T + 0.5GHSERAl + 0.5GHSERYB$	[32]
τ_1 Model: $(Al,Cu)_{0.923077}$ $(Er)_{0.076923}$	$G^{\tau1}_{Al:Yb} = -5209.485 + 0.01T + 0.923077GHSERAL + 0.076923GHSERYB$	This work
	$G^{\tau1}_{Cu:Yb} = -4739.485 + 0.2T + 0.923077GHSERCU + 0.076923GHSERYB$	This work
	$G^{\tau1}_{Al,Cu:Yb} = -73997.65$	This work
τ_2 Model: $(Al,Cu)_{0.894737}(Yb)_{0.105263}$	$G^{\tau2}_{Cu:Yb} = -12439.485 + 6.9T + 0.894737GHSERCU + 0.105263GHSERYB$	This work
	$G^{\tau2}_{Al:Yb} = -8539.485 + 6.2025T + 0.894737GHSERAL + 0.105263GHSERYB$	This work
	$G^{\tau2}_{Al,Cu:Yb} = -81000$	This work
τ_3 Model: $(Al)_{0.68}(Cu)_{0.231892}(Yb)_{0.108108}$	$G^{\tau3}_{Al:Cu:Yb} = -27999.98 + 1.0025T + 0.68GHSERAL + 0.231892GHSERCU + 0.108108GHSERYB$	This work
τ_4 Model: $(Al)_{0.128571}(Cu)_{0.728571}(Yb)_{0.142858}$	$G^{\tau4}_{Al:Cu:Yb} = -29050 + 6.0025T + 0.128571GHSERAL + 0.728571GHSERCU + 0.142858GHSERYB$	This work
τ_5 Model: $(Al)_{0.206207}(Cu)_{0.586897}(Yb)_{0.206896}$	$G^{\tau5}_{Al:Cu:Yb} = -30399.98 + 2.0025T + 0.206207GHSERAL + 0.586897GHSERCU + 0.206896GHSERYB$	This work
τ_6 Model: (Al)0.525(Cu)0.225(Yb)0.25	$G^{\tau6}_{Al:Cu:Yb} = -34585.01 + 1.0025T + 0.525GHSERAL + 0.225GHSERCU + 0.25GHSERYB$	This work
τ_7 Model: $(Al)_{0.333333}(Cu)_{0.333333}$ $(Yb)_{0.333334}$	$G^{\tau7}_{Al:Cu:Yb} = -34800.001 + 1.00249T + 0.333333GHSERAL + 0.333333GHSERCU + 0.333334GHSERYB$	This work

The calculated 870 K isothermal section for Al-Cu-Yb system with Pandat software [42] is shown in Fig. 2. Compared with the experimental data [29], it can be found that the intermetallic phases presented in the calculated three boundary systems are not consistent with the work of Stel'makhovych et al. [29].

According to the Al-Cu binary phase diagram, the θ phase is meta-stable at 870 K while it is stable in the isothermal section reported by Stel'makhovych et al. [29]. Also, the liquid phase should not be missing in the Al-Cu boundary system. On the Cu-Yb edge, there were only three phases in the Al-Yb boundary system (Cu_5Yb, Cu_2Yb, and CuYb) in the work of Stel'makhovych et al. [29]. Later, when Cacciamani and Riani [35] assessed this ternary system, the isothermal section was corrected in order to eliminate the above inconsistencies, i.e.θ didn't emerge at 870 K, and the liquid phase was presented itself in both Al-Cu and Cu-Yb boundary systems, Cu_9Yb_2 and Cu_7Yb_2 phases were also presented in the Cu-Yb boundary system. From the work of Cacciamani and Riani [25], phase relationships along three boundary systems would be in better agreement with the accepted binary systems. Therefore, the assessed results of Cacciamani and Riani [25] were adopted in the present work. From the optimization results, it can be found that the homogeneity region of Al_2Yb and Cu_5Yb extends, up to 15 at.% Cu and 45 at.% Al, respectively, which agrees with the work of Stel'makhovych et al. [29].

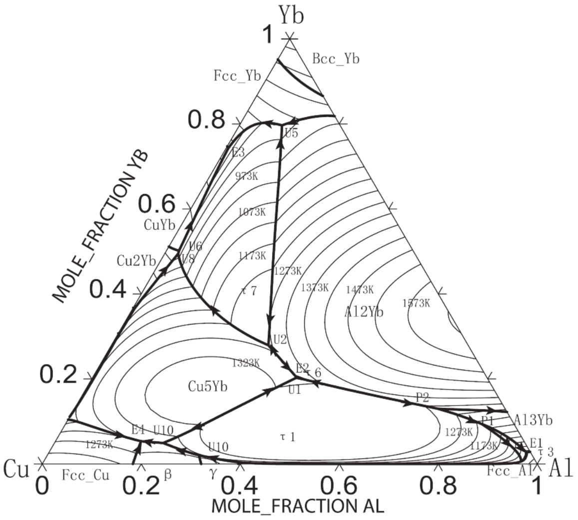

Figure 3. *The calculated liquidus projection of Al-Cu-Yb system*

Table 4. *Calculated invariant reactions and temperatures of Al-Cu-Yb ternary system*

Type	Reaction	T/K
E_1	Liquid $\Leftrightarrow$Fcc_Al+Al_3Yb+τ_3	899.54
E_2	Liquid $\Leftrightarrow$$Cu_5Yb$+$\tau_6$+ Al_2Yb	1287.82
E_3	Liquid $\Leftrightarrow$CuYb+Fcc_Yb+τ_7	746.5
E_4	Liquid $\Leftrightarrow$$Cu_5Yb$+Fcc_Cu+β	1219.99
U_1	Liquid +τ_2 $\Leftrightarrow$$Cu_5Yb$+$\tau_6$	1288.08
U_2	Liquid + Al_2Yb $\Leftrightarrow$ τ_7+Cu_5Yb	1261.6
U_3	Liquid +τ_6 $\Leftrightarrow$$\tau_2$+$\tau_7$	1263.42
U_4	Liquid +Al_2Yb $\Leftrightarrow$ τ_7+Fcc_Yb	893.68
U_5	Liquid +Cu_2Yb $\Leftrightarrow$ CuYb+τ_7	892.75
U_6	Liquid +Cu_5Yb $\Leftrightarrow$$\tau_7$+$Cu_2Yb$	899.16
U_7	Liquid +τ_1 $\Leftrightarrow$$Cu_5Yb$+β	1230.38
U_8	Liquid +γ $\Leftrightarrow$β+τ_2	1263.84
U_9	Liquid +γ $\Leftrightarrow$$\tau_2$+β	1223.63
U_{10}	Liquid +τ_3 $\Leftrightarrow$$Al_3Yb$ +τ_1	1204.07
U_{11}	Liquid +β $\Leftrightarrow$$\tau_1$+ε	1124.15
U_{12}	Liquid +Cu_9Yb_2 $\Leftrightarrow$$Cu_5Yb$+$Cu_7Yb_2$	1094.15
U_{13}	Liquid +Cu_7Yb_2 $\Leftrightarrow$ Cu_2Yb+Cu_5Yb	1024.24
U_{14}	Liquid +τ_1 $\Leftrightarrow$ θ+Fcc_Al	820.61
P_1	Liquid+τ_1+ Fcc_Al $\Leftrightarrow$$\tau_3$	909.64
P_2	Liquid +τ_1+Al_2Yb $\Leftrightarrow$$Al_3Yb$	1303.44
P_3	Liquid +τ_2+Al_2Yb $\Leftrightarrow$$\tau_6$	1299.69
P_4	Liquid+τ_1+ε$\Leftrightarrow$η	898.11
P_5	Liquid +η+$\tau_1$$\Leftrightarrow$ θ	868.85

The optimized standard enthalpies of formation of several assumed compounds: Cu_2Yb compound with Cu_2Mg structure, Al_5Yb with $CaCu_5$ structure and Al_2Yb compound with $CeCu_2$ structure are -13.92 kJ/mol, -14.639 kJ/mol and -32.792 kJ/mol respectively, which is consistent with those from first-principles calculations (-13.251 kJ/mol, -14.6986 kJ/mol and -32.4892 kJ/mol), as shown in Table 2. The results from CALPHAD optimization and first-principles calculations of the two end members of τ_1-$(Al,Cu)_{12}Yb$ and τ_2-$(Al,Cu)_{17}Yb_2$ ($Al_{12}Yb$ and $Cu_{12}Yb$ with $Mn_{12}Th$ structure, $Al_{17}Yb_2$ and $Cu_{17}Yb_2$ with Th_2Zn_{17} structure) are compared. It can be found out from Table 2 that reasonably good agreements have been achieved. Also, it can be found that the optimized standard enthalpies of formation of ternary compounds (τ_4-Al_4Cu_2Yb and τ_7-AlCuYb) are close to the results from first-principles calculations.

The calculated liquids projection is shown in Fig. 3. Note that the invariant equilibria involving the Al-Cu binary phases in Fig. 3 is too close with the Al-Cu binary subsystem to be visible. The calculated invariant reactions and temperatures involved liquid in the Al-Cu-Yb ternary system are summarized in Table 4. Further experimental data are needed to verify the liquids projection.

5. Conclusions

The Al-Cu-Yb ternary system has been assessed thermodynamically based on the reported experimental data of phase diagrams and thermodynamic properties. Reasonable agreement between calculation and experimental data has been achieved and the thermodynamic parameters for various phases in this ternary system have been obtained.

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