

## Section III: Phase Diagram Updates

**Table 1 Thermodynamic Model of the Ba-Yb System**

**Lattice stability parameter, J/mol**

$$G^0(\text{Ba,L}) = 0$$

$$G^0(\text{Yb,L}) = 0$$

$$G^0(\text{Ba,bcc}) = -7120 + 7.105T$$

$$G^0(\text{Yb,bcc}) = -7660 + 7.014T$$

**Excess Gibbs energy of mixing, J/mol**

$$\Delta_{\text{mix}}G^{\text{ex}}(\text{L}) = 0$$

$$\Delta_{\text{mix}}G^{\text{ex}}(\text{bcc}) = (7011 - 2458X)X(1 - X)$$

Note: *T* is temperature in K. *X* is atomic fraction of Yb.

minimum melting point at  $40 \pm 5$  at. % Yb. However, the liquidus is convex on both sides of the minimum point with inflection points near the minimum point. [91Oka2] pointed out that occurrence of two inflection points located close to one another is thermodynamically unlikely. In addition, the opening angles between the liquidus and solidus near pure Ba and pure Yb are too wide according to criteria given in [91Oka2]. The diagram in [78Zuk] was probably drawn schematically only to show that the melting points of Ba and Yb decrease on alloying the other elements.

The Ba-Yb phase diagram (Fig. 1) was calculated assuming an ideal solution for the liquid phase and a subregular solution for the solid phase using the minimum melting point as an anchor point. The actual thermodynamic properties of the liquid and solid phases may be somewhat different, but the calculated phase boundaries are not seriously influenced by the selected thermodynamic model [91Oka1]. The thermodynamic model assumed here is given in Table 1. The calculated solidus is very similar to that proposed by [78Zuk], but the calculated L + (Ba,βYb) two-phase field is much narrower than that of [78Zuk]. The phase boundaries between (Ba,βYb) and (αYb) are drawn as proposed by [78Zuk].

**Cited References**

78Zuk: M.A. Zukuritdinov, A.V. Vakhobov, and T.D. Dzburayev, *Izv. Akad. Nauk SSSR, Met.*, (2) 225-226 (1978) in Russian; TR: *Russ. Metall.*, (2), 179-180 (1978).

88Gsc: K.A. Gschneidner, Jr. and F.W. Calderwood, *Bull. Alloy Phase Diagrams*, 9(3), 224-225 (1988).

91Oka1: H. Okamoto, to be published in *J. Phase Equilibria* (1991).

91Oka2: H. Okamoto and T.B. Massalski, *J. Phase Equilibria*, 12(2), 148-168 (1991).

# Cu-La (Copper-Lanthanum)

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The Cu-La phase diagram in [Massalski2] was adopted from [81Cha]. [85Mey] reinvestigated the concentration range 0 to 33 at. % La and found two new phases; X(7.5 at. % La) and Cu<sub>4</sub>La. In addition, [87Yam] found that orthorhombic Cu<sub>6</sub>La is monoclinically distorted below ~500 K (~227 °C). The orthorhombic to monoclinic transformation is common to all Cu<sub>6</sub>RE compounds, but the transition temperatures are below room temperature except for RE = La [90Nak]. Fig. 1 has been modified according to the information above. Crystal structure data (Table 1) are from [81Cha] with additional information on Cu<sub>6</sub>La and Cu<sub>4</sub>La.

**Cited References**

81Cha: D.J. Chakrabarti and D.E. Laughlin, *Bull. Alloy Phase Diagrams*, 2(3), 302-305 (1981).

85Mey: F. Meyer-Liautaud, C.H. Allibert, and J.M. Moreau, *J. Less-Common Met.*, 110, 81-90 (1985).

87Yam: K. Yamada, I. Hirose, Y. Noda, Y. Endoh, Y. Onuki, and T. Komatsubara, *J. Phys. Soc. Jpn.*, 56, 3553 (1987).

90Nak: M. Nakazato, N. Wakabayashi, and Y. Onuki, *J. Phys. Soc. Jpn.*, 59, 4004-4009 (1990).

**Table 1 Cu-La Crystal Structure Data**

Phase	Composition, at. % La	Pearson symbol	Space group	Strukturbericht designation	Prototype
(Cu).....	~0	cF4	Fm $\bar{3}$ m	A1	Cu
X.....	7.5	...	...	...	...
βCu <sub>6</sub> La.....	14.3	oP28	Pnma	...	CeCu <sub>6</sub>
αCu <sub>6</sub> La.....	14.3	mP*	...	...	...
Cu <sub>5</sub> La.....	16.6	hP6	P6/mmm	D2 <sub>d</sub>	CaCu <sub>5</sub>
Cu <sub>4</sub> La.....	20	tI90	I4m2	...	...
Cu <sub>2</sub> La.....	33.3	hP3	P6/mmm	C32	AlB <sub>2</sub>
CuLa.....	50	oP8	Pnma	B27	FeB
(γLa).....	~100	cI2	Im $\bar{3}$ m	A2	W
(βLa).....	~100	cF4	Fm $\bar{3}$ m	A1	Cu
(αLa).....	~100	hP4	P6 <sub>3</sub> /mmc	A3'	αLa