Aluminium – Copper – Erbium

Paola Riani, Laura Arrighi, Pierre Perrot

Literature Data

A critical review of the literature data up to 1989 has been made by [1991Ran] and later literature considered in a general review of the crystallochemical and phase equilibria of the R-Cu-Al systems (R = rare-earth) by [2003Ria]. Different compounds have been identified and their crystal structures determined: (1) ErCuAl by [1968Dwi, 1973Oes, 1989Kuz], with a high pressure modification reported by [1987Tsv1, 1987Tsv2], (2) $ErCuAl_3$ by [1988Kuz, 1989Kuz], (3) $ErCu_4Al$ by [1978Tak], (4) $Er_2Cu_7Al_{10}$ by [1982Pre, 1989Kuz], (5) $ErCu_4Al_8$ by [1976Bus, 1979Fel, 1989Kuz], (6) $ErCu_6Al_6$ by [1980Fel, 1981Fel] and (7) $ErCu_{0.9}Al_{2.1}$ reported by [1992Kuz].
The alloys generally were prepared from 99.5% to 99.9 mass% Er and higher purity Cu and Al. They were melted either by arc melting or under argon protection in induction furnaces using MgO crucibles; followed by homogenization heat treatments. [1989Kuz] studied the phase equilibria at 600°C by X-ray powder analysis on 107 samples and reported trends in the lattice parameters for a number of solid solutions.
[1974Oes] studied the homogeneity ranges of $Er(Cu_{1-x}Al_x)_2$ and $Er(Cu_xAl_{1-x})_2$ and determined the limits of solubility by the appearance of X-ray diffraction lines characterizing a new phase. The results reveal that copper in $ErCu_2$ can be replaced by up to about 1.5 mole% aluminium and that in $ErAl_2$ up to about 15 mole% aluminium can be replaced by copper.

Binary Systems

The reported ternary experimental data are limited and can be summarized in the isothermal section at 600°C, which is consistent in its binary boundaries with (a) the Al-Er phase diagram by [1988Gsc], the Al-Cu phase diagram by [2003Gro] and Er-Cu as reported by [1994Sub]. Amendments have been made to the reported crystal structure data based on [2003Ria].

Solid Phases

According to [1980Fel] the $ThMn_{12}$ type structure is observed for RCu_4Al_8 and RCu_6Al_6, where R = rare earth from Gd to Lu and Y. From the literature it is not always explicit whether the two compositions 1:4:8 and 1:6:6 correspond to two different phases or whether they are the limits of a solid solution range. [1989Kuz] found τ_1,$ErCu_4Al_8$ to be stoichiometric and did not confirm the existence of τ_1,$ErCu_6Al_6$. However, on the basis of [1980Fel], we considered the τ_1,$Er(Cu_xAl_{1-x})_{12}$ as non stoichiometric with $0.33 \le x \le 0.5$. Obviously its range changes with the temperature, as [1980Fel] and [1989Kuz] observed it at different compositions at different temperatures, see Table 1. The existence of a homogeneity range for the compounds $R(Cu_xAl_{1-x})_{12}$, where R is a rare earth, was recently suspected by the same team for R = Y [2003Kra] and confirmed for R = Sc [2003Kan].
The crystal structure of the RCu_4Al phases (R = La to Sm and Gd to Tm) has been studied by [1978Tak]; this composition is included by [1989Kuz] in the homogeneity range of the phase τ_3,$Er(Cu_xAl_{1-x})_5$ with $0.46 \le x \le 0.82$.
Subsequently [1992Kuz] determined the crystal structure of the τ_4,$ErCu_{0.9}Al_{2.1}$ phase as pertaining to the $PuNi_3$ type (*hR*36).
Crystallographic data for all solid phases are given in Table 1.

Isothermal Sections

Figure 1, an isothermal section at 600°C is based on the work of [1989Kuz], corrected at the Al-Cu boundary to be in agreement with the accepted binary diagram. At the Cu-Er edge of the ternary isothermal section, however, the two compounds Er_2Cu_7 and Er_2Cu_9 are omitted, although they are reported in the accepted binary, as they were not observed at this temperature in the ternary alloys by [1989Kuz]. These

two compounds, designated Er_2Cu_7 and Er_2Cu_9 by [1994Sub] have been designated as $ErCu_x$ and $ErCu_y$ by [1970Bus], who assumes that $ErCu_x$ forms peritecticaly at 940°C, that $ErCu_y$ melts congruently at 1010°C. By lack of data in the Cu-Er system these assumptions are based on the melting behavior of other similar rare earth-copper compounds.
Inside the ternary system there are four ternary solid solutions: (1) τ_1,$Er(Cu_xAl_{1-x})_{12}$ ($ThMn_{12}$ type), which is shown as a stoichimetric phase at this temperature according to [1989Kuz], (2) τ_2, $Er_2(Cu_xAl_{1-x})_{17}$ with Th_2Zn_{17} type structure and a solution range of $0.41 \le x \le 0.56$, (3), τ_3, $Er(Cu_xAl_{1-x})_5$ in a range of $0.46 \le x \le 0.82$ and with a $CaCu_5$ type structure and (4) the τ_6, ErCuAl with a small solubility range and ZrNiAl type structure.
Three stoichiometric compounds have been found. (I) $Er_5Cu_6Al_9$ ($PuNi_3$ type) for which [1992Kuz] suggested that it assimilates with $ErCu_{0.9}Al_{2.1}(\tau_4)$ ($PuNi_3$ type) in samples annealed at 600°C, (II) the τ_5,$ErCuAl_3$ being of $HoCuAl_3$ type structure and (II) the τ_7,$Er_2Cu_3Al_5$ whose structure is unknown. At 600°C $ErCu_2$ dissolves up to ~1 at.% aluminium, ErCu dissolves up to ~20 at.% aluminium and $ErAl_2$ up to about 13 at.% copper. The τ_8,$Er_6Cu_{16}Al_7$ (Th_6Mn_{23} type) identified by [1990Ste] has not been observed at 600°C by [1989Kuz]. Its position in the phase diagram is shown in Fig. 1, but it is not possible to draw reliable equilibrium lines between τ_8 and its surrounding phases.

Notes on Materials Properties and Applications

[1979Fel] studied the magnetism and hyperfine interactions of ^{151}Eu, ^{155}Gd, ^{161}Dy, ^{166}Er and ^{170}Yb in RCu_4Al_8 and [1995Cac] reported neutron spectroscopy studies of crystal-field interaction in RT_4Al_8 compounds (R = Tb, Ho, Er; T = Mn, Fe, Cu).
[1973Oes] measured the Curie temperature of the ErCuAl compound as 17 K. [1996Jav] found that ErCuAl orders ferromagnetically below T_c= 6.8 K with the magnetic moments parallel to the *c*-axis, a behavior which [1998Jav] confirmed later by measuring susceptibility, magnetization and specific heat.
[1996Mit] studied the interaction of H_2 with RCuAl (R = Dy, Ho, Er).
For the $ErCu_4Al_8$ compound, a type 1 antiferromagnetic structure is observed by neutron powder diffraction in [1997Bai].

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Table 1: Crystallographic Data of Solid Phases

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
(Al) <660.45	*cF*4 $Fm\bar{3}m$ Cu	a = 404.96	at 25°C [Mas2] Cu solubility 2.48 at.% [Mas2] no appreciable solubility of Er [1988Gsc]
(Cu) < 1084.62	*cF*4 $Fm\bar{3}m$ Cu	a = 361.46	at 25°C [Mas2], 0 to 19.7 at.% Al [Mas2] no appreciable solubility of Er [1994Sub]
$Cu_{1-x}Al_x$		a = 361.52 a = 365.36	[1991Ell], x = 0, quenched from 600°C [1991Ell], x = 0.152, quenched from 600°C

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
(Er) <1529	*hP*2 *P6$_3$/mmc* Mg	*a* = 355.92 *c* = 558.50	pure Er at 25°C [1994Sub] solubility: < 1 at.% Al, [1988Gsc] <0.5 at.% Cu [1994Sub]
β, Cu_3Al(h) 1049-559	*cI*2 *Im$\bar{3}$m* W	 *a* = 294.6 *a* = 295.64	~70 to 82 at.% Cu [1985Mur], [1998Liu] at 580°C at 672°C in two-phase (Cu)+β alloy
α_2, $Cu_{100-x}Al_x$ < 363	*t*** $TiAl_3$ long period super-lattice	 *a* = 366.8 *c* = 368.0	22 ≤ *x* ≤ 23.5 [1985Mur] 76.5 to 78.0 at.% Cu at 76.4 at.% Cu (subcell only)
γ_0, $Cu_{100-x}Al_x$ $Cu_{\sim 2}Al$ 1037-800	cI52 *I$\bar{4}$3m* Cu_5Zn_8		31.5 ≤ *x* ≤ 37 [Mas2], 32 ≤ *x* ≤ 38 [1998Liu]
γ_1, Cu_9Al_4 < 890	*cP*52 *P$\bar{4}$3m* Cu_9Al_4	 *a* = 870.23	62 to 68 at.% Cu [Mas2, 1998Liu]; from single crystal [V-C2] at 68 at.% Cu
δ, $Cu_{100-x}Al_x$ < 686	*hR** *R$\bar{3}$m*	 *a* = 1226 *c* = 1511	38.1 ≤ *x* ≤ 40.7 [1985Mur] 59.3 to 61.9 at.% Cu at *x* = 38.9 [V-C2]
ε_1, $Cu_{100-x}Al_x$ 958-848	cubic?		37.9 ≤ *x* ≤ 40.6 59.4 to 62.1 at.% Cu [Mas2, 1985Mur]
ε_2, $Cu_{2-x}Al$ 850-560	*hP*6-x *P6$_3$/mmc* Ni_2In	*a* = 414.6 *c* = 506.3	0.47 ≤ *x* ≤ 0.78 55 to 61 at.% Cu [Mas, 1985Mur, V-C2], NiAs in [Mas2, 1994Mur]
ζ_1, ~$Cu_{47.8}Al_{35.5}$(h) 590-530	*oF*88 - 4.7 *Fmm2* $Cu_{47.8}Al_{35.5}$	*a* = 812 *b* = 1419.85 *c* = 999.28	55.2 to 57 at.% Cu [Mas2, 2003Gro] structure: [2002Gul]
ζ_2, $Cu_{11.5}Al_9$(r) < 570	*oI*24 - 3.5 *Imm2* $Cu_{11.5}Al_9$	*a* = 409.72 *b* = 703.13 *c* = 997.93	55.2 to 56.3 at.% Cu [Mas2, 1985Mur] structure: [2002Gul]
η_1, CuAl(h) 624-560	*o**32	*a* = 408.7 *b* = 1200 *c* = 863.5	49.8 to 52.4 at.% Cu [V-C2, Mas2, 1985Mur] Pearson symbol: [1931Pre]
η_2, CuAl(r) < 560	*mC*20 *C2/m* CuAl	*a* = 1206.6 *b* = 410.5 *c* = 691.3 β = 55.04°	49.8 to 52.3 at.% Cu [V-C2]
θ, $CuAl_2$ < 591	*tI*12 *I4/mcm* $CuAl_2$	 *a* = 606.7 *c* = 487.7	32.05 to 32.6 at.% Cu at 549°C 31.9 to 33 at.% Cu at 250°C [1996Goe] single crystal [V-C2, 1989Mee]

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
$ErCu_{1-x}Al_x$	*cP*2	*a* = 343.1	at *x* = 0 [1994Sub]
ErCu	$Pm\bar{3}m$		0 ≤ *x* ≤ 0.4 at 600°C [1989Kuz]
< 1065	CsCl	*a* = 341.0	at *x* = 0
		a = 347	at *x* = 0.4
$Er(Cu_{1-x}Al_x)_2$	*oI*12		0 ≤ *x* ≤ 0.015 (1 at.% Al) [1974Oes]
$ErCu_2$	*Imma*	*a* = 427.4	at *x* = 0, [1988Sub] [1994Sub]
< 935	$CeCu_2$	*b* = 673.3	
		c = 726.6	
Er_2Cu_7	?		[1994Sub]
< 940			
Er_2Cu_9	?		[1994Sub]
< 1010			
$ErCu_5$	*cF*24	*a* = 700.3	[1994Sub]
<1005	$F\bar{4}3m$		at 600°C dissolves up to ~2 at.% Al
	$AuBe_5$		according to the figure in [1989Kuz]
$ErAl_3$	*cP*4	*a* = 421.4	[1988Gsc]
< 1070	$Pm\bar{3}m$		
	$AuCu_3$		
$ErAl_2$	*cF*24		0 ≤ *x* ≤ 0.38 (~19 at.% $ErCu_2$) at 600°C
< 1455	$Fd\bar{3}m$		[1989Kuz]
$ErCu_xAl_{2-x}$	Cu_2Mg	*a* = 779.3	at *x* = 0 [1988Gsc, 1989Kuz]
		a = 773.7	at *x* = 0.38 [1989Kuz]
ErAl	*oP*16	*a* = 580.1	[1988Gsc]
< 1140	*Pbcm*	*b* = 1127	
	ErAl	*c* = 557.0	
Er_3Al_2	*tP*20	*a* = 812.3	[1988Gsc]
< 1060	$P4_2/mnm$	*c* = 748.4	
	Gd_3Al_2		
Er_2Al	*oP*12	*a* = 651.6	[1988Gsc]
< 1040	*Pnma*	*b* = 501.5	
	Co_2Si	*c* = 927.9	
* τ_1, $Er(Cu_xAl_{1-x})_{12}$	*tI*26		0.33 ≤ *x* ≤ 0.5 (*x* range tentatively
	I4/mmm		assigned)
$ErCu_4Al_8$	$ThMn_{12}$	*a* = 866.3	*x* = 0.33 at 600°C [1989Kuz]
		c = 510.5	
		a = 869.1	at *x* = 0.33, as-cast sample [1979Fel]
		c = 511.9	
$ErCu_6Al_6$		*a* = 863.0	at *x* = 0.5 at 800°C [1980Fel]
		c = 502.9	
* τ_2, $Er_2(Cu_xAl_{1-x})_{17}$	*hR*57		0.41 ≤ *x* ≤ 0.56 at 600°C [1989Kuz]
	$R\bar{3}m$	*a* = 880.4	at *x* = 0.41 [1982Pre]
	Th_2Zn_{17}	*c* = 1285.1	
		a = 871.0	at *x* = 0.56 [1989Kuz]
		c = 1274.6	

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
* τ_3, $Er(Cu_xAl_{1-x})_5$	*hP*6		$0.46 \le x \le 0.82$ at 600°C [1989Kuz]
	P6/mmm	$a = 502.9$	at $x = 0.82$ [1989Kuz]
	$CaCu_5$	$c = 413.9$	
$ErCu_4Cu$		$a = 503.9$	at $x = 0.8$ [1978Tak]
		$c = 413.9$	
		$a = 524.1$	at $x = 0.46$ [1989Kuz]
		$c = 407.1$	
* τ_4, $ErCu_{0.9}Al_{2.1}$	*hR*36	$a = 542.1$	[1992Kuz]
	$R\bar{3}m$	$c = 2529.9$	Previously reported as $Er_5Cu_6Al_9$
	$PuNi_3$		[1989Kuz]
* τ_5, $ErCuAl_3$	*oI*10	$a = 418.4$	[1988Kuz]
	Immm	$b = 411.2$	
	$HoCuAl_3$	$c = 977.3$	
* τ_6, ErCuAl	*hP*9	$a = 697.40$	$x = 0$ [1968Dwi]
$ErCu_{1+x}Al_{1-x}$	$P\bar{6}2m$	$c = 400.19$	$-0.02 \le x \le 0.1$ at 600°C [1989Kuz]
	ZrNiAl		
* τ_7, $Er_2Cu_3Al_5$			[1989Kuz]
* τ_8, $Er_6Cu_{16}Al_7$	*cF*116	$a = 1224.0$	[1990Ste]. Not observed by [1989Kun] in the investigation of the isothermal section at 600°C
	$Fm\bar{3}m$		
	Th_6Mn_{23}		

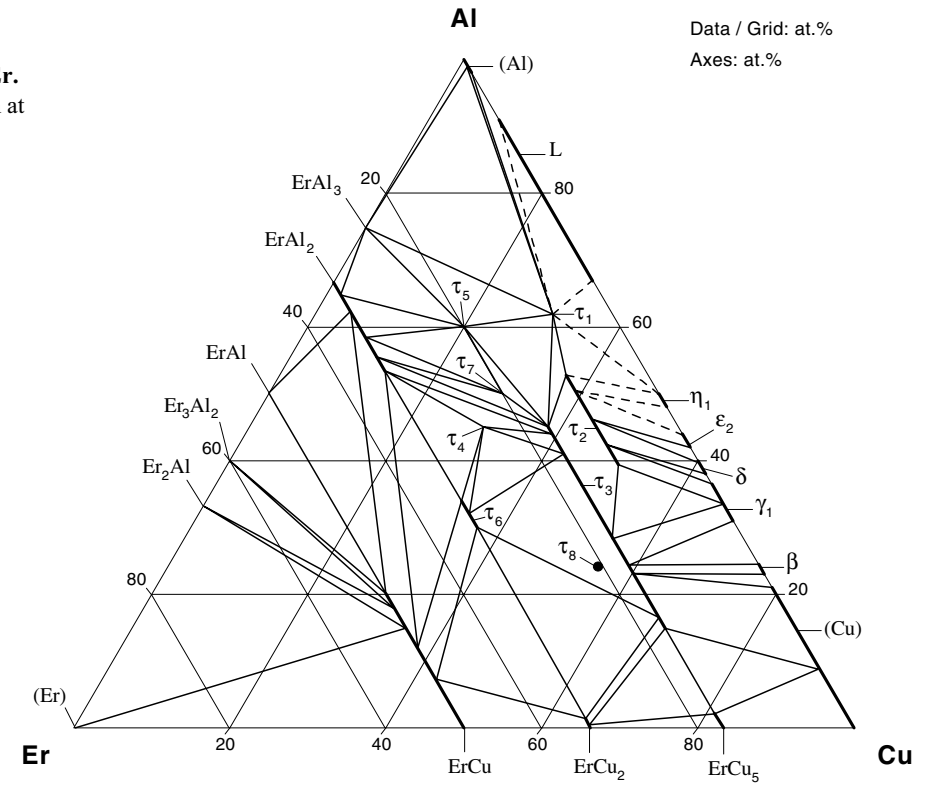

Fig. 1: Al-Cu-Er. Isothermal section at 600°C