

Aluminium – Copper – Ruthenium

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Introduction

The first work on the system was performed in 1986 [1986Rae], [1986Yan]. Authors presented isothermal section of the system at 770 K (500°C). In addition, the composition region where as cast alloys were clearly immiscible was delineated. Neither ternary compounds nor any noticeable (>2 at.%) solubility of third component in binary phases were detected.

The general interest in the system is due to the existence of a stable icosahedral quasicrystalline phase (IQC) in the Al rich region. This phase was discovered by [1988Tsa] at the composition of $\text{Al}_{65}\text{Cu}_{20}\text{Ru}_{15}$ both in conventionally solidified and annealed state. The alloys were obtained by arc melting. Its quasicrystalline nature was examined by X-ray diffraction, DTA, as well as by optical and transitional electron microscopy (TEM). [1989Gur] showed that the quasicrystalline order in this phase is one of most perfect among all known IQC phases. [1989Hir2] found that liquid quenching provides disordered IQC which gets ordered after a series of transformations.

In addition to IQC, two crystalline phases with X-ray pictures close to the IQC were found [1992Shi1]. Like the latter, their structures may be represented as projection of high-dimensional hyperlattices into common 3-dimensional space. But contrary to the IQC, this projection is to be done in rational directions (rational values of tangent of projection angle in the units of hyperlattice constants). Those are called *rational approximants* of icosahedral quasicrystals, and may be identified by projection directions.

The phase relations concerning IQC were studied first by [1992Shi1] using samples, obtained by melt spinning from liquid with subsequent grinding (this technique later became essentially standard for their preparation). The study of the transformations under DTA conditions revealed the following sequence: disordered IQC - periodic phases - ordered IQC based on face-centered quasilattice. In addition, a study of the equilibria at 800°C was performed on samples annealed for various time (24 h to a week). Clear DTA peak at 690 to 710°C was ascribed to formation of IQC as stable phase: a conclusion was drawn that the latter is stable only at high temperatures. Later [1994Gru], [1998Ath] and finally [2004Mi] tracked down the stability of IQC phase to at least 600°C (most probably, it is stable to room temperature). The reaction at about 700°C proved to be a peritectic with participation of IQC [1994Gru], [2004Mi]. The region of existence of IQC phase was also presented by [1993Shi1] and [1993Was].

[1997Kam] and [2002Guo] found the compositions and cooling regimes which provide single grains of IQC of millimeter size. The grains obtained had clear morphology of pentagonal dodecahedron.

[1993Ara] found the composition region where IQC forms at liquid quenching to be close to a line with the valence electrons to atoms ratio $e/a \approx 1.75$ indicating a possible electronic nature of its stabilization.

The melting region was studied by [1996Log] and [2002Guo], but the results are mutually incompatible and neither can be considered as quite satisfactory (see below for details). The equilibria with liquid phase still need further investigation.

[2004Mi] performed very thorough investigation of the phase equilibria in the region of Al compositions above 50 at.%. Alloys were produced from the constituent elements by levitation induction melting in a water-cooled copper crucible under an Ar atmosphere. The nominal purity of Al was 99.999%, of Ru 99.9% and of Cu 99.99%. The ingots were typically of about 5g. The dissolution of Ru in Al being difficult, the samples were re-melted if after inspection undissolved particles of Ru were detected in the broken ingots. This procedure was repeated until microscopically homogeneous ingots were obtained. Annealing temperatures from 600 to 1100°C were applied depending on the sample compositions. The phase morphology of the annealed samples was compared to that of the as-cast samples in order to verify whether equilibrium had been achieved. Additional annealing was applied if required. At 600°C the annealing time was up to 4392 h, at 680°C up to 864 h, at 800°C up to 2712 h, at 890°C up to 690 h, at 1000°C up to 117 h and at 1100°C up to 40 h. The alloys were studied by powder X-ray diffraction (XRD) and scanning electron microscopy (SEM). The local phase compositions were determined by SEM using energy-dispersive X-ray

analysis (EDX) on polished unetched cross sections. The samples were also studied by electron diffraction in a transmission electron microscope (TEM) operated at 200 kV. The compositions of selected single-phase samples were examined by inductively coupled plasma optical emission spectroscopy. These compositions were used to correct the EDX data. The vertices of the tie triangles were determined on the basis of the EDX measurements of equilibrated three-phase samples. The melting temperatures of the phases were determined by differential thermal analysis (DTA) at the rate of $20^{\circ}\text{C}\cdot\text{min}^{-1}$.

Authors [2004Mi] presented the projection of phase compositions to concentration triangle to indicate the compositions of all the phases found in the region studied at all the temperatures, and the isothermal sections at 1100, 1000, 890, 800, 680 and 600°C . For constructing the 600°C section their results were complemented by some data from unpublished PhD thesis, performed in the same laboratory. In addition to the experimental work, a critical analysis of nearly all published data was performed.

The structure of the stable IQC phase was generally established by [1989Gur], [1989Hir1]. [1992Hu] tested the models of projection from 6-dimensional hyperspace as well as Penrose tiling as models of the structure of IQC; the former proved to be more adequate. Further refinement of the structure was performed by [2004Yam], who used synchrotron radiation. Structural data were obtained also by [1997Ham] (positron annihilation).

[1993Shi2] suggested the structure of $\{1/1\}$ approximant phase to be identical to $\alpha'\text{AlMnSi}$. [2000Sad] studied this phase in more details on a single-crystal sample and found another structure, though close to $\alpha'\text{AlMnSi}$ and some other approximant phases. This was confirmed also by [2004Mi].

The structure of the phase considered as $\{1/0\}$ approximant to IQC was suggested by [1993Ara], [1993Was] to be of UH_3 type ($cP32$). [1998Sug] re-determined the structure of this phase on a quaternary sample $\text{Al}_{55.1}\text{Cu}_{14.6}\text{Ru}_{20.2}\text{Si}_{10.1}$, using single-crystal X-ray diffraction, and found that it has its own structural type instead of the UH_3 one. This phase was called (Al–Cu–Ru–Si). Later the same structure was found for $\{1/0\}$ approximant phase in the ternary [2004Mi].

The structure of a tetragonal phase found by [1992Shi1] as stable at 500°C , was determined by [1993Shi2] to be of $\text{Al}_7\text{Cu}_2\text{Fe}$ type ($tP40$); it is not related to IQC.

As thermodynamics concerns, only heat capacity data seem to exist. [1990Miz] measured heat capacity of IQC sample $\text{Al}_{68}\text{Cu}_{17}\text{Ru}_{15}$ at 1.5 to 6 K. Low temperature heat capacities of $\text{Al}_{61.5}\text{Cu}_{25}\text{Ru}_{13.5}$ and $\text{Al}_{65}\text{Cu}_{20}\text{Ru}_{15}$ IQC were studied by [1994Nak]; only the values of the electronic specific heat coefficient γ_{el} and Debye temperatures are reported. [1996Ina] measured heat capacities of $\text{Al}_{65}\text{Cu}_{20}\text{Ru}_{15}$ as perfect quasicrystal and quasicrystal with phason disorder as well as approximant phase with $\text{Al}_{70}\text{Cu}_{20}\text{Ru}_{10}$ composition, all for 1 to 350 K. Results were presented as the values of γ_{el} and graphs of temperature dependence of apparent Debye temperature. Those were used only for comparing electronic contribution to heat capacity and vibrational spectra for IQC with different structural states; no attempt to extract standard thermodynamic values was performed. The same data are discussed in more details in [1997Ina].

A number of other physical properties of IQC and related phases was measured, mostly as a tool for the study of their electronic structure. [1990Miz] studied resistivity of IQC at 4.2 to 300 K, in addition to the heat capacity, for samples with different degree of quasicrystalline order. Transport properties of quasicrystalline phase (resistivity and Hall coefficient) were studied by [1995Lal], [1994Nak] and [1994Tam1, 1994Tam2]; strong dependence on degree of quasicrystalline order was found. [1992Shi2], [1993Sha], [1994Hil], and [1995Sha] studied IQC using NMR technique. In addition experimental investigations of the IQC band structure were performed by [1994Sta] and [1996Bel], who used spectroscopic techniques. Theoretical analysis of resistivity of IQC was made by [2000Mac].

[2002Boz] performed theoretical prediction of distribution of a number of elements, including Cu, between sublattices of $B2$ phase RuAl .

[1991Aka], [1998Sad] and [2000Sad] determined volume of IQC under high pressures. Fitting the data to Murnaghan equation, bulk modulus and its pressure dependence were calculated.

[2001Sur] reviewed the formation of quasicrystals in the processes of mechanical alloying for various systems.

[2004Gru] presented general review of formation of quasicrystalline phases (not only icosahedral) in Al–3d metal alloys.

Details of the experimental investigations of phase relations, crystal structure and thermodynamics are listed in Table 1.

Binary Systems

For the Al–Cu and Cu–Ru binaries new MSIT evaluations [2004Gro], [2002Du] are accepted. For the Al–Ru edge the results of recent investigation [2003Mi] are accepted. These were not accounted for by [2004Oka] but were performed in the same group as most detailed investigation of the ternary Al–Cu–Ru system [2004Mi].

Solid Phases

Contrary to [1986Yan], Cu solubility in the binary Al–Ru phases is indeed measurable. The Al₆Ru phase dissolves up to 5 at.% Cu and its homogeneity range extends along a constant Ru line. The AlRu takes about 50 at.% Cu with simultaneous increase of Ru content, so its homogeneity range extends towards the ω phase of the Al–Cu edge. The solubility of Cu in other Al–Ru phases, as well as of Ru in the Al–Cu phases, is small (app. 1 to 3 at.%).

The results obtained for ternary phases are in good mutual agreement. In addition to the thermodynamically stable quasicrystalline phase *I*, three periodic phases are established. Two of these, namely *C*, called also “AlCuRu” [1993Ara] and having composition around Al₅₈Cu₃₀Ru₁₂, and *C_I*, formed at compositions between Al₇₁Cu_{8.5}Ru_{20.5} and Al₇₂Cu_{6.5}Ru_{21.5} have structures considered as rational approximants to the quasicrystals, of {1/1} and {1/0} type, respectively. The structure of the third periodic phase called ω was identified by [1993Shi2] and confirmed by [2004Mi]; it is not related to the quasicrystals.

For the *C_I* phase [2002Guo] provides the formation temperature as 1090°C based on DTA, but [2004Mi] found this phase at 1100°C, and its formation temperature must be somewhat higher. It decomposes between 890 and 800°C [2004Mi]; DTA study of [2002Guo] give for its decomposition the temperature of ~940°C, but its presence on isothermal section at 890°C [2004Mi] suggests lower value. The *C* phase forms also between 890 and 800°C [2004Mi], and the ω phase melts peritectically at about 730°C [2004Mi]. The quasicrystalline *I* phase is formed at 1057°C; contrary to early observations [1992Shi1], [1993Shi1], it remains stable to low temperatures [1998Ath], [2004Mi].

For the structure of *C* phase ({1/1} rational approximant to IQC) we accepted the results of [2000Sug] confirmed by [2004Mi].

[2004Mi] also identified the structure of *C_I* ({1/0} approximant phase) with that of γ (Al–Cu–Ru–Si), investigated by [1998Sug]. This was also accepted. [1993Shi1], [1993Ara] and [1993Was] suggested other versions, but those were based on more limited data. In particular, the technique, used by [1993Shi1], who suggested for this phase a cubic structure with two times smaller *a* value, may reveal the structure of local atomic configuration instead of the lattice, as was noted by author himself.

Models of structure of quasicrystalline phase are constructed by [1992Hu] and, in more detail, [2002Hir] and [2004Yam]. For general review of quasicrystalline structures see [1993Kel].

The structures of “disordered” and “ordered” quasicrystals [1989Hir2] are not much different; only the latter is thermodynamically stable, and transitions found by [1992Shi1] are clearly irreversible. For concept of phason disorder which prevails in IQC see [1989Gur] (experimental data), [1991Fra] (theory), and [1992Poo] and [1993Kel] (reviews).

All the phases are presented in Table 2, except for numerous metastable ones of the Al–Cu edge, which do not influence the ternary equilibria. For the quasicrystalline phase the so-called “quasilattice constant” a_R is provided, which is calculated by the equation $a_R = \pi\tau^3/q_{422222}$ (τ is golden section ratio, q_{422222} is the scattering vector for the (422222) plane). It is related to period of modeling 6-dimensional hyperlattice [1993Ara]; see also [1998Ath] for its treatment in terms of Penrose tiling model.

Invariant Equilibria

Only the reactions which are related to the IQC formation were more or less studied, and even for those the results are still contradicting. Peritectic reaction is definitely established [1996Log], [1998Ath], [2002Guo]

for the formation of the IQC phase, but the reported temperatures and participating phases are not in agreement. In particular, [1996Log] suggests a reaction $L + Al_{13}Ru_4 + Al_2Ru \rightleftharpoons I$ at $\sim 1200^\circ C$, whereas [2002Guo] gives this reaction as $L + Al_{68}Cu_{17}Ru_{15} \rightleftharpoons I$ (the “ $Al_{68}Cu_{17}Ru_{15}$ ” phase of [2002Guo] was identified by [2004Mi] with C_1 phase) which occurs at $1020^\circ C$. [1998Ath] and [2004Mi] found for the peritectic melting of I phase the value of $1057^\circ C$, which confirms the second version. Peritectic formation of C phase found by [2002Guo] is also accepted. A shift of the temperature of both peritectic temperatures for about $25^\circ C$ brings the data of [2002Guo] into agreement with [2004Mi]. We had to reject all the three reactions, suggested by [1996Log], as being incompatible with the accepted data.

Neither [1996Log] nor [2002Guo] determined the compositions of phases participating in the suggested reactions, so those can not be tabulated.

Liquidus, Solidus and Solvus Surfaces

The miscibility gap in the liquid phase, which exist in the Cu–Ru binary, extends into the ternary up to ~ 30 at.% Al [1986Rae], [1986Yan].

The partial liquidus projection suggested by [1996Log] shows a wide field of primary crystallization of IQC. Contrary to that, [2002Guo] found it to be narrow. The composition sets of alloys which give IQC as primary crystallizing phase as indicated by [1996Log] and by [2002Guo] are mutually exclusive: *e.g.*, for the section with 65 at.% Al [1996Log] indicates primary crystallization of IQC up to 12 at.% Ru, whereas [2002Guo] found an alloy with 4 at.% Ru not to form the IQC as primary phase. The results of [2002Guo] are also in broad agreement with [1998Ath], where a narrower field is suggested.

In addition, the field of primary crystallization of Al_2Ru was found by [2002Guo] to extent down to 4.5 at.% Ru along the section with 62 at.% Ru; this could not be brought into agreement with liquidus projection of [1996Log]. For reasons given in the previous section and above we accepted the results of [2002Guo] against [1996Log]. The field of primary crystallization of IQC is at about 30 to 40 at.% Cu, ~ 4 at.% Ru [2002Guo].

Isothermal Sections

Only the Al rich region (≥ 50 at.%) is studied in detail. For the Al poor region, no data seem to exist except for those from [1986Rae], [1986Yan].

All the sections presented here are taken from [2004Mi], as they are based both on detailed experimental data and on critical analysis of previous results. Thus, the fragmentary sections suggested by [1992Shi1], [1993Shi1] are considered to be superseded by those presented here.

We had to make some corrections to the compositions of some binary phases in Figs. 1 to 6 below, especially those of Al–Cu edge, as they were somewhat misplaced in the original figures of [2004Mi]. Moreover, the binary phases of the Al–Ru edge are given by [2003Mi] without homogeneity ranges, whereas [2004Mi] indicates for those a variable Ru content. To remove this discrepancy we reduced homogeneity ranges of the binary phases when approaching Al–Ru binary to zero, though in principle this point needs experimental clarification.

The partial isothermal section at $1100^\circ C$ is presented in Fig. 1; the sample of gross composition $Al_{60}Cu_5Ru_{35}$ could not be brought to equilibrium, and this part of section is provisional. The above-mentioned shift of the temperature of peritectic formation of C phase removes contradiction between the peritectic temperature from [2002Guo] and appearance of this phase on the $1100^\circ C$ section.

The section at $1000^\circ C$ is given in Fig. 2 and at $890^\circ C$ in Fig. 3.

Figure 4 displays the section at $800^\circ C$. The compositions of C , I and Al_2Ru phases on this section are in excellent agreement with those measured by [2000Sug] for the same temperature; so does the phase composition in $Al_{56}Cu_{31}Ru_{13}$ sample, annealed at this temperature by [1996Fre].

Partial section at $680^\circ C$, presented in Fig. 5, agrees well with the phase composition of the $Al_{70.3}Cu_{19}Ru_{10.3}$ alloy, annealed by [1996Fre] at $650^\circ C$.

Partial section at $600^\circ C$ is presented in Fig. 6. As was noticed above, in its constructing authors of [2004Mi] complemented their data by some results of unpublished PhD thesis, performed in the same laboratory.

The schematic isothermal section at 500°C, provided by [1986Rae], [1986Yan] can not be accepted, as no tendency for decomposition of the ternary phases *I*, ω or *C*, stable at 600°C with decreasing temperature, can be seen in the sequence of isothermal sections of [2004Mi].

Temperature – Composition Sections

The main part of the isopleth $\text{Al}_{62}\text{Cu}_{38-x}\text{Ru}_x$ ($x = 2.5$ to 25 at.%), as constructed by [2002Guo], is in drastic contradiction with the accepted phase equilibria after [2004Mi]. So it can not be accepted, though the temperatures of formation of both *C*₁ and *I* phases, if raised for about 25°C, are in general agreement with isothermal sections of [2004Mi].

Thermodynamics

Only the heat capacity data were reported, and no standard thermodynamic functions were ever extracted. Low-temperature data do not fit to standard equation $C_p = \gamma_{el}T + C^D(\theta/T)$. The value of electronic specific heat coefficient γ_{el} strongly varies on degree of quasicrystalline order, from $\sim 0.05 \text{ mJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-2}$ for perfectly ordered sample to $0.75 \text{ mJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-2}$ for sample with phason disorder; the latter value is close to $0.81 \text{ mJ}\cdot\text{mol}^{-1}\cdot\text{K}^{-2}$ measured for the sample of approximant *C* phase of close composition [1996Ina], [1997Ina]. For high-temperature limit of Debye temperature θ the extrapolated values of 462, 442 and 428 K are given correspondingly for perfect quasicrystal, disordered quasicrystal and approximant phase [1997Ina].

Miscellaneous

[1991Aka] found that IQC retains the quasicrystalline structure under pressure up to 30.8 GPa. [1998Sad], [2000Sad] confirmed this up to 35 GPa, though starting from ~ 10 GPa some degree of phason disorder appears. Fitting the pressure-volume data to Murnaghan equation, the latter authors obtained the bulk modulus at zero pressure $B = 128 \text{ kbar}$ and its pressure derivative $BP = 5$.

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Table 1: Investigations of the Al-Cu-Ru Phase Relations, Structure and Thermodynamics

Reference	Method/Experimental Technique	Temperature/Composition Phase Range Studied
[1986Rae]	Metallography, hardness measurement, EPMA	500°C, 0 to 100% Cu and Ru
[1986Yan]	Metallography, hardness measurement, EPMA	500°C, 0 to 100% Cu and Ru

Reference	Method/Experimental Technique	Temperature/Composition Phase Range Studied
[1988Tsa]	XRD, DTA, metallography, TEM	700 to 1400 K, 15 to 25 at.% Cu, 10 to 20 at.% Ru
[1989Gur]	XRD using usual and synchrotron radiation	850°C, Al ₆₅ Cu ₂₀ Ru ₁₅
[1989Hir1]	HREM, electron diffraction	Al ₆₅ Cu ₂₀ Ru ₁₅ : as cast, rapid quenched from liquid and annealed at 750°C, 30 min
[1989Hir2]	XRD, HREM	As cast and annealed at 1118 K, Al ₆₅ Cu ₂₀ Ru ₁₅
[1991Aka]	XRD and electrical resistivity under high pressure	4 to 270 K (resistivity), 270 K (XRD), 0 to 28 GPa, <i>i</i> -Al-Cu-Ru sample
[1992Hu]	Anomalous X-ray powder diffraction	Annealing at 1130 K, Al ₆₅ Cu ₂₀ Ru ₁₅
[1992Mat]	Anomalous X-ray powder diffraction	Annealing at 1130 K, Al ₆₅ Cu ₂₀ Ru ₁₅
[1992Shi1]	XRD, TEM, DTA	500°C, 10 to 27 at.% Cu, 5 to 20 at.% Ru
[1993Ara]	XRD and TEM	Liquid quenching with subsequent annealing at 800°C, 5 to 27 at.% Cu, 10 to 23 at.% Ru, app. along the line $e/a \approx 1.75$
[1993Sad]	Extended X-ray absorption fine-structure	Al ₆₅ Cu ₂₀ Ru ₁₅
[1993Shi1]	XRD, TEM, DTA	800 and 500°C, 10 to 27 at.% Cu, 5 to 20 at.% Ru
[1993Shi2]	TEM, converged beam electron diffraction	Liquid quenching with subsequent annealing at 800°C for Al ₆₀ Cu ₂₅ Ru ₁₅ and at 560°C for Al ₆₅ Cu ₂₃ Ru ₁₂
[1993Was]	XRD and TEM	Liquid quenching with subsequent annealing at 800°C for 1 <i>h</i> ; Al ₆₁ Cu ₂₅ Ru ₁₄ , Al ₇₁ Cu ₁₁ Ru ₁₈ , and Al ₇₁ Cu ₇ Ru ₂₂ compositions
[1994Sha]	Nuclear quadrupole resonance of ²⁷ Al at 4.2K	Al ₇₀ Cu ₁₅ Ru ₁₅ (number of nonequivalent Al positions in the structure)
[1994Gru]	SEM, XRD and DTA	Annealing at 800 and 600°C, Al _{70.3} Cu _{19.4} Ru _{10.3} , Al _{67.8} Cu _{22.3} Ru _{9.9} , Al _{61.0} Cu _{27.4} Ru _{11.6} , and Al _{65.3} Cu _{19.7} Ru _{11.0} compositions
[1996Log]	DTA, powder XRD, metallography, energy dispersive spectroscopy	Melting region of samples with 27, 30 and 35 at.% (Cu+Ru), 0 to 20 at.% Ru
[1996Fre]	Powder XRD with Rietveld refinement	650°C, Al _{70.3} Cu ₁₇ Ru _{10.3} and 800°C, Al ₅₆ Cu ₃₁ Ru ₁₃ (two-phase samples)
[1996Ina]	Adiabatic calorimetry (above 5 K) and isoperibolic calorimeter in ³ He cryostat (below 5 K)	1 to 310K, Al ₆₅ Cu ₂₀ Ru ₁₅ (two samples: perfect and with phason disorder) and Al ₇₀ Cu ₂₀ Ru ₁₀ (all contained 0.2 to 0.3 at.% O)

Reference	Method/Experimental Technique	Temperature/Composition Phase Range Studied
[1997Ina]	Adiabatic calorimetry (above 5 K) and isoperibolic calorimeter in ^3He cryostat (below 5 K)	1 to 310K, $\text{Al}_{65}\text{Cu}_{20}\text{Ru}_{15}$ (two samples: perfect and with phason disorder) and $\text{Al}_{70}\text{Cu}_{20}\text{Ru}_{10}$
[1997Kam]	Search for heat treatment for obtaining single grains of quasicrystals	$\text{Al}_{58}\text{Cu}_{30.8}\text{Ru}_{11.2}$, and $\text{Al}_{61.6}\text{Cu}_{24.8}\text{Ru}_{13.6}$ gross compositions
[1998Ath]	XRD, DTA	$\text{Al}_{70}\text{Cu}_{12}\text{Ru}_{18}$
[1998Sad]	XRD	$\text{Al}_{65}\text{Cu}_{20}\text{Ru}_{15}$, pressure up to 35 GPa
[2000Sad]	XRD, EXAFS	$\text{Al}_{65}\text{Cu}_{20}\text{Ru}_{15}$, pressure up to 24.5 GPa
[2000Sug]	Single-crystal XRD, EPMA	Annealed between 1073 and 1203 K $\text{Al}_{58}\text{Cu}_{30}\text{Ru}_{12}$ gross composition
[2002Guo]	DTA; search for conditions of single grains of quasicrystals	22.5 to 42.5 at.% Cu, 2.5 to 25 at.% Ru
[2004Mi]	XRD, SEM using energy-dispersive X-ray analysis, inductively-coupled optical emission spectroscopy, DTA	600, 680, 800, 890, 100 and 1100°C; 90 to 60 at.% Al, 0 to 50 at.% Ru
[2004Uch]	XRD	$\text{Al}_{62}\text{Cu}_{25}\text{Ru}_{15}$

Table 2: Crystallographic Data of Solid Phases

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
(Al) < 660.452	<i>cF4</i> <i>Fm$\bar{3}m$</i> Cu	$a = 404.96$	at 25°C [Mas2]
(Cu) < 1084.62	<i>cF4</i> <i>Fm$\bar{3}m$</i> Cu	$a = 361.46$	at 25°C [Mas2] melting point [1994Sub]
(Ru) < 2334	<i>hP2</i> <i>P6₃/mmc</i> Mg	$a = 270.58$ $c = 428.16$	at 25°C [Mas2]
θ , Al_2Cu < 591	<i>tI12</i> <i>I4/mcm</i>	$a = 606.7$ $c = 487.7$	31.9 to 33.0 at.% Cu [2004Gro]
η_1 , CuAl(h) 624 - 560	<i>oP16</i> <i>Pban</i>	$a = 401.5$ $b = 1202$ $c = 865.2$	49.8 to 52.3 at.% Cu [2004Gro]
η_2 , CuAl(r) < 560	<i>mC20</i> <i>C2/m</i> CuAl(r)	$a = 1206.6$ $b = 410.5$ $c = 691.3$ $\beta = 55.04^\circ$	49.8 to 52.3 at.% Cu [2004Gro]
ζ_1 , $\sim \text{Cu}_4\text{Al}_3(\text{h})$ 590 - 530	<i>hP42</i> <i>P6/mmc</i>	$a = 810$ $c = 1000$ (or 1237)	55.2 to 59.8 at.% Cu [2004Gro]

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
$\zeta_2 \sim \text{Cu}_4\text{Al}_3(\text{r})$ 590 - 530	$m\bar{2}1$	$a = 707$ $b = 408$ $c = 1002$ $\beta = 90.63^\circ$	55.2 to 56.3 at.% Cu [2004Gro]
ϵ_1 958 - 848	-	-	59.4 to 62.1 at.% Cu [2004Gro]
$\epsilon_2, \text{Cu}_{2-x}\text{Al}$ 850 - 560	$hP6$ $P6_3/mmc$ Ni_2In	$a = 414.6$ $c = 1000$	$0.47 \leq x \leq 0.78$ 55.0 to 61.1 at.% Cu [2004Gro]
δ , < 686	hR^* $R3m$	$a = 1226$ $c = 1511$	$38.1 \leq x \leq 40.7$ 59.3 to 61.9 at.% Cu at $x = 38.9$ [2004Gro]
$\gamma_0, \text{Cu}_{100-x}\text{Al}_x$ 1037 - 800	$cI52$ $\bar{I}4m$ Cu_5Zn_8	$a \approx 890$	$31 \leq x \leq 40.2$ [Mas2] [2004Gro]
$\gamma_1, \text{Cu}_9\text{Al}_4$ < 890	$cP52$ $P43m$ Cu_9Al_4	$a = 870.68$	[V-C2], [2004Gro]
$\beta, \text{Cu}_{100-x}\text{Al}_x$ 1049 - 559	$cI2$ $Im\bar{3}m$ W	$a = 295.64$	at 672°C in $\beta + (\text{Cu})$ alloy [2004Gro]
Al_6Ru < 734	$oC28$ $Cmcm$ MnAl_6	$a = 748.82 \pm 0.04$ $b = 655.59 \pm 0.03$ $c = 896.05 \pm 0.05$	[2003Mi]
		$a = 750.2 \pm 0.4$ $b = 651.2 \pm 0.4$ $c = 890.4 \pm 0.5$	at $\text{Al}_{82.0}\text{Cu}_{3.6}\text{Ru}_{14.4}$ composition [2004Mi] dissolves to 5 at.% Cu [2004Mi]
$\text{Al}_{13}\text{Ru}_4$ < 1420	$mC102$ $C2/m$ $\text{Fe}_4\text{Al}_{13}$	$a = 1586.2 \pm 0.6$ $b = 818.8 \pm 0.3$ $c = 1273.6 \pm 0.4$ $\beta = 107.77 \pm 0.08^\circ$	[2003Mi] dissolves to 2.5 at.% Cu [2004Mi]
Al_5Ru_2 1492 - 1340	$oC24$ $Cmcm$ Al_5Fe_2	$a = 780$ $b = 660$ $c = 420$	[2003Mi] electron diffraction data space group by analogy with Al_5Fe_2 dissolves to 2 at.% Cu in as cast samples [2004Mi]
Al_2Ru < 1805	$tI6$ $Fddd$ MoSi_2	$a = 801.2 \pm 0.2$ $b = 417.7 \pm 0.1$ $c = 878.5 \pm 0.2$	[2003Mi] dissolves to 1.5 at.% Cu [2004Mi]

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
β , AlRu < 2069	$cP2$ $Pm\bar{3}m$ CsCl	$a = 295$ $a = 297.0$ $a = 296.3$ $a = 295.5$	[2004Oka] [2003Mi] at Al ₅₀ Cu _{31.5} Ru _{18.5} [2004Mi] at Al ₄₇ Cu ₄₂ Ru ₁₁ [2004Mi] at Al _{44.5} Cu _{50.5} Ru ₅ [2004Mi]
* C < ~ 845±45	$cP148$ $Pm\bar{3}$ $C (= \alpha\text{AlCuRu})$	$a = 1237.73 \pm 0.08$	at Al _{57.3} Cu _{31.4} Ru _{11.3} [2000Sug] {1/1} rational approximant to IQC in original work the phase is called “ αAlCuRu ” after [1993Ara]
* C_I (1100) - (~ 845±45)	$cF368$ $Fm\bar{3}$ $\gamma(\text{Al-Cu-Ru-Si})$	$a = 1551.1 \pm 0.4$	Al _{69.5-72} Cu _{6.5-9.5} Ru _{21-21.5} [2004Mi] {1/0} rational approximant to IQC
* ω , Al ₇ Cu ₂ Ru < 730	$tP40$ $P4/mnc$ Al ₇ Cu ₂ Fe	$a = 643.3 \pm 0.2$ $c = 1489 \pm 1$	[2004Mi]
* I < 1057	FCI*	$a_R^{**} = 451$ $a_R = 452.87$	[1993Ara], after annealing [1998Ath] Al ₆₁ Cu ₂₆ Ru ₁₃ to Al _{70.5} Cu _{12.5} Ru ₁₇ [2004Mi]

* Face-centered icosahedral quasicrystal [1989Gur]. For detailed structural model see [2002Hir], [2004Yam]

** A “quasi-lattice” constant (see *Solid Phases* section for details).

Fig. 1: Al-Cu-Ru.
Partial isothermal
section at 1100°C

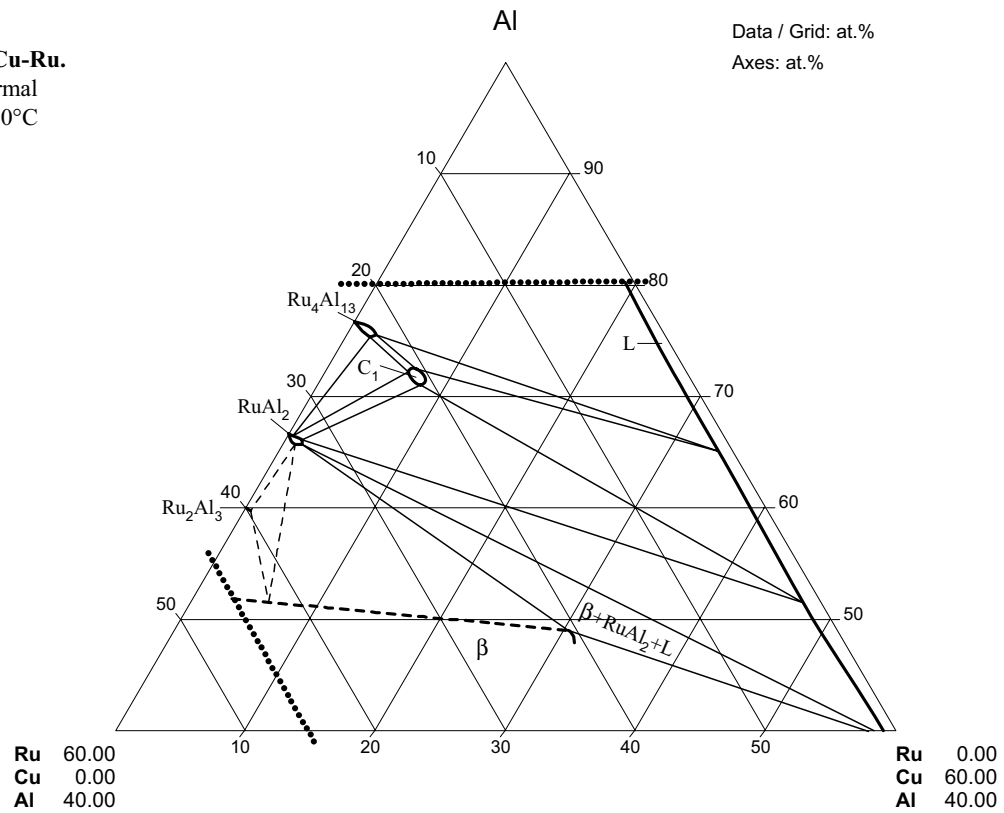


Fig. 2: Al-Cu-Ru.
Partial isothermal
section at 1000°C

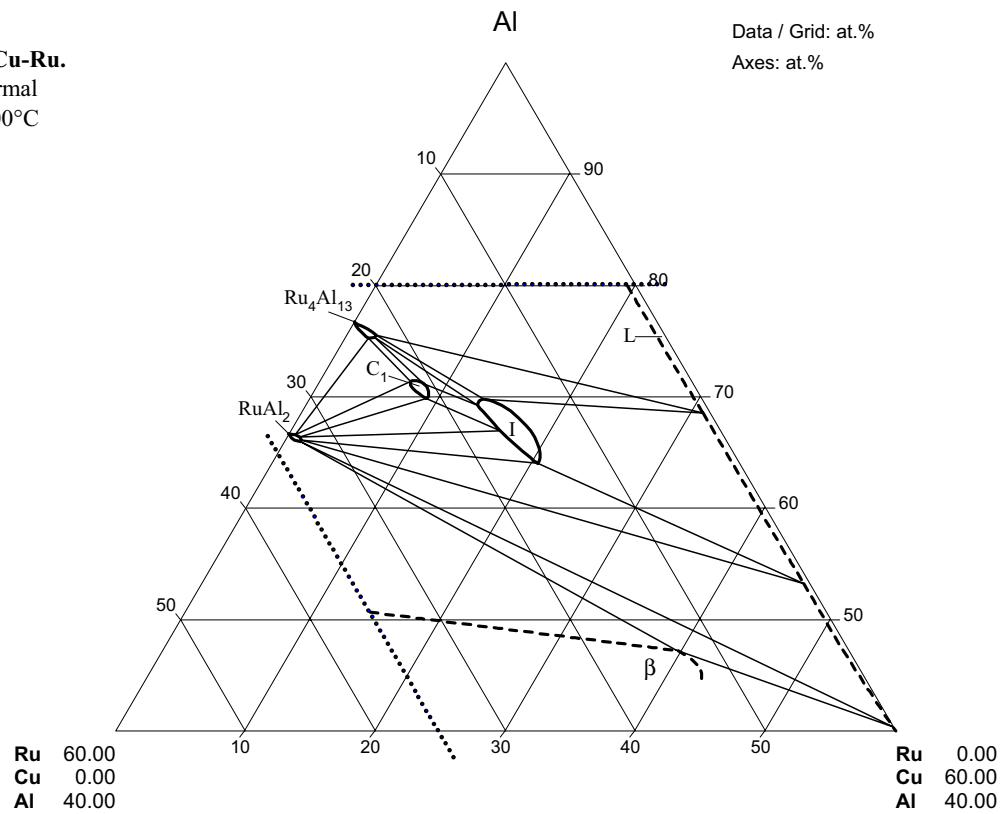


Fig. 3: Al-Cu-Ru.
Partial isothermal
section at 890°C

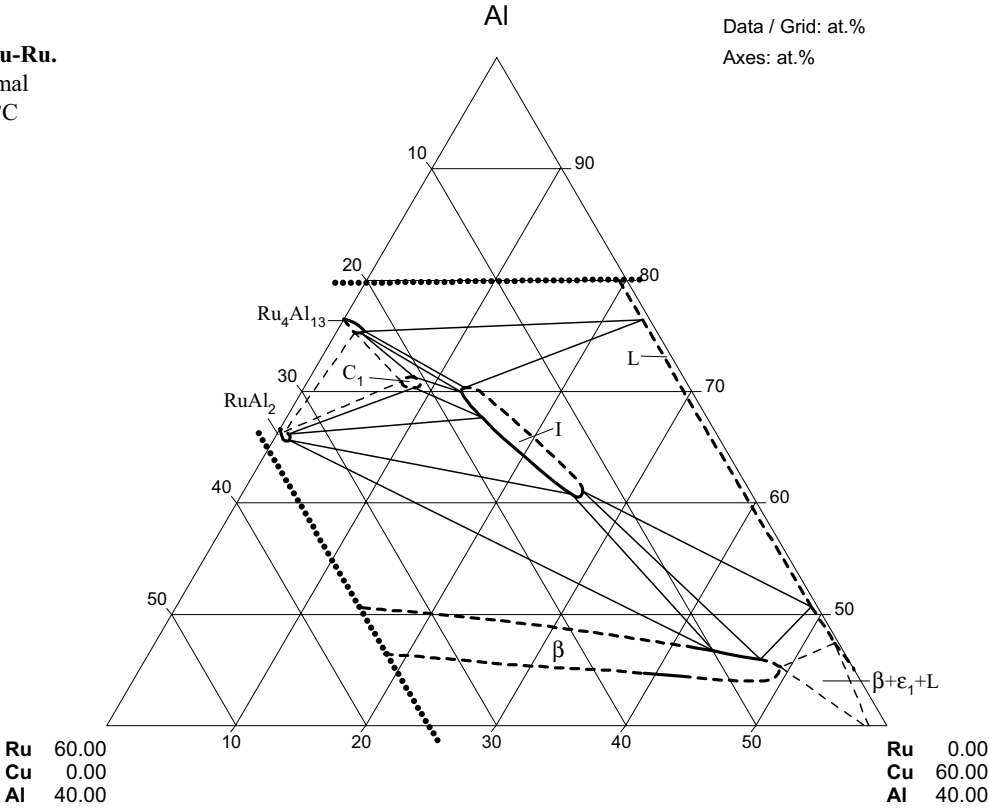


Fig. 4: Al-Cu-Ru.
Partial isothermal
section at 800°C

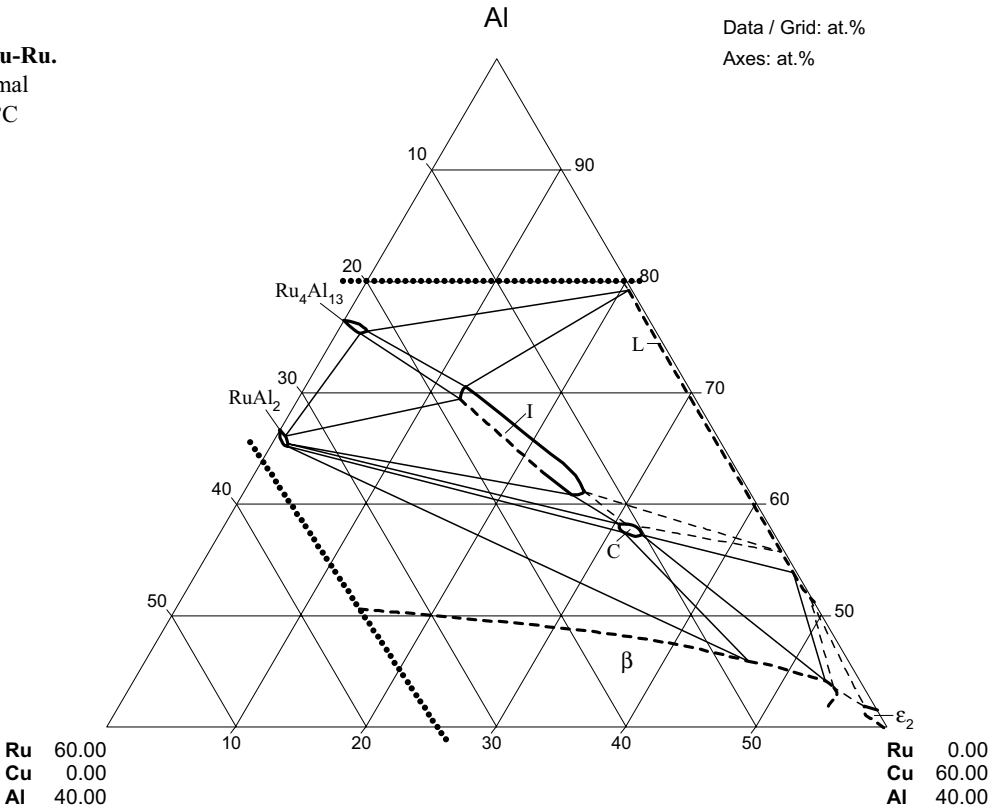


Fig. 5: Al-Cu-Ru.
Partial isothermal
section at 680°C

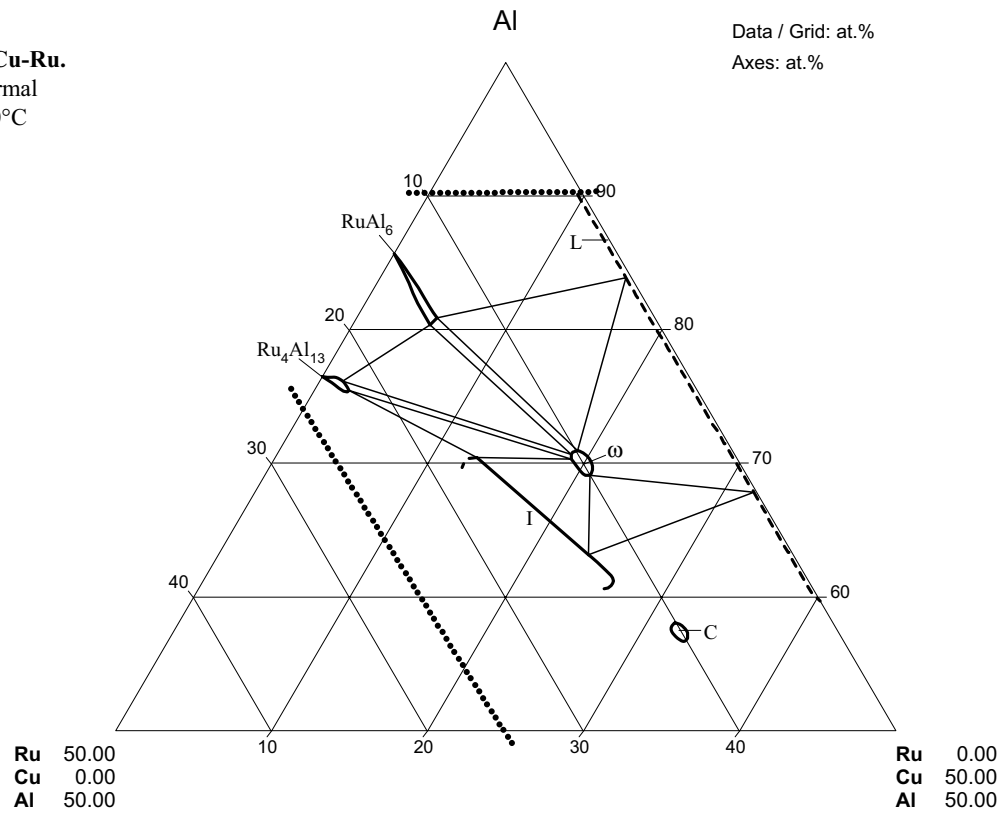


Fig. 6: Al-Cu-Ru.
Partial isothermal
section at 600°C

