How to Evaluate and Publish Ternary Phase Diagram Data

Best Practice Guidelines for Evaluation
&
Notes for Authors

6th Edition, 2012

Authoring team: MSIT®

Editors: G. Effenberg and R. Schmid-Fetzer

These guidelines give detailed instruction to those which want to contribute to the *MSIT® Ternary Evaluation Program* and/or want to publish own research data.

Under the auspices of APDIC, the Alloy Phase Diagram Commission, the MSIT® programs have set internationally agreed standards. The guide lines to meet these standards are made public here.

The instructions, conventions and the terminology matured over 28 years of joined evaluation work within MSIT®, the Materials Science International Team.
Starting in the year 1984 the members of MSIT® have undertaken the effort to cast their insight in materials constitution in guidelines. In particular colleagues like Leo Lukas, Allan Prince, Michael Hoch, Ibrahim Ansara, Riccardo Ferro, Peter Rogl and many others have been engaged over years to standardize evaluation and interpretation of constitutional data.

MSIT® has applied and refined the standards during evaluation of some 50 000 publications – resulting in almost 4000 system reports and 16 000 consistent and non-redundant phase diagrams, until now.

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Within the *MSIT® Ternary Evaluation Program* these Notes for Authors are binding.

Dr. G. Effenberg
Materials Science International Services, GmbH
Data and Knowledge Base for Materials Development
Postfach 800749
D-70507 Stuttgart
Federal Republic of Germany

Prof. R. Schmid-Fetzer
TU Clausthal
Institut für Metallurgie
Robert-Koch-Str. 42
D-38678 Clausthal-Zellerfeld
Federal Republic of Germany

9 783932 120497

Interested scientists are welcome to download and printout "Critical Evaluation of Ternary Phase Diagram Data. Best Practice Guidelines for Evaluation & Notes for Authors" for own academic use. For current information go to:
http://www.msiport.com/msi-research/ternary-evaluations/

In publications please refer to:

G. Effenberg and R. Schmid-Fetzer (Eds.), *Critical Evaluation of Ternary Phase Diagram Data. Best Practice Guidelines for Evaluation & Notes for Authors. Edition 6*, MSI, Stuttgart (2012)

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CONTENTS

Introduction

The knowledge base *MSI Eureka* and the print series *Ternary Alloys* provide concise and consistent descriptions of entire ternary material systems, as far as published data allow.

The approach used is to discuss the phase relationships and to consider changes in state and phase reactions with decreasing temperature. This has influenced the terminology employed and is reflected in the tables and the reaction schemes presented.

The world literature is thoroughly and systematically searched back to the year 1900. Then, the published data are critically evaluated by experts in materials science and reviewed under the authority of the MSIT[®] Program Board.

Conflicting information is commented upon and errors and inconsistencies removed wherever possible.

The system reports present concise descriptions and hence do not repeat in the text facts which can clearly be read from the diagrams. For most purposes the use of the compendium is expected to be self-sufficient. However, a bibliography with MSIT Keywords, is given to enable users to study the individual papers, if required.

Chapter 1.
The Authors' Job and the Workflow

The author prepares critical evaluation of the world literature, writes it down in a System Report and communicates with MSI and the board of reviewers to back the decisions made during the evaluation.

Different from manuscript supply to traditional journals the work within MSIT® is team work.

Each report will be thoroughly reviewed by the MSI panel of reviewers.

Critical evaluation of the published data means, for example:

- conflicts within the published data will be pointed out, settled wherever possible and the arguments for rejecting or accepting data will be given by the author.

- the author draws conclusions from the information gained from the many different articles. The Author does not speculate, *but sticks to the facts*. Reliably known data + the rules of heterogeneous equilibria + the competence of the author lead to new valuable information.

- to verify validity of experimental approach, the author checks purity of starting material, methods of sample preparation (materials specific), conditions of heat treatment (equilibrium reached), experimental methods used (with respect to materials, *etc*.), compatibility with thermodynamic data & estimates.

- conflicting diagrams are to be discussed in the evaluation report and one diagram has to be selected, even if the other may be equally good or bad. Decisions to be justified in the text. If necessary the author re-interprets published measured data *vs* published conclusions.

- the author draws new diagrams from that data that appear to be reliable. Figure captions do not contain citations; reference to other diagrams can be made in the text.

- finally the author double-checks his/her work carefully for internal consistency throughout text, tables and figures; checks consistency of intersecting cuts, compatibility of binary and ternary diagrams.

An Evaluation report is an authentic publication by the MSIT author(s)

- Diagrams are the diagrams of the MSIT author(s).
- Evaluation Reports take decisions to the benefit of less experienced users.
- The author takes the reader with him, so he can follow and understand why particular decisions, choices or preference have been taken by the author(s).
- If no decision is taken, the author in detail justifies to the reader why he is left alone with the problem.
- Specific proposals for further experiments are very helpful to direct future research; in particular if the expected scientific progress can be outlined!

An Evaluation Report is not a compilation/ collection of summaries

> -- and it should not look like this --

An Evaluation Report has

- Figure captions do not cite other publications; all explanations are given in the text. Diagrams are the diagrams of the MSIT author(s). If and how these diagrams are based on other peoples results has to be explained in the text

- Conflicting diagrams from other publications can be shown in the *MSI Eureka* "Diagrams as Published". Reference can be made to this in the Evaluation Report. These diagrams have no place in the Evaluation Report.

WORKFLOW in the MSIT Evaluation Programs

1)   MSI sends the copy-write transfer form to the author, by email.

2)   Author returns the signed copy-write transfer form to MSI as soon as possible, by fax or post.

3)   MSI makes on-line access to the literature collection of MSI. References are available in .html format and can be easily imported into *the report template* by the author.

4)   Report templates can be requested from mailto:evaluation@msiport.com

5)   For updating existing system reports MSI sends to the author the existing manuscripts in electronic form.

6)   MSI sends to the author the respective boundary binary systems, if available as evaluated by the MSIT Binary Evaluation Program.

7)   The author checks if literature provided by MSI is complete.

8)   The author adds missing references and searches the articles at home library.

9)   The author sends to MSI copies (electronic or carbon) of the articles found outside of the MSI collection.

10)   The author carefully reads the literature and separates non-relevant papers, if there are any and marks them in the reference list.

11)   The author writes critical evaluation of the published data according to the Notes for Authors.

12)   The author sends the manuscript with drawings included to MSI as soon as possible, before the deadline.
Diagrams will be redrawn by the MSI editorial office and may be delivered to MSI in any clearly readable, undistorted form; that might be electronic, hard-copies, scanned or hand-drawn.

REVIEW

13)   MSI forwards the manuscript to the reviewer. The reviewer has at hand the same literature which is available at the MSI data base and cited by the author.

14)   The author makes revision of the manuscript according to the guiding remarks of the reviewer. MSI may suggest including the reviewer in the list of co-authors if his/her contribution substantially improved the manuscript. Final decision is with the author.

15)   MSI editorial office makes layout of the system report, when manuscript is accepted by the reviewer.

16)   MSI sends the final version to the author for approval.

17)   The author sends approval back as soon as possible.

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Chapter 2.
Structure of a Ternary System Report

Structure of a Ternary System Report

Heading

Introduction	***concise summary of other people's work***

Binary Systems
Solid Phases
Quasibinary Systems
Invariant Equilibria
Liquidus Surface
Isothermal Sections
Temperature-Composition Sections
Thermodynamics
Notes on Materials Properties and

                Applications

This is the authors intellectual work, evaluating critically the existing data, amending and completing diagrams and tables; justifying the conclusions made, etc.

Miscellaneous
References
Tables
Figures

Topics without sufficient data are skipped.

2.0. Heading

25.02.01 Ag-Cu-Ti 1

Aluminium – Copper – Titanium

Rainer Schmid-Fetzer

Introduction

……………………

Please include page numbering for all pages in a headline!

Please denote your full name here!

Insert the date as follows: day.month.year, 25.02.12. Do NOT use options that amend the date when the document is opened.

2.1. Introduction

This chapter consists of two parts:

TEXT PART: This part should be easily digestible and generate general interest in the system, *e.g.* giving a brief historical review on how the knowledge developed over time, outline what triggered the interest in the investigations and may give the names of those scientists or groups to whom we owe the major scientific insight. Finally this text part may project into the future and make the reader aware what of the present interest in this system, if any.

TABLE PART: This table lists **all original investigations** on phase relations, structures & thermodynamics, NOT on properties.
(All experimental work, calculations such as Calphad or Ab-initio, NOT review)

Who made what investigations by which methods!

Experimental methods used in investigation should not be described in the <u>text</u>, but should be compiled <u>in this table</u>:

Table 1: Investigations of the X-Y-Z Phase Relations, Structures and Thermodynamics

Reference	Method/Experimental Technique	Temperature/Composition/Phase Range Studied

Such a table is **mandatory** if experimental information is published. See, for example, the system report on the Al-Fe-Ni on page 66".

Thermodynamic studies also should be listed in Table 1 of the "Introduction" section, however the details, data and functions should be **not** given in Table 1, but in the corresponding tables of section "Thermodynamics".

Work on Materials Properties and Applications is discussed in the chapter "Notes on Materials Properties and Applications" where a similar table is given, see page 16.

2.2. Binary Systems

For binary phase diagrams refer to standard compilations if the binary diagram which you accept is from one of the following compilations: [Mas2, Mas, S, E, H] (see "General References").

If the accepted diagram is from the MSIT[®] Binary Evaluation Program do not reproduce it but make a regular (not general) reference, *e.g.*

[2002Leb] Lebrun, N., "Cu-Ni (Copper - Nickel)", MSIT[®] Binary Evaluation Program, in *MSI Eureka*, Effenberg, G. (Ed.), MSI, Materials Science International Services GmbH, Stuttgart; Document ID: 20.14832.1.20, (2002) (Crys. Structure, Phase Diagram, Assessment, 28)

In all other cases reproduce and include the accepted binary diagram in the ternary evaluation report.

If ternary findings conflict with a binary subsystem, the author should mention this explicitly in the later sections.

2.3. Solid Phases

The assessed information is mainly presented in the Table "Solid Phases".

The Table "Solid Phases" should incorporate all phases of the ternary system; or a specified selection (see examples in Chapter 3.4), *starting* with unary, proceeding to binary and closing with the ternary phases. Two binary phases originating from different boundary systems and forming a continuous solid solution in the ternary are considered as *one* phase only and should be put behind the binary phases and before the ternary phases.

Each phase appears only once. Different phases are separated by horizontal lines.

Binary phases of no relevance to ternary information should be omitted (see example Al-Ge-Yb, Chapter 4).

Authors should indicate whether the original work has truly proved the existence of a ternary phase or merely the presence of a metastable phase, or a solid solution based on one of the binary phases.

For solid solutions between two binary phases the formulae of the terminal binary phases should be given together with their lattice parameters.

Examples for the Table "Solid Phases" are given in Chapter 3.4.

Column 1:

Phase/ Temperature Range (°C)	Person Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments
The *first column* of the table contains the formulae (at least an approximate one) of the phases. Whenever Greek letters are used to denote phases, these symbols must also appear in the first column. <u>Two phases must not have the same name and one phase can not have two different names</u>. A one to one relation between symbol and phase is necessary. If the same Greek symbol is used for different phases, they must be distinguished by suffixes. The sequence of the elements in the formula of a phase has to be according to the *chemical order* specified by Pettifor, see Chapter 3.5. We use SiC (instead of CSi) in the C-Si system. Different phases with the same formulae are distinguished by: – different symbols ε, ε', for allotropic transformations – Roman letters (I), (II), for pressure modifications – the temperature range of phase stability. Different temperature modifications can further be indicated by lower case letters in parenthesis behind the phase designation, with – (h) = high temperature modification – (r) = room temperature modification – (l) = low temperature modification ($l_1 > l_2$). These letters are used in the sequence h_2, h_1, r, l_1, l_2. Also, αMn, βMn or αPr, βPr, $αPr_3Al_{11}$ and $βPr_3Al_{11}$ are possible within one system report. All ternary phases are indicated with asterisks (*) in front of the formula. Generally, $τ_1$, $τ_2$ should be used as Greek letters for ternary phases.			

Column 2:

Phase/ Temperature Range (°C)	**Pearson Symbol/ Space Group/ Prototype**		Lattice Parameters (pm)	Comments
	The *second column* characterizes the crystal structure by the Pearson symbol, space group and its prototype, which also has to be given in *chemical order*. The prototype is the first phase where this structure was reported. If a sentence "is isotype to A_2XY [refs.]" is given in the literature, please check for prototype of A_2XY. If the structure is not known exactly (for example Bravais lattice and/or number of atoms per unit cell are unknown), the crystal system is sufficient (such as c^{**}, t^{**}, h^{**}, o^{**}, ...). No prototype may appear.			
	In some cases it may be helpful to give an incomplete Pearson symbol such as (o^*60).			
	Example for construction of Pearson symbol:			
	$aP7$; a – anorthic (triclinic) crystal system, P – primitive Bravais lattice type, 7 – number of atoms in unit cell.			
	Bravais lattice types : P, C, I, F, R			
	If the structure is known completely the prototype must be reported.			
	Technical requirement:			
	To denote inversion axis in the Space Group, use minus in front of the value, *e.g.* -3 for $\bar{3}$. It will be converted to a bar with final editing. Do not use Equation Editor in MS Word for that.			

Column 3:

Phase/ Temperature Range (°C)	Person Symbol/ Space Group/ Prototype	**Lattice Parameters (pm)**	Comments
		The *third column* gives the lattice parameters in pm and if necessary the angle of inclination of the crystal lattice.	
		Conversion must be made to pm :	
		$1Å = 0.1$ nm $= 100$ pm ; 1 kX $= 1.00202$ Å	
		For rhombohedral lattices the hexagonal setting is mandatory. For convenience, the relationships between the cell parameters a, c of the triple hexagonal cell and the cell parameters a', α' of the primitive rhombohedral cell are listed:	
		$a = 2a' \sin(\alpha'/2)$	
		$c = a' \sqrt{3}\sqrt{1+2\cos\alpha'}$	
		The Pearson symbol hR... should show the number of atoms in the hexagonal unit cell, *e.g.* αSm : $hR9$, but not $hR3$ with reference to the number, 3, of atoms contained in the primitive rhombohedral unit cell.	
		Best practice:	
		If in the literature (*e.g.* [V-C2]) many values are reported with a large scatter, present two values in Table "Solid Phases": one – close to the minimum value; second – close to the maximum value	
		If scatter of values is not too big, select one and include it in the Table.	
		For the phases with a range of homogeneity present 2 or 3 different values, specify composition.	
		Do not include in Table "Solid Phases" an average value from different values reported in literature!	

Phase/ Temperature Range (°C)	Person Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	**Comments**
			Column four allows the inclusion of additional information, such as: references, solubility ranges, concentrations, comments on accuracy, *etc*. The source of data has to be referenced. In the case of ternary phases, [V-C] as the reference is not enough, the original reference must be given.

2.4. Quasibinary Systems

Note: Terms „Pseudobinary" and „Quasibinary" have the same meaning. They describe equilibria in a ternary *T-x* section with all tie-lines in-plane. Compositions of the co-existing equilibrium phases can be read in the same way as in a binary phase diagram. Any other section is to be treated as a vertical section (isopleth or polythermal section).

The notation used in quasibinary systems is the same as that of vertical sections, which are reported under "Temperature-Composition Sections".

2.5. Invariant Equilibria

The invariant equilibria of a system are listed in the table "Invariant Equilibria" and, where possible, are described by a constitutional "Reaction Scheme". While the table "Invariant Equilibria" is self-explanatory, the conventions have been adopted for standard presentation of the "Reaction Scheme". The authors must design a layout of the reaction scheme according to

[1986Luk] Lukas, H.L., Henig, E.T., Petzow, G., "50 Years Reaction Scheme after Erich Scheil", *Z. Metallkunde*, **77**, 360-367 (1986)

The basic principles are briefly outlined below (see Fig. 4 in Chapter 3.3).

Glossary:

L = ternary liquid, l = binary liquid

Temperature in reaction schemes is always given in °C

Binary three-phase equilibria and ternary maxima and minima.

$l' \rightleftharpoons l'' + \alpha$ $l \rightleftharpoons \alpha + \beta$ $\alpha \rightleftharpoons l + \beta$ $\alpha \rightleftharpoons \beta + \gamma$ $\beta_1 \rightleftharpoons \alpha + \beta_2$	monotectic reaction eutectic reaction metatectic reaction eutectoid reaction monotectoid reaction	e-type reactions "decomposition"
$l' + l'' \rightleftharpoons \alpha$ $l + \alpha \rightleftharpoons \beta$ $\alpha + \beta \rightleftharpoons \gamma$	syntectic reaction peritectic reaction peritectoid reaction	p-type reactions "formation"

Ternary four-phase equilibria.

$L' \rightleftharpoons L'' + L''' + \alpha$ $L' \rightleftharpoons L'' + \alpha + \beta$ $L \rightleftharpoons \alpha + \beta + \gamma$ $\alpha \rightleftharpoons \beta + \gamma + \delta$	bitectic reaction monotectic reaction eutectic reaction eutectoid reaction	E-type reactions "decomposition"
$L' + \alpha \rightleftharpoons L'' + L'''$ $L' + \alpha \rightleftharpoons L'' + \beta$ $L' + L'' \rightleftharpoons \alpha + \beta$ $L + \alpha \rightleftharpoons \beta + \gamma$ $\alpha + \beta \rightleftharpoons \gamma + \delta$	liquid transition reactions solid transition reaction	U-type reactions "transition" or "transformation"
$L' + L'' + L''' \rightleftharpoons \alpha$ $L' + \alpha + \beta \rightleftharpoons L''$ $L + \alpha + \beta \rightleftharpoons \gamma$ $\alpha + \beta + \gamma \rightleftharpoons \delta$	syntectic reaction – peritectic reaction peritectoid reaction	P-type reactions "formation"

Binary reactions are represented in the following way:

779	e_1
$l = (Ag) + (Cu)$	

Ternary reactions are represented as follows:

665	L =(Ag) + (Cu) + β	E

630	L + γ = ε + β	U_1

665	L + γ + β = δ	P

Quasibinary three-phase equilibria (ternary maxima or minima) are indicated by a convention similar to that adopted for binary invariant reactions. They are numbered together with the binaries, see Fig. 4 in Chapter 3.3.

Univariant three-phase equilibria are <u>not</u> written in boxes. Those existing down to "room temperature" are underlined, those starting in one ternary and ending in another ternary reaction are indicated without underlining. Univariant three-phase equilibria starting or ending at a binary reaction are indicated by a line to this binary reaction.

Univariant three-phase equilibria starting or ending at a critical point (c) are represented as:

● 1500(c_1)

$L_1 + L_2 + \beta$ $L_1 + L_2 + \beta$

● 800(c_2)

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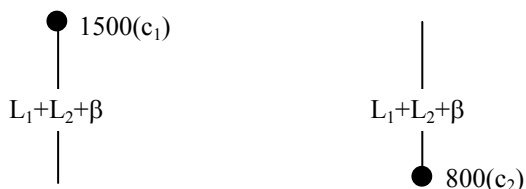
The sequential numbering of invariant equilibria increases with decreasing temperature, one numbering for all binary and ternary systems.

Equilibria notations are used to indicate the reactions by which phases will be

- decomposed (e- and E-type reactions)

- formed (p- and P-type reactions)

- transformed (U-type reactions)

For transformed or transition reactions the letter U (Übergangsreaktion) is used in order to reserve the letter T to denote temperature. The letters d and D indicate degenerate equilibria which do not allow a distinction according to the above classes. Lower case letters denote three-phase equilibria and upper case letters four-phase equilibria.

Degenerate reactions:

In systems with stoichiometric phases some of the invariant equilibria may be degenerate. This means, no decision can be made between e- and p-type in a binary system respectively, between E- and U-type or between U- and P-type or even between all the 3 types in a ternary system.

For a more detailed discussion of the treatment of degenerated reactions (d-type or D-type) authors may refer to a paper

[1986Luk] Lukas, H.L., Henig, E.T., Petzow, G., "50 Years Reaction Scheme after Erich Scheil", *Z. Metallkunde*, **77**, 360-367 (1986)

See example in System Report Al–Cu–Mg, page 34.

Table "Invariant Equilibria".

In addition to the reaction scheme, this section should include a table showing the details of the invariant equilibria present in the ternary system. Invariant equilibria should be listed in Table "Invariant Equilibria" in sequential order by decreasing temperature. Four columns are necessary: reaction, temperature (°C), type, phase and composition. For example, the ternary peritectic reaction in a system should be tabulated as follows:

Reaction	T (°C)	Type	Phase	Composition (at.%)		
				Ag	Cu	Mg
L + β' + γ ⇌ ε	505	P	L	9.8	15.5	74.7
			β'	36.5	6.8	56.7
			γ	2.5	30.0	67.5
			ε	14.0	15.2	70.8

2.6. Liquidus, Solidus and Solvus Surfaces

The projection of the *liquidus surface* should be included. All monovariant curves separating the regions of primary crystallization of individual phases are to be drawn with two closelyspaced arrows pointing to descending temperatures. Ternary invariant points are to be labeled with the appropriate letters E, U and P or the designations e and p in the case Max. and Min., defined in corresponding tables.

If more than one liquid phase is involved in an invariant reaction, the phase designations e'$_1$, e"$_1$,

E'_1, E''_1 should be attached to the appropriate invariant points, where e_1, E_1 designate the *reaction* and the ' and " designate the different *liquid phases/compositions* (see Chapter 3.3).

The regions of primary crystallization are to be labeled with the appropriate phase designation, e.g. (Ag), MgO, etc.

Isotherms should be inserted on the liquidus surface.

Comment should be made on specific features of the liquidus surface in the text.

2.7. Isothermal Sections

Isothermal sections should be presented as needed.

All single-phase regions and all three-phase regions should be designated, *e.g.* L, (Ag), AgAl, *etc.* Inside the three-phase fields put an asterisk (*).

If Greek symbols are used, they must be identical with those used for the phase names in the table of solid phases, and in the text.

If only vertical sections (temperature-composition) through a ternary diagram are available, the author is asked to determine the corresponding isothermal sections, but not to speculate.

2.8. Temperature – Composition Sections

All non-quasibinary *T-x sections* (vertical sections, isopleths) can be presented here.

2.9. Thermodynamics

Depending on data available for a system, generally there are two ways to report on thermodynamic data:

Case A: An accepted Calphad assessment exists.

- Report **diagrams** of those calculated thermodynamic data that are supported by **direct measurements** (enthalpy of mixing, activities,…). In that case, do not report individual experimental data in tables.

- If a thermodynamic quantity is not given in a diagram, tabulated values may be reported (generally best choice only) (data for stoichiometric phases,…)

- The author may **modify** a calculated phase diagram and/or a calculated thermodynamic quantity if that results in a better overall description of the system. Make a note in the text in that case.

- If experimental data are published after that assessment:

    (i)   if the data agree, then just state that in the text.

    (ii)   if the data disagree, then also report the actual values in the form of case B (see below). A new assessment may be proposed in that case. Show the phase diagram of the previous assessment (or your best choice) **and** show the new experimental thermodynamic data, comment in the text.

Case B: No accepted Calphad assessment exists.

- Report **only the directly measured** thermodynamic data. Use table form specified below.

- In principle, this is asking for a Calphad type assessment, but this is out of the scope of a system report

2 ways of graph presentations are acceptable:

"$RT\ln p_{O_2}$ *vs T*"   or   "$\log p_{O_2}$ *vs* $10^4/T$"

However, if within one system report data from different original sources are reported, a uniform presentation of data should be used, and "$RT\ln p_{O_2}$ vs T" is preferred.

Table N: Thermodynamic Data of Reaction or Transformation

Reaction or Transformation	Temperature (°C)	Quantity, per mol of atoms (kJ, mol, K)	Comments
¼ {A(α) + 3 B(β) $\Rightarrow$ AB$_3$(s)}	25	$\Delta H = -11.2 \pm 0.8$	[1995Abc] dir.cal.
1/3 {A(α) + 2 B(β) $\Rightarrow$ AB$_2$(s)}	25	$\Delta H = -17.8$	[1996Mno] Calphad
1/3 {A(α) + 2 B(β) $\Rightarrow$ AB$_2$}	25 - 800	$\Delta G = -14.0 + 0.003\ T$	[1996Abc] derived from emf measurements
1/(2.56) {Ce + 1.56 Si $\Rightarrow$ CeSi$_{1.56}$}	800	$\Delta H = xxx$	[1996Abx]
(1-x) A(L) + x B(L) $\Rightarrow$ A$_{(1-x)}$B$_x$(L)	1000	$\Delta H = -15.0 \pm 1$ -14.0 ± 1	$x = 0.3$ $x = 0.4$ [1996Def] solution cal.
A(L) $\Rightarrow$ L (n=∞, x_B=0.5)	1200	$a_A = 0.5$	[1994Ghi] emf
A(α, 25°C) + L(n=∞, 800°C) $\Rightarrow$ L (x_B = 0.2, 800°C)	25 - 800	$\Delta H'_A = 1.5 \pm 0.3$	[1997Jkl] drop cal.
A(L) + L(n=∞) $\Rightarrow$ L (x_B=0.2)	800	$\Delta H'_A = -0.5 \pm 0.3$	[1997Jkl] drop cal. H_A ($\alpha \rightarrow$L) from [Din]
A(α, 25°C) + L(n=∞, 800°C) $\Rightarrow$ L (x_B = 1, 800°C)	25 - 800	$\Delta H'_A = 1.2 \pm 0.3$	[1997Jkl] drop cal. Infinite dilution
½(H$_2$)(g) + L(n=∞) $\Rightarrow$ L (x_H = 0.01)		$\Delta H'_H = xxx$	

Note: derived/calculated quantities only if the actual measurements are not available.

$\Delta H'_A$: users of MS Word should use prime to denote partial quantities. It will be denoted by a bar with final editing. Do not use Equation Editor in MS Word for that.

Table N+1: Thermodynamic Properties of Single Phases

Phase	Temperature Range (°C)	Property, per mole of atoms (J, mol, K)	Comments
1/3 AB$_2$	200 - 800 400 - 500 25	$C_p = 23.68 + 5.44\ 10^{-3}\ T$ $C_p = 27 \pm 0.5$ $S° = 38.9 \pm 2.1$	[1992Abc] DSC [1993Def] drop cal. (calculated from ΔH) [1998Ghi]
¼ AB$_3$	25 - 500	$H(773)–H(298) = 12400 \pm 500$	[1995Jkl] drop cal.
α	25 - 500	$H(773)–H(298) = 12800 \pm 500$	[1997Jkl] drop cal.

Table N+2: Vapor Pressure Measurements

Phase(s)	Temperature (°C)	Pressure (bar)	Comments
A(α)	700	$p_A = 0.2$	[1999Acb] Knudsen effusion
AB(s) + AB$_2$(s)	650	$\log 10(p_{B2}) = -4.5$	

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2.10. Notes on Materials Properties and Applications

This chapter is important as it can relate applications and properties with the temperature / concentration regime; i.e. showing the significance of phase diagrams.

No specific literature search is performed for this section. However all relevant and noteworthy materials properties (mechanical, magnetic, electrical, optical, etc.) and applications / possible applications (functional or structural application areas, processing, etc.) found in the constitutional literature should be reported briefly here.

In this chapter *type* of properties studied, kind of measurements and phases / alloy compositions for which they are measured should be described. It is not required to present original values reported in the articles, unless these are outstanding properties.

In this chapter the following table is helpful if a larger number of original work is to be referenced:

Table #: Investigations of the X-Y-Z Materials Properties

Reference	Method/Experimental Technique	Type of Property

2.11. Miscellaneous

This paragraph should include noteworthy features not covered by the preceding form of presentation. For example, for systems containing gas other kinds of presentation may be chosen for the description of the system, e.g. (log $p(O_2)$ *vs T*). In this case no instruction for the size and the form of diagrams is given for the authors.

Note: It is recommended to suggest further experiments which are crucial for a more complete understanding of the system, if applicable. Specify what kind of information is wanted from these experiments.

2.12. References

All references should be included. General references used in the text need not to be included in the reference list of each individual system. These are:

General References

[E]   Elliott, R.P., Constitution of Binary Alloys, First Supplement, McGraw-Hill, New York (1965)
[Eff1]   Effenberg, G., Petrova, L.A., Red Book. Phase Diagrams of Metallic Systems (published in 1990), MSI, Stuttgart, Vol. 35 (1993)
[Eff2]   Effenberg, G., Petrova, L.A., Red Book. Phase Diagrams of Metallic Systems (published in 1991), MSI, Stuttgart, Vol. 36 (1994)
[Eff3]   Effenberg, G., Petrova, L.A., Red Book. Phase Diagrams of Metallic Systems (Summaries of the publication year 1992), MSI, Stuttgart, Vol. 37 (1997)
[Eff4]   Effenberg, G., Bodak, O.I., Petrova, L.A., Red Book. Constitutional Data and Phase Diagrams of Metallic Systems (Summaries of the publication year 1993), MSI, Stuttgart, Vol. 38 (1997)
[Eff5]   Effenberg, G., Bodak, O.I., Petrova, L.A., Red Book. Constitutional Data and Phase Diagrams of Metallic Systems (summaries of the publication year 1994), MSI, Stuttgart, Vol. 39 (1997)
[Eff6]   Effenberg, G., Bodak, O.I., Petrova, L.A., Red Book. Constitutional Data and Phase Diagrams of Metallic Systems (summaries of the publication year 1995), MSI, Stuttgart, Vol. 40 (1998)
[Eff7]   Effenberg, G., Bodak, O.I., Yanson, T.I., Red Book. Constitutional Data and Phase Diagrams

(summaries of the publication year 1996), MSI, Stuttgart, Vol. 41 (1999)

[G]   Gmelin Handbook of Inorganic Chemistry, 8th ed., Springer-Verlag, Berlin

[H]   Hansen, M. and Anderko, K., Constitution of Binary Alloys, McGraw-Hill, New York (1958)

[L-B]   Landolt-Boernstein, Numerical Data and Functional Relationships in Science and Technology (New Series). Group 3 (Crystal and Solid State Physics), Vol. 6, Eckerlin, P., Kandler, H. and Stegherr, A., Structure Data of Elements and Intermetallic Phases (1971); Vol. 7, Pies, W. and Weiss, A., Crystal Structure of Inorganic Compounds, Part C, Key Elements: N, P, As, Sb, Bi, C (1979); Group 4: Macroscopic and Technical Properties of Matter, Vol. 5, Predel, B., Phase Equilibria, Crystallographic and Thermodynamic Data of Binary Alloys, Subvol. a Ac-Au ... Au-Zr (1991); Springer-Verlag, Berlin.

[Mas]   Massalski, T.B. (Ed.), Binary Alloy Phase Diagrams, ASM, Metals Park, Ohio (1986)

[Mas2]   Massalski, T.B. (Ed.), Binary Alloy Phase Diagrams, 2nd edition, ASM International, Metals Park, Ohio (1990)

[P]   Pearson, W.B., A Handbook of Lattice Spacings and Structures of Metals and Alloys, Pergamon Press, New York, Vol. 1 (1958), Vol. 2 (1967)

[S]   Shunk, F.A., Constitution of Binary Alloys, Second Supplement, McGraw-Hill, New York (1969)

[V-C]   Villars, P. and Calvert, L.D., Pearson's Handbook of Crystallographic Data for Intermetallic Phases, ASM, Metals Park, Ohio (1985)

[V-C2]   Villars, P. and Calvert, L.D., Pearson's Handbook of Crystallographic Data for Intermetallic Phases, 2nd edition, ASM, Metals Park, Ohio (1991)

All other references are to be given by the 4 figures of the year and the first three letters of the name of the first author. If two different papers would have the same abbreviation a number index is added.

Examples are:

" ... it has been shown by [1968Joh1] that ... " or

" ... experiments with calcium [1968Joh2], potassium [1975Dal] ... "

Other abbreviations are:

Gürtler   [1943Gue]

El-Boragy   [1971ElB]

McKisson   [1979McK]

von Unterrichter   [1976Unt].

Use for ä = ae, ö = oe, ü = ue and Å = A.

The reference list should be written in the following style:

[2009Ria]   Riani, P., Cacciamani, G., Parodi, N., Borzone, G., Marazza, R., Nanni, F., Gusmano, G., "Phase Equilibria in the In-Sn-Rich Part of the Cu-In-Sn Ternary System", *J. Alloys Compd.*, **487**(1-2), 90-97 (2009), DOI: 10.1016/j.jallcom.2009.07.129 (Experimental, Phase Diagram, Phase Relations, 24)

For a journal article as mentioned in the example all authors are given, even when there are many, followed by the title of the paper in quotation marks. The title is always given in English. The original language, if not English, is indicated in brackets after the title. The abbreviation of the journal is given as listed in *"Chemical Abstracts, List of Periodicals"*. Names of journals or other periodical publications not listed there should be written in full. The volume number is bold and the first and last page numbers must be given.

For journals that start the pagination of each issue with 1, the issue number must be given in parentheses

following the volume number, if there is any:

[1986Pay1]   Paygai, I.N., Khairidinov, S.Kh., Vakhobov, A.V., "The Ba-La Phase Diagram", *Russ. Metall.*, **3**(1), 213-214 (1986), translated from *Izv. Akad. Nauk. SSSR, Metally*, **3**(1), 216-217 (1986) (Experimental, Phase Diagram, Phase Relations, Magn., Electr. Prop., #, *, 4)

Where an English translation exists, this should be first referenced and followed by the data on the original publication, as shown by the example above.

For pamphlets, bulletins or any publications other than "regular" books or journals give all the information available and do not use abbreviations.

Keywords at the end of references should indicate the nature of the data available in the article.

Keywords are as follows:

A)   Mandatory **subject-** keywords:

Crys. Structure for Crystal Structure	Morphology	Phase Diagram	Phase Relations	Thermodyn. for Thermodynamics

B)   Mandatory **type of work-** keywords:

Abstract	Assessment	Calculation	Experimental	Review	Theory

C)   Optional keywords (only in combination with one or more **A**-field(s))

Catalysis	Electronic Structure	Electr. Prop. for Electrical Properties	Electrochemistry	Interface Phenomena
Kinetics	Magn. Prop. for Magnetic Properties	Mechan. Prop. for Mechanical Properties	Optical Prop. for Optical Properties	Phys. Prop. for Physical Properties
Semicond. for Semiconductivity	Supercond. for Superconductivity	Transport Phenomena		

In addition the following symbols are used:

\#   – indicates accepted phase diagram in the paper

*   – indicates key papers, important reference for the proposed diagram

Number   – number of references in the paper

Do not use other keywords or abbreviations.

Examples.

Report:

[1961Eng]   English, J.J., "Binary and Ternary Phase Diagrams of Columbium, Molybdenum, Tantalum and Tungsten", *Defense Metals Information Center Report*, Battelle Memorial Institute, Columbus, OH, Report No. 152, 1-53 (1961) (Phase Diagram, Review, #, 7)

Book (without Editor)**:**

[1982Kub]   Kubaschewski, O., *Iron Binary Phase Diagrams*, Springer Verlag, Berlin, Verlag Stahleisen, Düsseldorf, 152-156 (1982) (Phase Diagram, Review, 26)

Book (with Editor)**:**

[1978Mis]   Mister, X.Y., "Title of the article" in "*Title of the book*", Name, A., Name, B. (Eds.), **Vol. 2**, Publisher, City, Country(not mandatory), 69-74 (1978) (Phase Diagram, Review, 79)

Chapter of Book:

[1961Sem]   Semchysen, M., Barr, R.Q., "Molybdenum and Molybdenum-Containing Refractory Alloys" in "*Refractory Metals and Alloys*", *AIME Metall. Soc. Conf.*, Vol. 11, Interscience Publishers, Inc., New York, 283-317 (1961) (Crys. Structure, Review, 34)

Proceedings:

[1978San]   Sankar, S.G., "Magnetic Properties of Er(Fe$_{1-x}$Mn$_x$)$_2$" in "*The Rare Earths in Modern Science and Technology*", Proc. Conf., Wheeling, W. Virginia, 1977, 69-74 (1978) (Experimental, 7)

If a reference is not available but quoted in a given literature or even in Chemical Abstracts, then it should be presented in the following form:

[1964Tiv]   Tivilivi, E.T., "The Al-Ar-He Phase Diagram", *Moldavian Chemical Congress*, **1**, 23-27 (1964) as quoted by N.V. Ageev, "Phase Diagrams of Metallic Systems" (in Russian), 1965 (Publ. 1968)

[1989Ham]   Hamalainen, M., Jaaskelainen, K., Luoma, R., Taskinen, P., Teppo, O. Vanninen, M. "Thermodynamic Analysis of the Binary Systems Cu-Cr, Cu-Nb and Cu-V", *Metall., 1989, Tkk-V-B47,* 24 pp., (1989) as quoted in C.A. 111-158477F

This form may only appear, if the primary source is definitely not available.

Chapter 3.

Best Practice of Authors & Editorial Office

The MSIT® Evaluation program is based on jointly developed rules and editorial instructions. Substantial support is provided by the editorial office and the reviewers, which only can become effective if the author obeys strictly the agreed layout rules given below.

3.1. Diagrams

At MSI the diagrams will be reproduced in a digital format, by editorial assistants, one-to-one as submitted by the author. Errors that enter the databases at this stage cause multiple correspondences, correction activities with the author and a substantial delay of publication. To minimize the avoidable errors the author sends diagrams that are clearly readable, free of obvious mistakes and without general instructions.

Several points require special attention.

1. The diagrams are to be labeled with the concentrations/temperatures of at least three points, normally the three corners of the diagram, in order to enable digitizing by computer means. *This labeling has to occur in the units of the diagram itself.*

Make labeling of diagrams as shown below (**obligatory**):
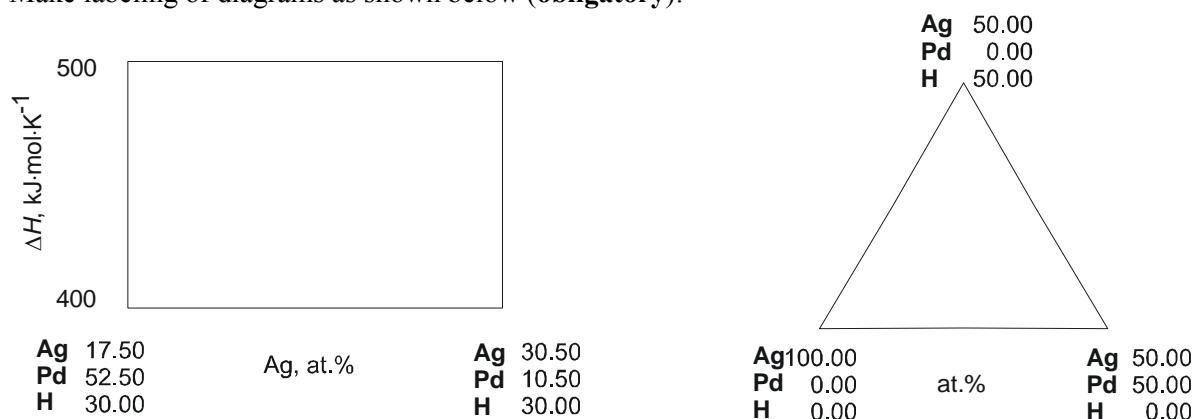
3. No general correction remarks should be included on the diagrams, e.g. "please change all liquidus curves to dashed".

4. If it is necessary to allocate to a specific point a numerically known concentration/temperature, these should be denoted on the diagram in an unambiguous way.

5. If *by exception* copies of diagrams from the literature are used as base for drawings, these copies have to comply fully with the Notes for Authors!
Make sure that:
 – continuous lines are not interrupted due to low copying quality;
 – separated lines do not intersect or overlay;
 – the phase labels on the original are removed and re-labeled by the author according to the table "Solid Phases". If the readability becomes questionable do not use copies but redraw the diagram!

6. If already digitized diagrams require corrections of line curvatures or angles between lines, use a *thin* colour pen for the correction, denoting clearly the correct location of the line.

7. Line styles and thickness:

Dashed lines are used to denote uncertainties.

Dotted lines are used to show metastable equilibria or magnetic and second order transformations.

Magnetic transformation should be marked by the "T_C", "T_N", or "T_m" labels.

Rectangular diagrams are drawn by thin solid lines.

Triangular diagrams:

Tie lines	by thin lines,
Single phase borders	by thick lines.
Isothermal lines on liquidus, solidus, solvus surfaces	by thin lines
Monovariant lines on liquidus, solidus, solvus surfaces	by thick lines
Monovariant lines on liquidus	– add double arrow
Monovariant lines on solidus and solvus	– add single arrow

8. Always place references in square brackets [ ], do not use anything else. And do not use square brackets [ ] for anything else except for references.

3.2. Text and Tables

General

- Each page should be labelled in the upper right corner with the chemical symbols of the alloy system in alphabetical order. The pages should be numbered.

- In text the binary systems are indicated as: "The Au-Pb system ..."

- Use American spelling, e.g. *crystallization*, *homogenization*, *behavior*, *sulfur* (but *aluminium*, since this spelling is recommended by IUPAC).

- Within a report, reference may be made to individual sections of the report (not to chapters).

- Make complete sentences (*e.g.* "The solid phases are given in Table 1." but not "The solid phases see Table 1.").

- Do not capitalize the names of mineral forms (*e.g.* sphalerite, wurtzite).

- Omit the hyphen in phrases such as "a compound of Ag_2Te type" or "tie line" or "Cu-corner" or "Al-rich"; do not write "Ag_2Te-type" or "tie-line" or "Cu-corner" or "Al-rich".

- Use only lower case letter p (italic) to denote pressure (not P).

- Follow IUPAC recommendation and write the following symbols ***in italic:***

  - T for temperature; p for pressure; lattice parameters a, b, c; thermodynamic   quantities H, S, G, C_p.

  - In the notation of composition: write x or y ***in italic.***

- Differentiate between allotropic phases by using Greek letters only; do not use commas or dashes (*e.g.* αAgI neither α-AgI nor α,AgI) in Table 1.

- Capitalize all main words in the section and table headings. In figure captions capitalize only the first word.

- A statement of accuracy of the data should be given wherever it can be concluded from the published work. Use format: $a = 779.2 \pm 0.1$, not $a = 779.2(1)$

- All citations should be given in "References" and all the references listed in "References" should appear in the text or tables.

- Use only $\rightleftharpoons$ (and not =) in equations describing equilibria (e.g. L $\rightleftharpoons$ (Te) + μ; **not** L = (Te) + μ).

- Use only the Greek letter ρ (rho) to denote density, given in the units $g \cdot cm^{-3}$.

- Write the equation of equilibrium in one line,

  e.g. L + (Ag, Au) $\rightleftharpoons$ $AuTe_2$ + γAg_2Te,

  and not L + (Ag, Au) $\rightleftharpoons$

  $AuTe_2$ + γAg_2Te.

- There is a blank space before and after *equal*, *less than* and *more than* signs; *e.g.* κ = 10 and

$0 \leq \kappa \leq 1$, 779.2 ± 0.1.

- Do not write "isn't", "doesn't", *etc*. Use the unabbreviated forms "is not", "does not", *etc*.

- If a paper is referred to as, [1971Gly], then it is singular, *e.g.* "[1971Gly] finds", even if several authors have contributed to the paper. The plural should be used, for example, in the following manner: "The authors of [1971Gly] find that ...".

- [1962Mai] is to be used as a noun in sentences.

- For several references listed together the format is, *e.g.*: "[1962Mai, 1963Mai, 1972Ran, 1973Luk] have ...", or, where two references are used as different nouns: "... both [1962Mai] and [1963Sch] found by different techniques ...".

- There should be no space inside phase symbols; e.g. $Co_2Ni(h)$ or $Co_2Ni(r)$.

- Use prime to denote partial quantities (use H' for $\overline{H}$) and use minus to denote inversion axis in Space Group (use -3 for $\overline{3}$). They will be converted to bars with the final editing.

Abbreviations
- An alloy may be abbreviated, for example, 50Al-Cu-10Zn (at.%) or Ca-50Mg-10Y (mass%).

- Do not use the abbreviations "Fig." or "Figs." at the beginning of a sentence, but write out "Figure" or "Figures".

- Use emf for electromotive force, not EMF.

- Use h for hours, s for seconds, min for minutes, d for days.

- Use mol for mole.

Numbers and Numbering
- Decimal points should be used for decimal figures, (*e.g.* 1.23 not 1,23).

- If a list of numbered points is presented, number them "1. 2. 3. ..." (Not 1) 2) 3) or 1.) 2.) 3.)).

- Use a, b, c as an additional label to identify figures (e.g. Fig. 11a, 11c; not Fig. 11.1, 11.2).

- Number figures according to the order in their logical sequence.

- In formulae, write e.g. $5 \cdot 10^{10}$, **not** 5×10^{10}.

Units

- In the text all temperatures should be given in °C (not °). At very low temperatures Kelvin (K) may be used.

- All other physical and chemical properties should be expressed in SI units (see International Organization for Standardization ISO, International Standard ISO 1000, First Edition, 1973).

- Use "mass%" not "wt.%".

- Leave a space between a number and its unit (*e.g.* 0.28 eV, 260 h, 6.5 at.%.)
  Exception: no blank space between number and °C. (e.g. 286°C not 286 °C).

Tables

- Footnotes are denoted in tables by superscripts in lower case letters without brackets and without full stop, e.g. xyz^a or xyz^b, (not xyz$^{a.}$ nor xyz$^{b)}$). Do not use subscripts for footnotes.

- In the Table "Solid Phases" use "to" when giving the ranges of lattice parameters, e.g. 543.3 to 550 (not 543.3-550).

- In the Table "Solid Phases" write lattice parameters, their ranges and accuracy in one line, e.g. $a = 1654 \pm 3$.

3.3. Liquid Miscibility Gaps

Example.

E'_1 denotes the composition of L' at the reaction E_1
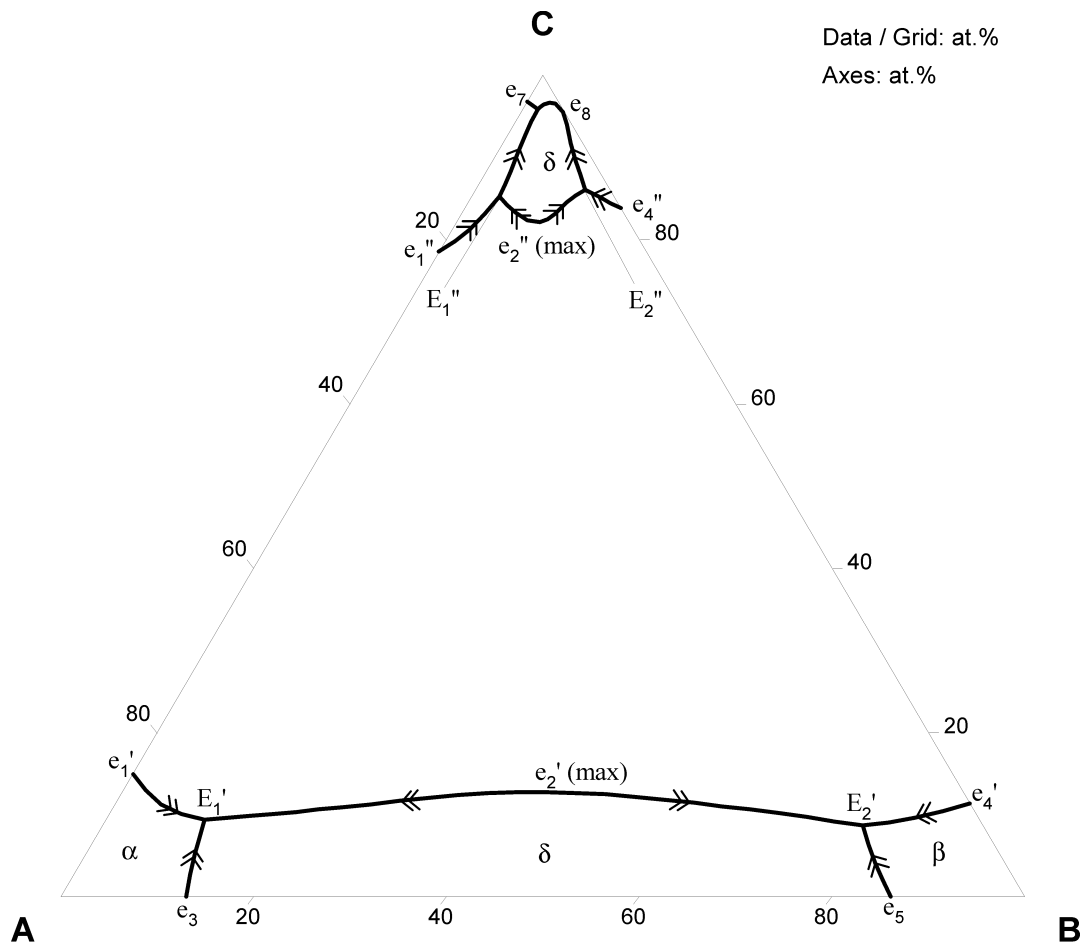
Fig. 1: Liquidus surface of A-B-C system with miscibility gap in the liquid

C

γ

e_6 (max)

e_7 e_8

20   E_3 E_4 80

40   60

δ

60   β

α

40

E_1'' E_2''

80   e_2'' (max)   20

e_4''

L'+L"

e_1''

A   20   40   60   80   B

Data / Grid: at.%

Axes: at.%

Fig. 2: Enlarged C-corner

l'

l"   l

e_1 l'   l"

e_3

e_5

e_7 e_8

γ   α   δ   β   γ

C   A   B   C

Fig. 3: Binary Systems

Reaction scheme — columns: **A-B**, **A-C**, **A-B-C**, **B-C**

A-B

- 923 | c_3 | $l \rightleftharpoons \alpha + \delta$
- 879 | c_5 | $l \rightleftharpoons \beta + \delta$

A-C

- 991 | e_1 | $l' \rightleftharpoons l'' - \alpha$
- 791 | e_7 | $l'' \rightleftharpoons \alpha + \gamma$

A-B-C

- 969 | e_3 (max) | $L' \rightleftharpoons L'' \cdot \alpha \cdot \delta$
- E_1
- 897 | $L' \rightleftharpoons L'' + \alpha + \delta$
- 860 | $L' \rightleftharpoons L'' + \alpha + \delta$
- E_2
- 793 | c_6 (max) | $L'' \rightleftharpoons \delta + \gamma$
- E_3
- 789 | $L'' \rightleftharpoons \alpha + \gamma + \delta$; $\alpha + \gamma + \delta$
- E_4
- 787 | $L'' \rightleftharpoons \beta + \gamma + \delta$; $\beta + \gamma + \delta$

B-C

- 917 | c_4 | $l' \rightleftharpoons l'' + \beta$
- 789 | e_8 | $l'' \rightleftharpoons \beta + \gamma$
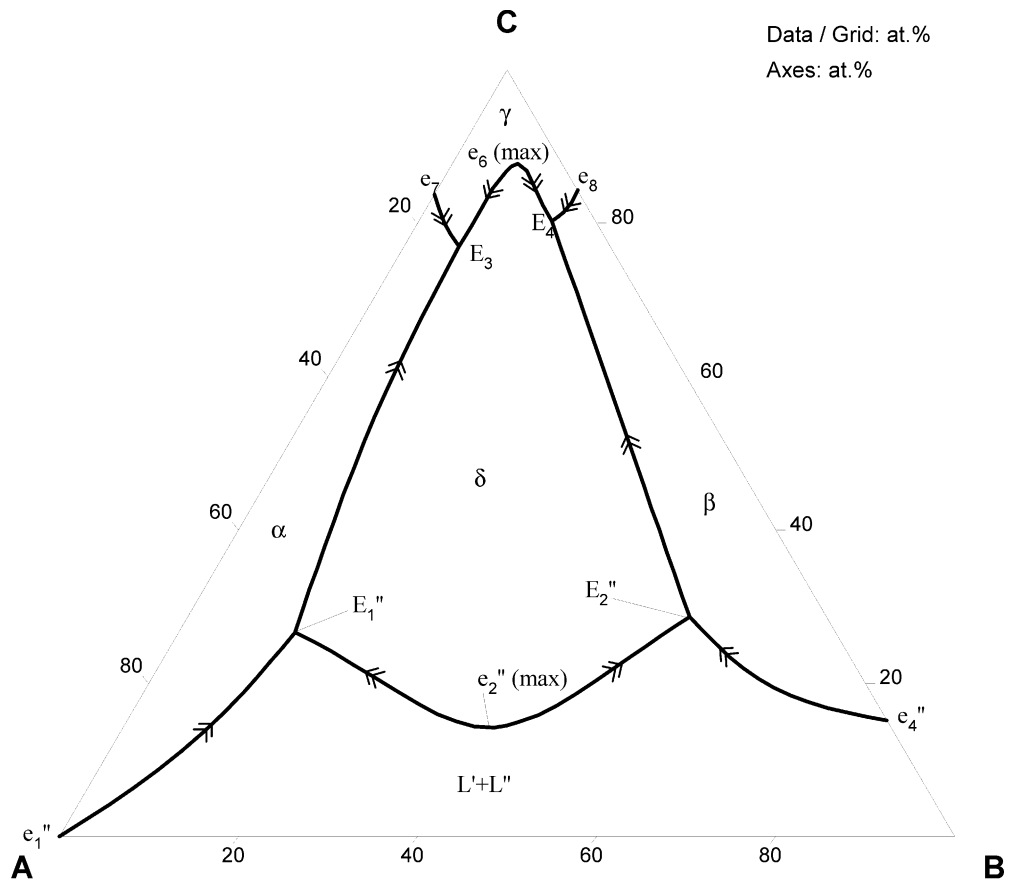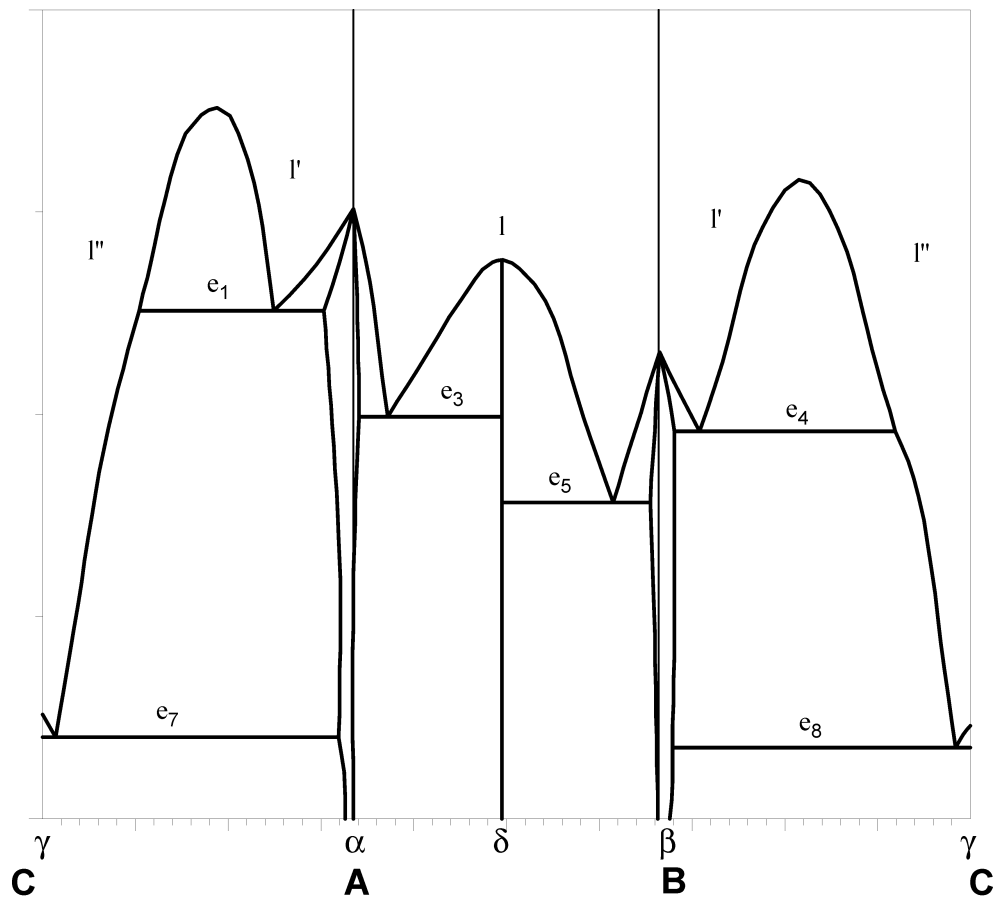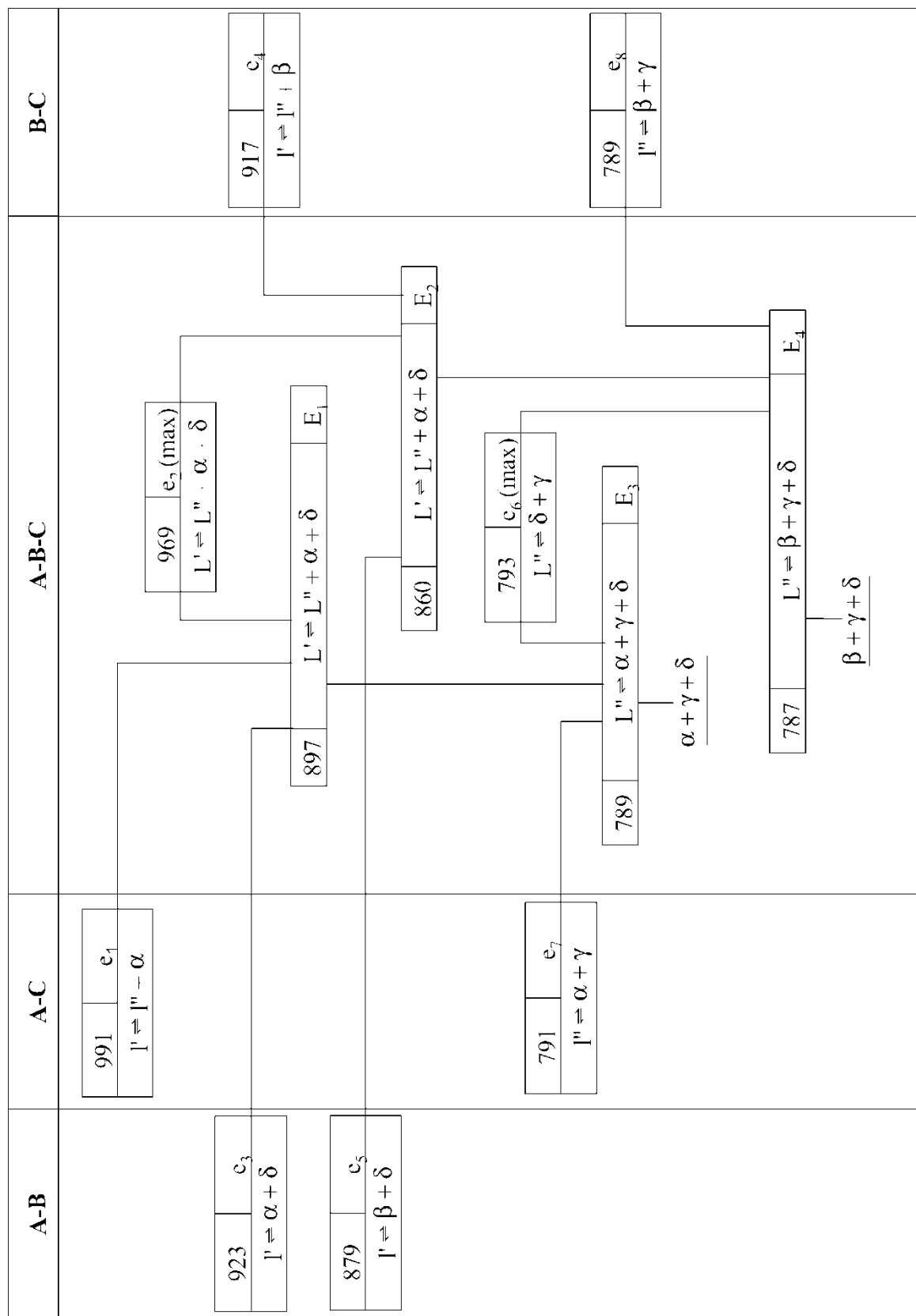
Fig. 4: Reaction scheme

3.4. Examples of the table "Solid Phases"

If not all phases are given in the table, the selection criterion should be indicated in the text.

Examples for selection criteria

1. All phases are given in Table 1.

2. All ternary phases...

3. All stable phases of the A-A$_2$B-C partial system...

4. The phases of the A$_2$B-A$_2$C qusibinary system...

5. All phases stable below (at, above) 900°C...

6. All phases known to be stable... (indicates, that there are reports on additional phases, assumed to be not stable)

but please do <u>not</u> give:

1. All phases shown in the diagrams... (this describes a subjective criterion of selection and gives the impression, that some phases arbitrary are omitted)

2. All known phases...(that is equivalent to "all phases", because nobody can include phases detected later than the date of the evaluation)

Examples for the Style of the Table:

Example 1: Binary, Complete Solutions and Ternary Phases- Note the sequence. See figure below the table

Table 1: Solid Phases

Phase/ Temperature Range (°C)	Person Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments
(Al) < 660.5	$cF4$ $Fm\bar{3}m$ Cu	$a = 404.88$	24°C[Mas, V-C]
$Y_{1-x}Er_xAl_3$ YAl$_3$ < 980	$hR12$ $R\bar{3}m$ BaPb$_3$	$a = 620.4$ $c = 2118.4$ $a = 618.5$ $c = 2114$	$0 \le x \le 0.4$ at 800°C, [1969Zal] at $x = 0$ [V-C] at $x = 0.09$ [1965Vuc]
$Y_xEr_{1-x}Al_3$ ErAl$_3$ < 1070	$cP4$ $Pm\bar{3}m$ AuCu$_3$	$a = 421.5$	$0 \le x \le 0.02$, at 800°C, [1969Zal] at $x = 0$ [1965Vuc, 1969Zal, V-C]
$Y_{1-x}Er_xAl_2$ ErAl$_2$ < 1455 YAl$_2$ < 1485	$cF24$ $Fd\bar{3}m$ Cu$_2$Mg	$a = 779.2\pm0.1$ $a = 785\pm1$	$0 \le x \le 1$ [1972Wil] at $x = 1$ and 27°C [1972Wil] at $x = 0$ and 27°C [1972Wil]

Phase/ Temperature Range (°C)	Person Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments
* τ_1, $Y_x Er_{1-x} Al_3$	$hR20$ $R\overline{3}m$ $HoAl_3$	$a = 604.3$ $c = 3578$ $a = 604.8$ $c = 3578$	$0.05 \leq x \leq 0.35$ [1969Zal] at $x = 0.05$ [1969Zal] at $x = 0.35$ [1969Zal]
* τ_2, $Y_x Er_{1-x} Al_3$	$hP16$ $P6_3/mmc$ $TiNi_3$	$a = 608.6$ $c = 953.0$ $a = 607.7$ $c = 951.9$	$0.4 \leq x \leq 0.55$ [1969Zal] at $x = 0.4$ [1969Zal] at $x = 0.55$ [1969Zal]
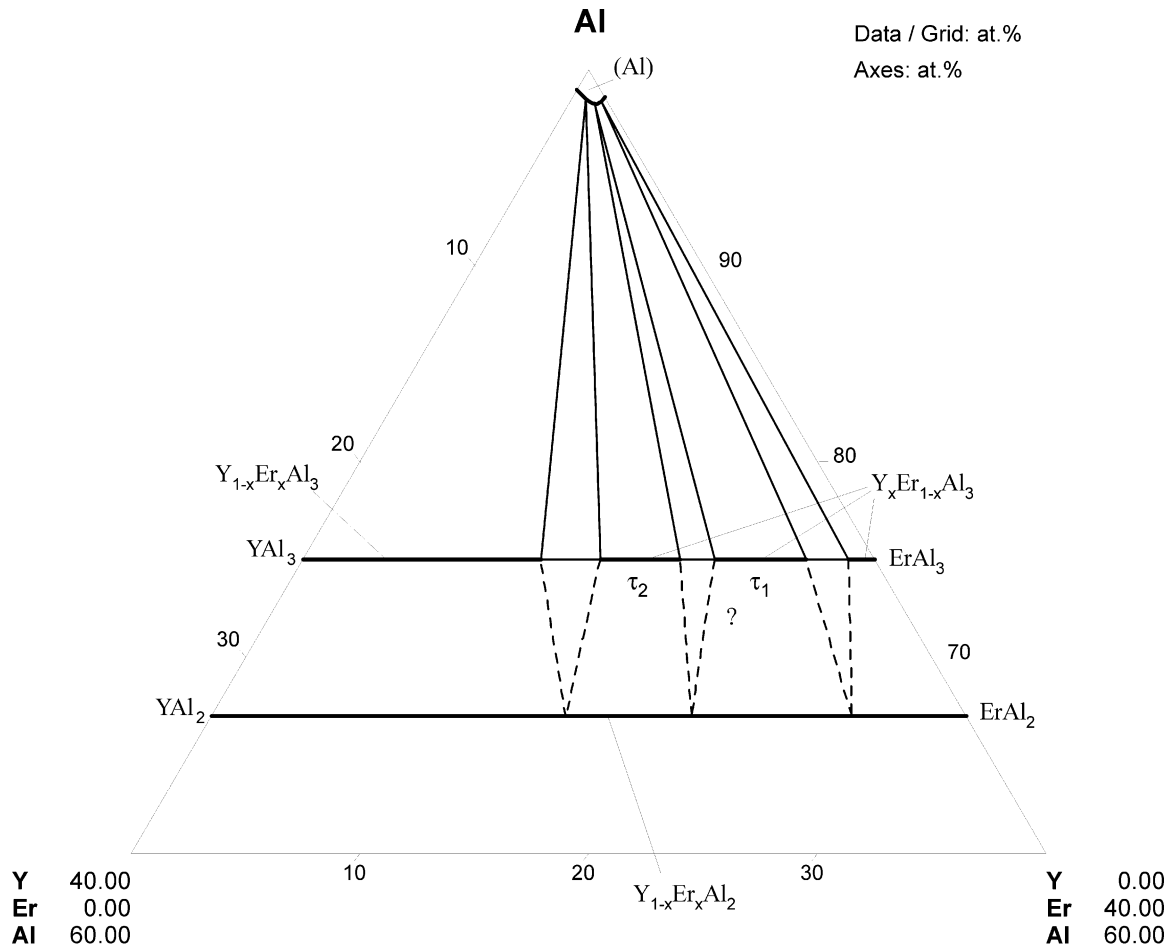
Fig. 5: Isothermal section of the system Al-Er-Y at 500°C in the range 66-100 at.% Al

Example 2: Binary and Ternary Phases - note the dual statement in x and at.%

Table 1: Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments
$U(Ni_xAl_{1-x})_2$ UAl₂ < 1622	cF24 $F d \bar{3} m$ Cu₂Mg	 $a = 776.3$ $a = 770.4$	$0 \leq x \leq 0.18$ [1978Dre] at $x = 0$ at $x = 0.18$ (12 at.% Ni)
$U(Ni_{1-x}Al_x)_2$ UNi₂ < 985	hP12 $P6_3/mmc$ MgZn₂	 $a = 496.17$ $c = 824.16$ $a = 500.3$ $c = 826.0$ $a = 503.9$ $c = 826.4$	$0 \leq x \leq 0.25$ [1978Dre] at $x = 0$ at $x = 0.15$ (10 at.% Al) at $x = 0.25$ (16.7 at.% Al)
* $U(Ni_{1-x}Al_x)_2$	hP9 $P\bar{6}2m$ Fe₂P	 $a = 674.4$ $c = 403.8$ $a = 666.4$ $c = 403.2$	$0.505 \leq x \leq 0.54$ [1978Dre] at $x = 0.505$ (33.6 at.% Al) at $x = 0.54$ (36 at.% Al)

Example 3: Quantitative data on solubility in two directions

Table 1: Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group Prototype	Lattice Parameters (pm)	Comments
β, $(Co_{1-x}Ni_x)Al_{1-y}$ $CoAl_{1-y}$ < 1645 $NiAl_{1-y}$ < 1638	cP2 $Pm\bar{3}m$ CsCl	 $a = 286.2$ $a = 288.7$	$0 \leq x \leq 1$ [09Abc] at $x = 0$ and y = 0 [V-C] $-0.04 \leq y \leq 0.73$ [Mas] (51 to 21 at.% Al) at $x = 1$ and y = 0 [V-C] $-0.30 \leq y \leq 0.55$ [Mas] (55 to 38 at.% Al)

The range of homogeneity of the phase is known to be due to vacancies on the (Co, Ni) sublattice at the Al-rich side and to Co or Ni atoms on the Al sublattice at the Al poor side, corresponding to the crystallographic formula:

$(Co_{1-x-y}Ni_x\square_y)(Al_{1-u-v}Co_uNi_v)$

Example 4: High temperature, high pressure modifications

Table 1: Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group Prototype	Lattice Parameters (pm)	Comments
Ag₂Se(h) 897 - 133	cI*	$a = 498$	[E]
Ag₂Se(r) < 133	oP12 $P222_1$ Ag₂Se(r)	$a = 705$ $b = 432.5$ $c = 782$	[V-C]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group Prototype	Lattice Parameters (pm)	Comments
In$_2$Se$_3$(h$_3$) 900 - 750	m**		[S]
In$_2$Se$_3$(h$_2$) 750 - 650	c**	a = 1010	[S, P]
In$_2$Se$_3$(h$_1$) 650 - 195	h**	a = 401 c = 1924	[E]
In$_2$Se$_3$(r) < 195	hP160 -	a = 1600 c = 1924	V-C]
* α', AgInSe$_2$(h) 778 - 625			[1966Pal1], [1967Pal]; most probably identical to □III, range of homogeneity
* α, AgInSe$_2$(r) < 695	tI16 $I\overline{4}2d$ FeCuS$_2$	a = 610.4 c = 1171.4	chalcopyrite structure, lattice parameter [1980Grz], range of homogeneity
* αIII, AgInSe$_2$(III)	hR12 NaFeO$_2$	a = 394.7 c = 1988.4	High pressure – high temperature phase [1977Jay, 1983Sch], lattice parameter at 1 bar [1977Jay]
* αII, AgInSe$_2$(II)	cF8 $F\overline{4}3m$ ZnS	a = 600 to 606	high pressure phase, sphalerite type structure [1968Ran, 1977Jay]
* αI, AgInSe$_2$(I)	cF8 $Fm\overline{3}m$ NaCl	a = 569 a = 551	(1 bar) non-equilibrium high pressure phase [1969Ran1] lattice parameter [1977Jay] (80 kbar)
* β', AgIn5Se$_8$(h) 811 - 662	cF8 $F\overline{4}3m$ ZnS sphalerite		[1966Pal3] peritectic melting point from [1967Pal]
* β, AgIn5Se$_8$(r) < 740	tP14 $P\overline{4}2m$ AgIn5Se$_8$(r)	a = 579.34 c = 1162.23	ordered defect structure □$_2$AgIn5Se$_8$ [1966Pal3, 1971Rob, 1983Ben], lattice parameters from single crystal [1983Ben]

Example 5:

Table 1: Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group Prototype	Lattice Parameters (pm)	Comments
(δFe) 1538 - 1394	cI2 $Im\overline{3}m$ W	a = 293.78	at 1480°C [V-C]
(αFe) < 912	cI2 $Im\overline{3}m$ W	a = 286.65	at 20°C [V-C]
(γFe) 1394 - 912	cF4 $Fm\overline{3}m$ Cu	a = 366.0	at 1167°C [V-C]

Comment: If the (αFe) and (δFe) solution range merges in the system, the designation of (αδFe) is recommended.

3.5. Sequential Order of the Elements

For system names: alphabetical order of element symbols

For compound names: chemical order according to G.D. Pettifor, *J. Phys. C*, **19**, 285-313 (1986)

For diagrams: chemical order – in the left bottom corner has to be element with lowest Pettifor number. At the top corner should be element with highest Pettifor number

Examples: HfC_{1-x} in the C–Hf system, or YAl_3 in the Al–Y system

Ac 48	Be 77	Cm 41	Fe 61	Ho 23	Md 36	No 35	Pr 31	Sb 88	Te 92	Yb 17	
Ag 71	Bi 87	Co 64	Fm 37	I 97	Mg 73	Np 44	Pt 68	Sc 19	Th 47	Zn 76	
Al 80	Bk 40	Cr 57	Fr 7	In 79	Mn 60	O 101	Pu 43	Se 93	Ti 51	Zr 49	
Am 42	Br 98	Cs 8	Ga 81	Ir 66	Mo 56	Os 63	Ra 13	Si 85	Tl 78		
Ar 3	C 95	Cu 72	Gd 27	K 10	N 100	P 90	Rb 9	Sm 28	Tm 21		
As 89	Ca 16	Dy 24	Ge 84	Kr 4	Na 11	Pa 46	Re 58	Sn 83	U 45		
At 96	Cd 75	Er 22	H 103	La 33	Nb 53	Pb 82	Rh 65	Sr 15	V 54		
Au 70	Ce 32	Es 38	He 1	Li 12	Nd 30	Pd 69	Rn 6	Ta 52	W 55		
B 86	Cf 39	Eu 18	Hf 50	Lr 34	Ne 2	Pm 29	Ru 62	Tb 26	Xe 5		
Ba 14	Cl 99	F 102	Hg 74	Lu 20	Ni 67	Po 91	S 94	Tc 59	Y 25		

Exception: if the ionic nature of a compound is to be emphasized.
$Mg(VO_3)_2$ may be used if the formation of Mg^{2+} and $(VO_3)_2^{-1}$ ions is discussed. However, the strict chemical order V_2MgO_6 is to be used instead of MgV_2O_6
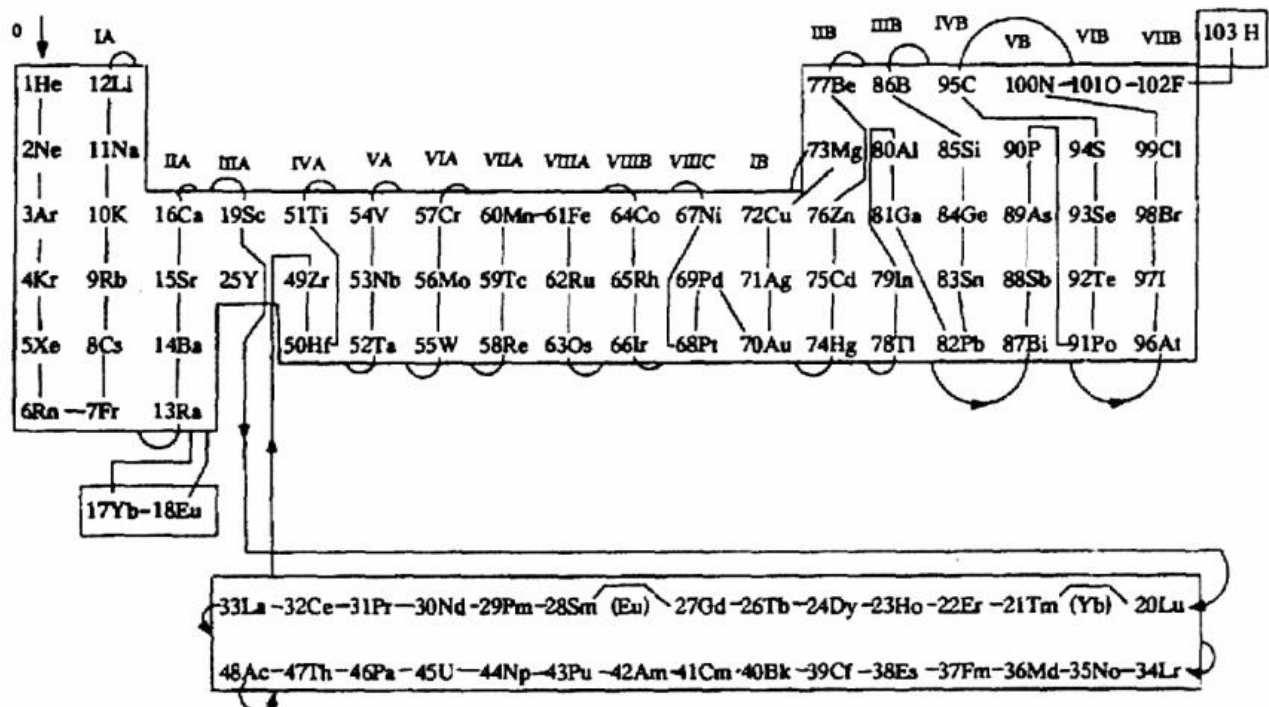
Chapter 4.
Examples of System Reports

Arsenic – Molybdenum – Ruthenium

Aluminium – Germanium – Ytterbium

Aluminium – Copper – Magnesium

Aluminium – Iron – Nickel

Cerium – Copper – Silicon

Arsenic – Molybdenum – Ruthenium

Peter Rogl

Introduction

Superconducting metallic glasses have been reported by [1979Joh] for the ternary composition $(Mo_{0.6}Ru_{0.4})_{1-x}As_x$ with $x = 0.24, 0.28$.

References

[1979Joh]   Johnson, W.L., Williams, A.R., "Structure and Properties of Transition Metal- Metalloid Glasses Based on Refractory Metals", *Phys. Rev.*, **B20**, 1640-1655 (1979)

Aluminium – Germanium – Ytterbium

Riccardo Ferro, Adriana Saccone, Stefano Delfino

Introduction

Ternary alloys of the compositions $YbAl_2Ge_2$ [1970Zar, 1972Mur] and YbAlGe 1974Rya, 1974Yan] have been studied. [1970Zar] prepared the alloys starting from Al 99.98 mass%, Ge 99.999 mass% and Yb 99.96 mass%. Powder X-ray analysis was then performed.

A compilation that includes several phases containing Al, Ge and rare earths has been presented by [1982Gla].

Solid Phases

The crystal data of two ternary phases are given in Table 1.

References

[1970Zar]   Zarechnyuk, O.S., Murav'eva, A.A., Gladyshevskii, E.I., "Some New Intermetallic Compounds with a Structure Similar to that of La_2O_2S" (in Ukrainian), Dopov. Akad. Nauk Ukr. RSR, (A), **8**, 753-756 (1970) (Crys. Structure, Experimental, 2)
[1972Mur]   Murav'eva, A.A., "Phase Equilibria and Crystal Structures of Compounds in the Ternary Systems of Al and Si (or Ge) with Rare Earth Metals" (in Russian), Thesis, Ivan Franko State University (1972) (Crys. Structure, Phase Diagram, Experimental, 7)
[1974Rya]   Ryabokov, T.I., "New Intermetallic Compounds RAlGe, where R is a Rare Earth Metal" (in Ukrainian), Visn. L'viv Univ., Ser. Khim., **15**, 26-28 (1974) (Crys. Structure, Experimental, 2)
[1974Yan]   Yanson, T.I., Zarechnyuk, O.S., Gladyshevskii, E.I., "New Rare Earth-Al-Ge Compounds" (in Russian), "Tezisy Dokl.-Vses. Konf. Kristallokhim. Intermet. Soedin.", 2nd, Ed: R.M. Rykhal, L'vov Gos. Univ.: Lvov, USSR, 35 (1974) (Crys. Structure, Experimental, 0)
[1982Gla]   Gladyshevskii, E.I., Bodak, O.I., "Crystallochemistry of Rare Earth-Metal Intermetallic Compounds" (in Russian), Ed. L'vov University (1982) (Crys. Structure, Review, 1702)

Table 1: Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
* $YbAl_2Ge_2$	$hP5$ $P\bar{3}m1$ La_2O_3	a = 418.4 c = 704.7 a = 418 c = 705	[1970Zar] [1972Mur]
* YbAlGe	$oC12$ DyAlGe	a = 430.7 b = 1057 c = 593.5	[1974Rya, 1982Gla]

Aluminium – Copper – Magnesium

Günter Effenberg, Alan Prince[†], updated by Nathalie Lebrun, Hans Leo Lukas, Mireille G. Harmelin

Introduction

This system was previously evaluated by [1991Eff]. Their evaluation has been used by two groups as the basis for thermodynamic assessments and phase diagram calculations [1993Zuo, 1996Zuo, 1997Che] and [1998Buh, 2003Jan]. Some experiments have been performed to support these calculations [1995Hua, 1995Kim, 1995Soa, 1998Fau] and [1999Fau]. The equilibria in the Al-Cu-Mg system are complicated by the existence of four ternary phases. There is need for experiments to clarify the ternary equilibria involving the three Laves phases, λ_{1-3}, which have clearly been identified as three separate phases. The λ_1 phase with a Cu_2Mg type structure is a solution phase of the binary Cu_2Mg compound with replacement of the Cu atoms by Al along the 33.3 at.% Mg section. At a composition close to the Cu_3Mg_2Al formula, the λ_1 phase melts congruently at ~910°C. Further replacement of Cu by Al stabilizes the λ_2 phase with a $MgNi_2$ type structure and then the λ_3 phase with a $MgZn_2$ type structure. A variety of polytype structures with different atom layer stacking sequences have been observed between the $MgNi_2$ and $MgZn_2$ type phases. The λ_{2-3} phases appear to be formed by peritectic reaction and each Laves phase is associated with a region in which it forms as the primary phase on solidification of melts. Four additional ternary compounds have also been studied extensively. The S phase is based on the $CuMgAl_2$ composition, V on $Cu_6Mg_2Al_5$ and Q on $Cu_3Mg_6Al_7$. These three phases exist over very limited homogeneity ranges. The T phase has a broad range of homogeneity. A formula $(Cu_{1-x}Al_x)_{49}Mg_{32}$ is derived from the crystal structure [1952Ber], but also some mutual replacement between Mg and Cu+Al takes place.

The liquidus projection, presented by [1952Ura], does not include the monovariant curves associated with the $L + \lambda_1 \rightleftharpoons \lambda_2$ and $L + \lambda_2 \rightleftharpoons \lambda_3$ peritectic reactions. The Laves phase λ_1 is the predominant primary phase, but also the regions for primary solidification of (Al) and (Mg) are relatively large. Six quasibinary reactions have been identified experimentally, and the quasibinary reaction e_3 (Table 2b) has been suggested. The invariant reactions associated with the primary (Al) phase region are well characterized by numerous workers. The invariant reactions associated with the primary V, Q and T phase regions have been elucidated by Russian workers, summarized by [1952Ura]. The liquidus surface across the Mg_2Al_3, T and $Mg_{17}Al_{12}$ phase regions is exceptionally flat and ranges in temperature from 420 to 475°C. [1952Ura] gave a complete reaction scheme. The thermodynamic calculations referred to above in principle reproduce this reaction scheme, but differ in some details.

Binary Systems

Assessments of the Al-Cu system by [2003Gro], of the Al-Mg system by [2003Luk] and of the Cu-Mg system by [2002Iva] are accepted. They are based on [1994Mur, 1998Liu] for Al-Cu, [1982Mur, 1998Lia1] for Al-Mg and [1994Nay] for Cu-Mg. The thermodynamic data set of the COST 507 action [1998Ans, 1998Buh] was updated recently in some details [2003Jan]. It was used for the calculated figures and the reaction scheme presented in this assessment. The homogeneity ranges of the phases Mg_2Al_3, ζ and δ were simplified to stoichiometric phases. η_1 and η_2 were treated as a single phase, η. ζ_1 and ζ_2 were also not distinguished and called ζ.

Solid Phases

There are four well-defined ternary phases, designated in the literature as Q, S, T and V phases. It is quite interesting to note that all ternary compounds in the Al-Cu-Mg system are formed at maxima of three-phase equilibria involving the liquid phase, except the V phase, which is formed in a four-phase peritectic reaction (P_1). In addition the section at 33.3 at.% Mg contains a complex series of ternary Laves-Friauf phases that are designated as λ_1, λ_2, λ_3, 5L, 6L, 9L and 16L in this assessment, Table 1. The Q phase is based on the chemical formula $Cu_3Mg_6Al_7$ [1947Str, 1951Mir1] and has a very limited homogeneity range. The S phase

has been extensively studied [1936Lav1, 1937Nis1, 1938Pet1, 1938Pet2, 1940Kuz, 1941Obi, 1943Per, 1944Lit, 1946Pet, 1946Ura, 1947Str, 1949Mir]. It also has a limited homogeneity range, based on the chemical formula $CuMgAl_2$. Its structure was determined by [1943Per] and confirmed by [1949Mir]. The T phase has been equally thoroughly investigated [1919Vog, 1923Gay, 1935Lav, 1937Nis1, 1940Kuz, 1943Gue, 1944Lit, 1946Pet, 1946Ura, 1948Str, 1949Ura1, 1949Ura2, 1950Phr, 1952Ber, 1966Aul, 2000Tak] and a variety of chemical formulae assigned to it. From the crystal structure determined by [1952Ber], the formula $(Cu_{1-x} Al_x)_{49}Mg_{32}$ is adequate. It is found that very few Al atoms occupy site A, which is the center of an isochahedral cluster being almost empty [2000Tak]. The V phase has a small region of homogeneity centered on the $Cu_6Mg_2Al_5$ formula [1936Lav1, 1936Lav2, 1937Sch, 1943Gue, 1947Str, 1948Str, 1949Sam, 1949Ura1, 1951Mir3, 1952Ura] although other chemical formulae have been quoted in the literature. Its structure was determined by [1949Sam] with the ideal formula $Cu_6Mg_2Al_5$. New recent results using DSC and EDS/WDX techniques [2001Fau] confirmed small solubility ranges of the Q and S phases. Moreover, the solubility domain of the V phase seems to be parallel to the Al-Cu binary edge [2001Fau]. Addittional experiments are needed to confirm it.

The Laves-Friauf phases, although well studied, have not been integrated experimentally into the ternary equilibria in a satisfactory manner. The λ_1 phase with a Cu_2Mg type structure is based on the Cu_2Mg binary compound with a substitution of Al atoms for Cu to form a solid solution series. At a composition close to Cu_3Mg_2Al, the λ_1 phase melts congruently [1936Lav1, 1952Ura]. With further replacement of Cu by Al on the 33.3 at.% Mg section, an $MgNi_2$ type phase is stable, λ_2. There is general agreement between [1953Kle, 1965Sli, 1977Kom, 1981Mel1] and [1981Mel2] on the extent of the λ_2 phase region. Earlier work did not detect λ_2 [1934Lav, 1943Gue, 1949Ura1] or regarded it as stable at high temperature only [1936Lav1]. The $MgZn_2$ type structure, λ_3, is formed with further substitution of Cu atoms by Al. The results from the different workers are summarized in Fig. 1. Polytype structure Laves phases with variations in the layer stacking sequences have been studied by [1962Kom, 1977Kit, 1977Kom] and [1981Mel1]. They are located between λ_1 and λ_2, but their ranges of stability could not exactly be separated from those of λ_1 and λ_2. [1998Che] proposed a "new intermetallic compound $Mg_{1.75}Cu_{1.0}Al_{0.4}$" at a composition, where [1991Eff, 2000Fau] and the calculations [1997Che, 1998Buh, 2003Jan] assume two phases, λ_1 and (Mg). The characteristics of this "new phase", however, clearly identify it as the λ_1 phase [2000Fau]. The presence of (Mg) and λ_1 phases were confirmed by [2000Fau] who made XRD experiments on alloys having the same composition as those reported by [1998Che]. Most probably the also present (Mg) phase was not detected in the X-ray patterns of [1998Che] due to line broadening by cold deformation.

Quasibinary Systems

A number of quasibinary systems have been reported. The calculation [2003Jan] found 13 maxima of three-phase equilibria, but some of them are less than 1 K above an adjacent four-phase equilibrium and must be taken as tentative only. The (Mg)-λ_1 section is a quasibinary eutectic [1932Por, 1933Bas, 1934Por, 1949Ura2], e_{13}, Table 2. The (Al)-S section contains a quasibinary eutectic e_{14} [1937Nis1, 1946Ura, 1948Bro, 1952Han]. The calculated temperatures [2003Jan] of both equilibria are far below those given by [1946Ura] and accepted by [1991Eff]. The sections Mg_2Al_3-T, e_{19}, and $Mg_{17}Al_{12}$-T, e_{16}, are also quasibinary eutectic sections at Cu contents below the beginning of the primary Q phase region. [1943Gue, 1949Ura1, 1949Ura2, 1951Mir2] and [2003Jan] are in agreement on the nature of these two sections, Table 2. The investigation [1951Mir2] of the region of primary solidification of Q led to the conclusion that the T phase is formed by peritectic reaction with Q at p_{13}, Fig. 2. A quasibinary reaction was indicated by [1946Ura] who found a maximum on the curve U_8U_{11} corresponding with the peritectic formation of S by reaction of liquid with a Laves phase. [1949Ura1, 1949Ura2] and [1952Ura] refer to the cubic Cu_2Mg type phase λ_1 or to a composition CuMgAl. They take no account of the λ_2 and λ_3 Laves phases. The calculation of [2003Jan] gives λ_2 as the Laves phase participating in this reaction, p_{10}, which is also favoured by [1991Eff]. [1938Pet1] regarded the $CuAl_2$-S section as a quasibinary, but later work has disproved this assumption.

Invariant Equilibria

Table 2 lists the invariant reactions following from the thermodynamic calculation of [2003Jan] for the Al-Cu-Mg ternary system and may be read in conjunction with Fig. 2. The reaction scheme, following from this calculation is given in Fig. 3. In this calculation, η_1 and η_2 as well as ζ_1 and ζ_2 were considered as single phases and called η and ζ, respectively. The ternary eutectic reaction E_5 has been widely studied, Table 3. The flat nature of the liquidus surface near to E_7 has led to a considerable scatter in quoted compositions and temperatures, Table 4. The reaction has normally been quoted as a ternary eutectic reaction and this is accepted. The transition reaction U_{16} has also been widely studied, Table 5. The work of [1946Ura, 1949Ura2] and [1948Bro] rests on an examination of a greater number of alloys than other work and allowed a more precise determination of the liquid composition at U_{16}. Ternary eutectic reactions in Mg-rich alloys occur at E_6 and E_9. The reaction temperature at E_6 is 1°C [1932Por, 1933Bas, 1934Por] or 2°C [1949Ura2] below the binary Cu-Mg eutectic temperature. The ternary eutectic E_9, Table 6, was initially regarded as involving a Laves phase, but the work of [1951Mir2] indicates that this eutectic involves the Q phase, which was not detected by the previous workers. Faudot et al. [1998Fau, 1999Fau] confirmed the eutectic, Table 6. The ternary eutectic reaction at E_9 was found by [1949Ura2] at 423°C, what agrees well with that calculated by [2003Jan], 424°C. The reaction at U_{13} was regarded as a transition reaction by [1937Nis1, 1952Han], as calculated by [2003Jan], whereas [1946Ura] and [1949Ura2] considered it to be a ternary peritectic reaction, $L+\lambda_1+S \rightleftharpoons T$. [1951Mir2] gives it as $L+\lambda_1+S \rightleftharpoons Q$. There is doubt about this reaction on two counts. The Q phase lies virtually on the L-λ_1 tie line [1952Ura] and it is unlikely that the Laves phase is λ_1. For the reactions U_{15} and U_{18} [2003Jan] reproduced those given by [1951Mir2] with 3°C deviation. For U_{18} Faudot et al. [1998Fau] gave 427°C as calculated by [1998Buh, 2003Jan]. But later [1999Fau] found it at 451°C with a more Al-rich liquid, Table 6. The transition reaction at U_{17} was given by [1951Mir2] as $L+\lambda_1 \rightleftharpoons (Mg)+Q$, but the work of [1981Mel2] indicates λ_3 as the reactant rather than λ_1, whereas [1998Fau, 1999Fau, 2003Jan] assume λ_2. The reactions in the Cu-rich corner have been little studied. In Table 2 are given those calculated by [2003Jan]. [1949Ura2] assumed an eutectic instead of U_2 and a transition reaction instead of E_4. The temperatures of the invariant equilibrium in this area calculated by the two groups [1997Che] and [1998Buh, 2003Jan] deviate up to 20°C. The regions of primary solidification of the Laves phases λ_1, λ_2 and λ_3 have not been experimentally defined, but the calculation [2003Jan] gives them as shown in Fig. 2. [1997Che] did not distinguish these Laves phases.

Liquidus Surface

A liquidus projection, Fig. 2b, is taken from the calculation of [2003Jan] with some minor modifications on the edges according to the binary systems accepted in this assessment. It should be compared with the projection, Figs. 2 and 2a, deduced also from the calculations of [2003Jan]. The liquidus in the ternary diagram was also calculated by [2001Che, 2002Che] using the multicomponent phase diagram calculation software PANDAT. [1999Xie] also studied the liquidus projection in the Al rich corner. Results are in agreemnt with those calculated by [2003Jan]. According to the liquidus of the binary systems accepted in this assessment, the liquidus projection was modified at the edge boundaries. The liquidus isotherms reproduce fairly well those assessed by [1991Eff]. The primary (Al) region has been widely studied with general agreement on the form of the liquidus. The isotherms for the region of primary solidification of the series of Cu-rich Al-Cu phases are uncertain.

Isothermal Sections

The calculated 400°C isothermal section calculated by [2003Jan], Fig. 4, agrees with Fig. 4 of [1991Eff] except the broadening of the homogeneity range of λ_1 near 25 at.% Al, which in calculation needs to model an anomaly in the Gibbs energy description at that composition, but there is no other evidence for an anomaly. The phase Mg_2Al_3 is simplified as a stoichiometric phase as well as the $CuMg_2$, η, ζ and δ phases. The solubility of Cu and Mg in Al-rich alloys at 460°C was determined by [1944Lit] and [1947Str], Fig. 5. [1944Lit] also produced data for 375°C. The results of [1932Dix] agree with the solubilities given in Fig. 5. [1946Pet] found lower Mg solubilities but used fewer alloys. [1955Zam] published solubility curves with a

series of cusps that cannot be reconciled with the alloy constitution. The solubilities of Mg and Cu in (Al) reported in the accepted binary systems have also been taken into account in Fig. 5. The calculated solvus isotherms of [1986Cha] and [2003Jan], Fig. 6, are in good agreement with [1944Lit] and [1947Str]. [1957Rog] reported the solubility of Al and Mg in (Cu), Fig. 7. No comparable work has appeared. In this area the calculation is less reliable, as it cannot be based on adjacent experimental data. More extensive isothermal sections were determined by [1946Pet] at 400°C in the region from Al to S and T. [1949Mir] reported on the S phase region at 420°C, [1949Ura1] on the T and λ_1 phase region at 400°C, [1951Mir1] on the Q phase region at 400°C, [1952Ura] on an almost complete isothermal section at 400°C and [1981Mel2] on the region from 33.3 to 100 at.% Mg at 400°C. [1944Lit] and [1947Str] studied the 460°C isothermal section from Al to the θ, S, Q and T phases.

Temperature – Composition Sections

The liquidus and solidus of the Al rich alloys along the isopleth Al-Cu$_{0.5}$Mg$_{0.5}$ were calculated by [1997Che, 1999Xie, 2000Lia] using thermodynamic descriptions. The measured solidus data found by [1988Mur] was found to be ~ 0.5 at.% higher than the model-calculated values, while the measured liquidus is in good agreement with the model-calculation. The inaccuracy for the solidus is explained by microsegregations occuring in ternary Al-Cu-Mg alloys [1999Xie].
Several isopleths were calculated by [1997Che, 2003Jan] from thermodynamic descriptions. Figs. 8 and 9a, 9b, 9c show isopleth sections at 33.3 at.% Mg and x mass% Al (x =60, 70 and 95.5) respectively. The calculated isopleth, taken from [2003Jan] and reported on Fig. 8, is in agreement with the experimental data reported by [1936Lav1] and [1953Kle]. The calculated isopleths reported on Figs. 9a, 9b and 9c are taken from [1998Buh] and describe quite well the experimental information reported by [1937Nis1, 1937Nis2, 1952Han] and [1946Ura]. The calculated isopleths at 37 at.% Al (Fig. 10a) and 43.75 at.% Al (Fig. 10b) show the λ_2 and the Q phases formations respectively [2003Jan].

Thermodynamics

[1972Pre] studied the enthalpy of formation of alloys on the 33.3 at.% Mg section. Substitution of Cu by Al increases the stability of the λ_1 phase although there is a decrease of stability at a valency electron concentration of 1.5 (76.9Cu, 17.3Mg). [1987Hoc] calculated the enthalpy of a ternary alloy containing 33.3% "MgAl$_2$"; agreement with [1972Pre] is fair. [1985Kuz] applied a thermodynamic model to predict the ternary solidus from the ternary liquidus and the binary solidus-liquidus for Al-rich alloys. [1973Dav] used quasi-chemical regular solution theory to calculate the monovariant curve e$_2$E$_5$ of Fig. 2a. With the introduction of a ternary interaction parameter the calculated ternary eutectic point E$_5$, Table 3, shows reasonable agreement with the assessed composition. [1987Lac] calculated the Al-rich region of the phase diagram using an extended Redlich-Kister formalism. Excellent agreement was obtained with the assessed liquidus, Fig. 2b. [1985Far] calculated the composition of the ternary eutectic E$_5$, Fig. 2a and Table 2, assuming both ideal solution behaviour and regular solution behaviour. The calculated eutectic compositions, 34.4Cu-8.8Mg (mass%) for ideal solutions and 30.3Cu-7.5Mg (mass%) for regular solutions, approximate to the assessed values. The calculated eutectic temperatures are surprisingly low at 273°C and 271°C, respectively. Recently two groups [1997Che] and [1998Buh, 2003Jan] calculated the whole ternary system, describing the Gibbs energies of all phases involved by the compound energy formalism. Both calculations show very similar results, only in the Cu-rich part there is some disagreement of the invariant temperatures (up to 20°C). The first group also calculated solidification paths using the model of Scheil [1993Zuo, 1996Zuo].
[1986Che] measured the enthalpy of fusion of the ternary eutectic E$_5$ as 365 J·g^{-1} corresponding to 11.8 kJ·mol^{-1} of atoms. [1986Not] measured the enthalpy of formation of the S phase as -63.2 ± 4.0 kJ·mol^{-1} of CuMgAl$_2$. [1995Kim] measured the enthalpy of mixing of ternary liquids by a high temperature calorimeter at 713°C along three lines with constant Al/Mg ratios up to 40 at.% Cu and along Al/Cu = 13/7 up to 27 at.% Mg. [1995Soa] measured the chemical potential of Mg in ternary melts by an isopiestic method.

Notes on Materials Properties and Applications

The mechanical properties such as tensile strengh were investigated by [2002Dav] on 0.02Zn-0.05Ti-0.42Mn-0.27Fe-4.5Cu-1.5Mg-Al-0.17Si alloys.
[2002Zhu] reported that a small addition of Ag (< 0.1 at.%) to an Al-Cu-Mg alloy with a high content of Al promote an increasing strength and creep resistance when compared to Al-Cu-Mg alloys that contain only the $CuAl_2$ precipitate.

Miscellaneous

[1940Kuz] and [1946Kuz] measured lattice spacings of the (Al) phase along sections from Al with various Cu:Mg ratios. [1951Poo] measured the lattice spacings of the (Al) phase along sections from 99 at.% Al, 1 at.% Mg to 99.5 at.% Al, 0.5 at.% Cu and from 98 at.% Al, 2 at.% Mg to 99 at.% Al, 1 at.% Cu, Table 7.
A small addition of Mg to Al-Cu alloys accelerates the formation of Guinier-Preston (GP) zones through the Mg/Cu/vacancy complexes mechanism [2000Hir, 2002Hir].
The crystal structure of a metastable variant of S on aging Al alloys was studied by [1950Bag]. Aging studies of single crystals of an alloy containing 1.2 at.% Cu, 1.2 at.% Mg [1978Ale] showed S particles to be coherent with the Al matrix. The effect of aging on mechanical properties of Al-rich alloys have been reported by [1939Han, 1941Mec] and [1948Sha]. More recent studies on metastable precipitates in (Al) are from [1990Gar] and [1991Jin].
[1959Pal] prepared thin film Al-rich ternary alloys by evaporation on to Al substrates. The constitution is claimed to correspond with bulk samples. There is a growing literature on the formation of a non-equilibrium icosahedral quasicrystalline phase by rapid solidification of alloys in the T phase region. [1986Cas] tentatively outlined the phase region that produces quasicrystals on rapid solidification as containing 10 to 13.5 at.% Cu, 35 to 37 at.% Mg. This composition range is on the low Mg side of the equilibrium T phase region. Annealing a rapidly solidified alloy with 1 at.% Cu, 5 at.% Mg for 100 h at 190°C gave both the icosahedral phase and the equilibrium T phase at the grain boundaries of the Al matrix. For anneals of 24 h at 250°C only the T phase was observed at the grain boundary [1986Cas, 1987Cas] with precipitation of the S phase in the Al matrix. [1987San1] and [1987San2] rapidly solidified an alloy corresponding to $CuMg_4Al_6$. This composition lies in the T phase region. DSC measurements gave a melting point of 474.9°C which is in good agreement with the assessed temperature of the quasibinary reaction p_6, L+Q⇌T, Fig. 3. A polymorphic transformation of the T phase, reported at 356.5°C, has not been noted by other workers. [1988She] rapidly solidified an alloy containing 12.5Cu-36.5Mg-51Al (at.%) and found it to be a single phase icosahedral quasicrystal. This composition is within the phase region given by [1986Cas]. A wider, but less exact, delineation of the icosahedral quasicrystal phase region was given by [1988Shi]. They quote the composition as typically $CuMg_4Al_5$, as proposed by [1937Nis1] for the stable T phase. [1988San] rapidly solidified the composition $CuMg_4Al_6$ and carried out a detailed X-ray study of the quasicrystalline phase and its transformation to the crystalline T phase by annealing for 1 h at 340°C. [1989She] used high resolution X-ray diffraction to study atomic distribution in quasicrystalline phases as well as differential scanning calorimetry (DSC) to get thermodynamic properties. [1991Wit] prepared and studied an icosahedral alloy with composition $Cu_{12.5}Mg_{36.5}Al_{51}$ by electrical resistivity measurements and DSC.

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Table 1: Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
(Al) < 660.452	$cF4$ $Fm\bar{3}m$ Cu	$a = 404.88$	at 24°C [V-C] 100 to 81.4 at.% Al at 450°C [1982Mur]
(Cu) < 1084.62	$cF4$ $Fm\bar{3}m$ Cu	$a = 361.46$	at 25°C [Mas2] 0 to 19.7 at.% Al [Mas2] melting point [1994Mur]
$Cu_{1-x}Al_x$		$a = 361.52$ $a = 365.36$	[1991Ell], $x=0$,quenched from 600°C [1991Ell], $x=0.152$,quenched from 600°C, linear da/dx
(Mg) < 650	$hP2$ $P6_3/mmc$ Mg	$a = 320.94$ $c = 521.01$	at 25°C [V-C2] 0 to 11.5 at.% Al at 437°C [1982Mur]
θ, $CuAl_2$ < 591	$tI12$ $I4/mcm$ $CuAl_2$	$a = 606.7$ $c = 487.7$	31.9 to 33.0 at.% Cu [1994Mur] single crystal [V-C2, 1989Mee]
η_1, CuAl(h) 624 - 560	$o*32$	$a = 408.7$ $b = 1200$ $c = 863.5$	49.8 to 52.4 at.% Cu, [V-C, Mas2, 1985Mur] Pearson symbol: [1931Pre]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
η_2, CuAl(r) < 569	$mC20$ $C2/m$ CuAl(r)	$a = 1206.6$ $b = 410.5$ $c = 691.3$ $\beta = 55.04°$	[1985Mur] 49.8 to 52.3 at.% Cu, [V-C2]
ζ_1, ~$Cu_{47.8}Al_{35.5}$(h) 590 - 530	$oF88$ - 4.7 $Fmm2$ $Cu_{47.8}Al_{35.5}$	$a = 812.67$ $b = 1419.85$ $c = 999.28$	55.2 to 59.8 at.% Cu [Mas2, 1994Mur] structure: [2002Gul]
ζ_2, $Cu_{11.5}Al_9$(r) < 570	$oI24$ - 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]
ε_1, $Cu_{100-x}Al_x$ 958 - 848	cubic (?)		$37.9 \leq x \leq 40.6$ 59.4 to 62.1 at.% Cu, [Mas2, 1985Mur]
ε_2, $Cu_{2-x}Al$ 850 - 560	$hP6$ $P6_3/mmc$ Ni_2In	$a = 414.6$ $c = 506.3$	$0.47 \leq x \leq 0.78$ 55.0 to 61.1 at.% Cu, [Mas, 1985Mur, V-C2], NiAs in [Mas2, 1994Mur]
δ, $Cu_{100-x}Al_x$ < 686	$hR*$ $R3m$	$a = 1226$ $c = 1511$	$38.1 \leq x \leq 40.7$ [Mas2, 1985Mur] 59.3 to 61.9 at.% Cu at $x = 38.9$ [V-C]
γ_0, $Cu_{100-x}Al_x$ $Cu_{\sim2}Al$ 1022 - 780	$cI52$ $I\bar{4}3m$ Cu_5Zn_8	-	$31 \leq x \leq 40.2$ [Mas2], 62 to 68 at.% Cu [1998Liu]
γ_1, Cu_9Al_4 $\leq$ 890	$cP52$ $P\bar{4}3m$ Cu_9Al_4	$a = 870.23$ $a = 870.68$	62 to 68 at.% Cu, [Mas2, 1998Liu]; powder and single crystal [V-C2] from single crystal [V-C2]
β, Cu_3Al(h) 1049 - 559	$cI2$ $Im\bar{3}m$ W	$a = 295.64$	70.6 to 82 at.% Cu [1985Mur][1998Liu] at 672°C in β+(Cu) alloy
$CuMg_2$ < 568	$oF48$ $Fddd$ $CuMg_2$	$a = 907$ $b = 528.4$ $c = 1825$ $a = 905$ $b = 528.3$ $c = 1824.7$ $a = 904.4 \pm 0.1$ $b = 527.5 \pm 0.1$ $c = 1832.8 \pm 0.2$	[Mas2, V-C2] [1994Nay] [1993Gin]
Cu_2Mg < 797	$cF24$ $Fd\bar{3}m$ Cu_2Mg	$a = 702.1$	64.7 to 69 at.% Cu [Mas2, V-C2]
Mg_2Al_3 $\leq$ 452	$cF1168$ $Fd\bar{3}m$ Mg_2Al_3	$a = 2823.9$	[1982Mur] 60-62 at.% Al [1982Mur, 2002Cze] 1168 atoms on 1704 sites per unit cell [1965Sam, 1982Mur]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
$Mg_{17}Al_{12}$ ≤ 458	$cI58$ $I\bar{4}3m$ αMn	$a = 1054.38$	[1982Mur] At 41.4 at.% Al, [V-C2] 39.5 to 51.5 at.% Al, [1998Lia11] 40 to 52 at.% Al, [2002Cze] Space group from [1998Don]
$Mg_{23}Al_{30}$ 410 - 250	$hR159$ $R\bar{3}$ $Mn_{44}Si_9$	$a = 1282.54$ $c = 2174.78$	54.5-56.5 at.% Al [1998Lia1, 1998Lia2, 2002Cze] Structure : 159 atoms refer to hexagonal unit cell [1968Sam]
λ_1, $(Cu_{1-x}Al_x)_2Mg$ Cu_2Mg < 900	$cF24$ $Fd\bar{3}m$ Cu_2Mg	$a = 701.3$ $a = 715.42$	$0 \leq x \leq 0.433$ [1936Lav1] space group from [1936Lav1] at $x = 0$ For $Mg_{1.75}Cu_{1.0}Al_{0.4}$ at 480°C [2000Fau]
* Q, $Cu_3Mg_6Al_7$	$cI96$ $Im\bar{3}m$ $CuFeS_2$	$a = 1208.7$	[1951Mir1] space group from [1991Eff]
* S, $CuMgAl_2$	$oC16$ $Cmcm$ BRe_3	$a = 401$ $b = 925$ $c = 715$	[1943Per] space group from [1991Eff]
* T, $(Cu_{1-x}Al_x)_{49}Mg_{32}$	$cI162$ $Im\bar{3}$ $Mg_{32}(Al,Zn)_{49}$	$a = 1428$ to 1435	[1952Ber] composition dependent space group from [1981Mel2]
* V, $Cu_6Mg_2Al_5$	$cP39$ $Pm\bar{3}$ Mg_2Zn_{11}	$a = 827$	[1949Sam] space group from [1991Eff]
* λ_2, $(Cu_{1-x}Al_x)_2Mg$ < 601.6	$hP24$ $P6_3/mmc$ $MgNi_2$	$a = 509.8$ to 510.2 $c = 1664$ to 1676	$0.492 \leq x \leq 0.576$ [1936Lav1] space group from [1936Lav1]
* λ_3, $(Cu_{1-x}Al_x)_2Mg$ < 537.8	$hP12$ $P6_3/mmc$ $MgZn_2$	$a = 507$ to 512 $c = 829$ to 839	$0.598 \leq x \leq 0.613$ [1936Lav1] space group from [1936Lav1]
* 5L, $(Cu,Al)_2Mg$	$hP30$	$a = 514$ $c = 2105$	stacking variation of Laves phases observed by electron diffraction [1962Kom]
* 6L, $(Cu,Al)_2Mg$	$hP36$ $P6m2$	$a = 510$ $c = 2500$ $a = 514$ $c = 2530$	stacking variation of Laves phases observed by electron diffraction [1977Kit] [1977Kom]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
* 9L, $(Cu,Al)_2Mg$	$hR18$	$a = 1297$ $\alpha = 22.50°$	[1962Kom], stacking variation of Laves phases observed by electron diffraction [1977Kom]
* 16L, $(Cu,Al)_2Mg$	$hP96$ $P6_3/mmc$	$a = 510$ $c = 6670$	stacking variation of Laves phases observed by electron diffraction [1977Kit]
		$a = 514$ $c = 6740$	[1977Kom]

Table 2a: Invariant Four-Phase Equilibria

Reaction	T (°C)	Type	Phase	Composition (at.%)		
				Al	Cu	Mg
$\gamma_0 + \varepsilon_1 \rightleftharpoons L + \gamma_1$	876.4	U_1	γ_0	34.2	65.8	0.0
			ε_1	36.8	62.8	0.4
			L	39.2	56.4	4.4
			γ_1	35.0	65.0	0.0
$\varepsilon_1 \rightleftharpoons L + \gamma_1 + \varepsilon_2$	827.6	E_1	ε_1	39.7	59.9	0.4
			L	43.4	52.4	4.2
			γ_1	36.1	63.9	0.0
			ε_2	42.0	58.0	0.0
$L \rightleftharpoons \gamma_0 + \gamma_1 + \lambda_1$	804.0	E_2	L	25.1	59.6	15.3
			γ_0	31.8	68.2	0.0
			γ_1	32.7	67.3	0.0
			λ_1	16.3	50.6	33.1
$L \rightleftharpoons \beta + \gamma_0 + \lambda_1$	800.3	E_3	L	21.8	62.8	15.4
			β	27.5	71.4	1.1
			γ_0	31.3	68.7	0.0
			λ_1	14.2	52.8	33.0
$L + \beta \rightleftharpoons (Cu) + \lambda_1$	782.8	U_2	L	12.9	70.2	16.9
			β	20.7	78.3	1.0
			(Cu)	17.8	81.1	1.1
			λ_1	8.6	58.7	32.7
$\gamma_0 + \lambda_1 \rightleftharpoons \beta + \gamma_1$	782.1	U_3	γ_0	31.2	68.8	0.0
			λ_1	14.0	53.0	33.0
			β	27.2	71.7	1.1
			γ_1	31.4	68.6	0.0
$L + \gamma_1 \rightleftharpoons \varepsilon_2 + \lambda_1$	739.9	U_4	L	38.7	48.4	12.9
			γ_1	36.3	63.7	0.0
			ε_2	42.5	57.5	0.0
			λ_1	23.4	43.4	33.2

Reaction	T (°C)	Type	Phase	Composition (at.%)		
				Al	Cu	Mg
$\varepsilon_2 + \gamma_1 \rightleftharpoons \delta, \lambda_1$	690.2	D_1	ε_2	42.8	57.2	0.0
			γ_1	36.3	63.7	0.0
			δ	40.0	60.0	0.0
			λ_1	23.4	43.3	33.2
$L + \varepsilon_2 + \lambda_1 \rightleftharpoons V$	683.9	P_1	L	46.5	41.0	12.5
			ε_2	44.2	56.8	0.0
			λ_1	27.1	39.8	33.1
			V	38.5	46.1	15.4
$\varepsilon_2 + \lambda_1 \rightleftharpoons \delta + V$	641.8	U_5	ε_2	43.6	56.4	0.0
			λ_1	25.0	41.8	33.2
			δ	40.0	60.0	0.0
			V	38.5	46.1	15.4
$L + \varepsilon_2 \rightleftharpoons \eta + V$	601.5	U_6	L	58.3	33.5	8.1
			ε_2	45.8	54.2	0.0
			η	49.0	51.0	0.0
			V	38.5	46.1	15.4
$\varepsilon_2 \rightleftharpoons \delta + \zeta, V$	582.7	D_2	ε_2	44.4	55.6	0.0
			δ	40.0	60.0	0.0
			ζ	45.0	55.0	0.0
			V	38.5	46.1	15.4
$\varepsilon_2 \rightleftharpoons \eta + \zeta, V$	579.3	D_3	ε_2	47.5	54.3	0.0
			η	48.9	51.1	0.0
			ζ	45.0	55.0	0.0
			V	38.5	46.1	15.4
$\beta \rightleftharpoons (Cu) + \gamma_1 + \lambda_1$	564.6	E_4	β	22.8	76.9	0.3
			(Cu)	20.4	79.3	0.3
			γ_1	29.6	10.4	0.0
			λ_1	10.2	56.7	33.1
$L + \lambda_1 \rightleftharpoons \lambda_2 + V$	562.0	U_7	L	60.0	26.6	13.4
			λ_1	32.9	34.1	32.9
			λ_2	36.6	30.9	32.5
			V	38.5	46.1	15.4
$L + \lambda_2 \rightleftharpoons S + V$	561.2	U_8	L	60.1	26.5	13.4
			λ_2	36.6	30.9	32.5
			S	50.0	25.0	25.0
			V	38.5	46.1	15.4
$L + \eta \rightleftharpoons \theta + V$	559.4	U_9	L	62.5	29.4	8.1
			η	49.6	50.4	0.0
			θ	67.0	33.0	0.0
			V	38.5	46.1	15.4
$L + V \rightleftharpoons \theta + S$	543.8	U_{10}	L	63.0	28.9	8.1
			θ	67.0	33.0	0.0
			S	50.0	25.0	25.0
			V	38.5	46.1	15.4

Reaction	T (°C)	Type	Phase	Composition (at.%)		
				Al	Cu	Mg
$L + \lambda_2 \rightleftharpoons \lambda_3 + S$	534.7	U_{11}	L	58.4	10.7	30.9
			λ_2	39.0	28.0	33.0
			λ_3	40.4	26.3	33.3
			S	50.0	25.0	25.0
$L + \lambda_3 \rightleftharpoons \lambda_2 + Q$	524.9	U_{12}	L	46.7	7.7	45.6
			λ_3	40.1	26.5	33.4
			λ_2	38.5	28.3	33.2
			Q	43.8	18.7	37.5
$L + \lambda_3 \rightleftharpoons Q + S$	513.2	U_{13}	L	58.6	8.2	33.2
			λ_3	41.0	25.6	33.3
			Q	43.8	18.7	37.5
			S	50.0	25.0	25.0
$L \rightleftharpoons \theta + (Al) + S$	502.1	E_5	L	73.9	15.5	10.6
			θ	67.8	32.2	0.0
			(Al)	95.7	1.7	2.6
			S	50.0	25.0	25.0
$L + \lambda_1 \rightleftharpoons \lambda_2 + (Mg)$	497.3	U_{14}	L	18.6	7.1	74.3
			λ_1	31.0	35.5	33.5
			λ_2	34.6	32.0	33.4
			(Mg)	3.8	0.0	96.2
$L \rightleftharpoons \lambda_1 + CuMg_2 + (Mg)$	481.2	E_6	L	1.1	16.6	82.3
			λ_1	19.2	47.1	33.7
			$CuMg_2$	0.0	33.3	66.7
			(Mg)	0.1	0.1	99.8
$L + Q \rightleftharpoons T + S$	479.0	U_{15}	L	64.1	5.5	30.4
			Q	43.8	18.7	37.5
			T	52.0	8.3	39.7
			S	50.0	25.0	25.0
$L + S \rightleftharpoons T + (Al)$	469.2	U_{16}	L	67.0	4.9	28.1
			S	50.0	25.0	25.0
			T	52.4	8.1	39.5
			(Al)	89.2	0.3	10.5
$L + \lambda_2 \rightleftharpoons Q + (Mg)$	454.6	U_{17}	L	26.3	4.1	69.6
			λ_2	37.2	29.4	33.4
			Q	43.8	18.7	37.5
			(Mg)	7.5	0.0	92.5
$L \rightleftharpoons T + Mg_2Al_3 + (Al)$	447.6	E_7	L	63.5	0.5	36.0
			T	55.4	4.1	40.5
			Mg_2Al_3	61.1	0.0	38.9
			(Al)	83.6	0.0	16.4
$L \rightleftharpoons T + Mg_2Al_3 + Mg_{17}Al_{12}$	447.6	E_8	L	57.4	0.3	42.3
			T	55.1	3.4	41.5
			Mg_2Al_3	61.1	0.0	38.9
			$Mg_{17}Al_{12}$	51.9	0.0	48.1

Reaction	T (°C)	Type	Phase	Composition (at.%)		
				Al	Cu	Mg
$L + Q \rightleftharpoons T + (Mg)$	426.8	U_{18}	L	31.1	1.7	67.2
			T	47.8	9.3	42.9
			Q	43.8	18.7	37.5
			(Mg)	11.0	0.0	89.0
$L \rightleftharpoons (Mg) + T + Mg_{17}Al_{12}$	424.7	E_9	L	31.6	1.8	66.6
			(Mg)	11.1	0.0	88.9
			T	47.9	9.2	42.9
			$Mg_{17}Al_{12}$	40.0	0.0	60.0
$Mg_2Al_3 + Mg_{17}Al_{12} \rightleftharpoons Mg_{23}Al_{30}$, T	409.8	D_4	Mg_3Al_2	61.1	0.0	38.9
			$Mg_{17}Al_{12}$	50.6	0.0	49.4
			$Mg_{23}Al_{30}$	56.6	0.0	43.4
			T	55.2	3.4	41.4
$Mg_{23}Al_{30} \rightleftharpoons Mg_2Al_3 + Mg_{17}Al_{12}$, T	250.1	D_5	$Mg_{23}Al_{30}$	56.6	0.0	43.4
			Mg_3Al_2	61.1	0.0	38.9
			$Mg_{17}Al_{12}$	46.4	0.0	53.6
			T	55.8	3.5	40.7

Table 2b: Invariant Maxima of Two- and Three-Phase Equilibria

Reaction	T (°C)	Type	Phase	Composition (at.%)		
				Al	Cu	Mg
$L \rightleftharpoons \lambda_1$	909.3	congruent	L	16.1	50.5	33.4
			λ_1	16.1	50.5	33.4
$L \rightleftharpoons \gamma_0 + \lambda_1$	804.4	e_3	L	24.2	60.4	15.4
			γ_0	31.6	68.4	0.0
			λ_1	15.8	51.1	33.1
$L \rightleftharpoons \gamma_1 + \lambda_1$	804.0	e_4	L	25.1	59.6	15.3
			γ_1	32.7	67.3	0.0
			λ_1	16.3	50.6	33.1
$L \rightleftharpoons \beta + \lambda_1$	800.4	e_5	L	20.9	63.5	15.6
			β	26.9	72.0	1.1
			λ_1	13.7	53.3	33.0
$L + \lambda_1 \rightleftharpoons \lambda_2$	601.6	p_8	L	51.5	16.4	32.1
			λ_1	33.9	32.9	33.2
			λ_2	37.0	29.9	33.1
$L \rightleftharpoons \lambda_1 + CuMg_2$	566.5	e_{10}	L	0.2	33.9	65.9
			λ_1	9.3	56.6	34.1
			$CuMg_2$	0.0	33.3	66.7
$L + \lambda_2 \rightleftharpoons S$	570.9	p_{10}	L	60.2	20.8	19.0
			λ_2	37.5	29.8	32.7
			S	50.0	25.0	25.0
$L + \lambda_2 \rightleftharpoons \lambda_3$	537.8	p_{11}	L	54.4	9.7	35.9
			λ_2	38.8	28.1	33.1
			λ_3	40.3	26.4	33.3

Reaction	T (°C)	Type	Phase	Composition (at.%)		
				Al	Cu	Mg
L ⇌ λ_1 + (Mg)	528.2	e_{13}	L	7.8	10.7	81.5
			λ_1	26.3	40.1	33.6
			(Mg)	1.1	0.0	98.9
L + λ_3 ⇌ Q	527.5	p_{12}	L	49.1	7.9	43.0
			λ_3	40.3	26.3	33.4
			Q	43.8	18.7	37.5
L ⇌ (Al) + S	505.5	e_{14}	L	73.5	12.6	13.9
			(Al)	95.2	1.1	3.7
			S	50.0	25.0	25.0
L + Q ⇌ T	495.4	p_{13}	L	53.5	4.8	41.7
			Q	43.8	18.7	37.5
			T	51.1	8.3	40.6
L ⇌ $Mg_{17}Al_{12}$ + T	457.2	e_{16}	L	48.0	0.9	51.1
			$Mg_{17}Al_{12}$	47.1	0.0	52.9
			T	52.4	5.4	42.2
L ⇌ Mg_2Al_3 + T	449.3	e_{19}	L	60.5	0.4	39.1
			Mg_2Al_3	61.1	0.0	38.9
			T	55.3	3.8	40.9

Table 3: Reported Data for the Invariant Reaction E_5, L ⇌ (Al) + S + θ

Temperature (°C)	Liquid composition (mass%)		References	Comment
	Cu	Mg		
500	26.8	6.2	[1937Nis1]	-
500	29.7	7.2	[1946Ura, 1949Ura2]	-
507	33	6.1	[1948Bro]	-
-	29	6.5	[1950Phr]	scaled from figure
506.5	33.1	6.8	[1952Han]	-
506	33	7	[1967Coo]	unidirect solidification
506	33.1	6.25	[1972Gar]	unidirect solidification
507	33	7.1	[1973Dav]	-
507	34	7.6	[1973Dav]	calculated
507	30	6	[1976Mon]	-
506±1	-	-	[1980Bir]	d.s.c
506.6	33.4	7.2	[1987Lac]	calculated
503	32	7.2	[1995Hua]	DTA
503±2	33.4	6.95	[1997Che]	calculated
503	30.4	8	[1998Buh]	calculated
502.1	30.4	8	[2003Jan]	calculated

Table 4: Reported Data for the Invariant Reaction E_7, $L \rightleftharpoons T + (Al) + Mg_2Al_3$

Temperature (°C)	Liquid Composition (mass%)		References
	Cu	Mg	
451	~0.0	35	[1919Vog]
447	3	32	[1937Nis1]
445	1.5	33	[1946Ura, 1949Ura2]
451	~2.7	~ 32	[1948Bro]
450	~ 3.5	~ 32	[1952Han]
-	4	31.5	[1950Phr]
~ 450	2.8	32	[1951Mir2]
443	3.4	34	[1987Lac]
448±5	1.34	34.2	[1997Che]
448	1.5	33.3	[1998Buh]
447.6	1.3	33.4	[2003Jan]

Table 5: Reported Data for the Invariant Reaction U_{16}, $L + S \rightleftharpoons T + (Al)$

Temperature (°C)	Liquid Composition (mass%)		References	Comment
	Cu	Mg		
471	10	27	[1919Vog]	-
465	11	25	[1937Nis1]	-
465	10	25.6	[1946Ura]	-
462	10	25.6	[1949Ura2]	-
467	10	26	[1948Bro]	-
465	9.3	26.5	[1951Mir2]	-
472.3	11.3	25.7	[1952Han]	scaled from figure
467	10	26	[1976Mon]	-
468	11.4	25.5	[1987Lac]	assessment
467±4	10.7	26.1	[1997Che]	calculated
469	11.1	24.6	[1998Buh]	calculated
469.2	11.2	24.4	[2003Jan]	calculated

Table 6: Reported Data for the Mg-Rich Invariant Reactions E_9, U_{17} and U_{18}

Temperature (°C)	Liquid Composition (mass%)		References	Invariant Reaction
	Cu	Mg		
412	17	56.5	[1933Bas, 1934Por]	$L \rightleftharpoons (Mg) + Al_{11}Mg_{17} + \lambda$
419-420	6	62.2	[1940Han]	$L \rightleftharpoons (Mg) + Al_{11}Mg_{17} + \lambda$
423	4.6	67	[1949Ura2]	$L \rightleftharpoons (Mg) + Al_{11}Mg_{17} + \lambda$
425	6	63	[1951Mir2]	$L \rightleftharpoons (Mg) + Al_{12}Mg_{17} + Q$
423.6	5.4	62.6	[1997Che]	$L \rightleftharpoons (Mg) + Al_{12}Mg_{17} + Q$
426	4.4	63.2	[1998Buh]	$L \rightleftharpoons (Mg) + Al_{12}Mg_{17} + Q$
424.9	4.3	63.3	[2003Jan]	$L \rightleftharpoons (Mg) + Al_{12}Mg_{17} + Q$
452.0	11.3	62.7	[1997Che]	$L + \lambda_2 \rightleftharpoons (Mg) + Q$
456.6	9.9	63.7	[2003Jan]	$L + \lambda_2 \rightleftharpoons (Mg) + Q$
444.0	6.0	52.9	[1997Che]	$L + T \rightleftharpoons Al_{12}Mg_{17} + Q$
428	4.4	62.3	[1998Buh]	$L + T \rightleftharpoons Al_{12}Mg_{17} + Q$
426.8	4.4	62.6	[2003Jan]	$L + T \rightleftharpoons Al_{12}Mg_{17} + Q$

Table 7: Lattice Parameter, a, of the (Al) Phase [1951Poo] at 25°C

Analysed Composition (at.%)		Observed a (pm)	Intended Composition (at.%)		Corrected a (pm)
Mg	Cu		Mg	Cu	
0.189	0.367	404.8	0.25	0.375	404.81
0.456	0.247	404.97	0.5	0.25	404.99
0.655	0.119	405.1	0.75	0.125	405.14
0.202	0.88	404.58	0.25	0.875	404.6
0.414	0.75	404.72	0.5	0.75	404.76
0.637	0.628	404.9	0.75	0.625	404.95
0.927	0.5	405.07	1	0.5	405.1
1.247	0.362	405.24	1.25	0.375	405.24
1.311	0.246	405.32	1.5	0.25	405.4
1.608	0.127	405.5	1.75	0.125	405.56
0.356	0.302	404.91	0.375	0.313	404.91
0.578	0.179	405.05	0.625	0.188	405.07
1.058	0.422	405.12	1.125	0.438	405.14
0.57	0.659	404.77	0.625	0.688	404.78
0.804	0.521	404.9	0.875	0.563	404.91

Fig. 1: Al-Cu-Mg.
Phases detected along
the 33.3 at.% Mg
section

$Cu_2Mg = \lambda_1$ $MgNi_2 = \lambda_2$ $MgZn_2 = \lambda_3$

stacking variants

| $MgNi_2$ | $MgZn_2$ | [1977Kom] |

$MgNi_2+MgZn_2$ [1962Kom] slowly cooled from melt

Cu_2Mg $MgNi_2$ $MgZn_2$ [1981Mel2]

Cu_2Mg $MgNi_2$ [1965Sli]

Cu_2Mg $MgNi_2$ $MgZn_2$ [1953Kle]

Cu_2Mg Cu_2Mg+ [1949Ura1]
$MgZn_2$

Cu_2Mg [1943Gue] annealed close to solidus

Cu_2Mg $MgNi_2$ $MgZn_2$ [1936Lav1]

Cu_2Mg Cu_2Mg+ $MgNi_2$ $MgZn_2$ [1936Lav1] as-cast
primary $MgNi_2$prim. primary primary

Cu_2Mg $MgZn_2$ [1934Lav]

↑AlCuMg

| 20 | 40 | 60 |

Al, at.%

0.0 **Al**   66.7 **Al**
33.3 **Mg**   33.3 **Mg**
66.7 **Cu**   0.0 **Cu**

Fig. 2: Al-Cu-Mg.
Liquidus univariant
lines and primary
phases

Al

Data / Grid: at.%

Axes: at.%

Mg   **Cu**
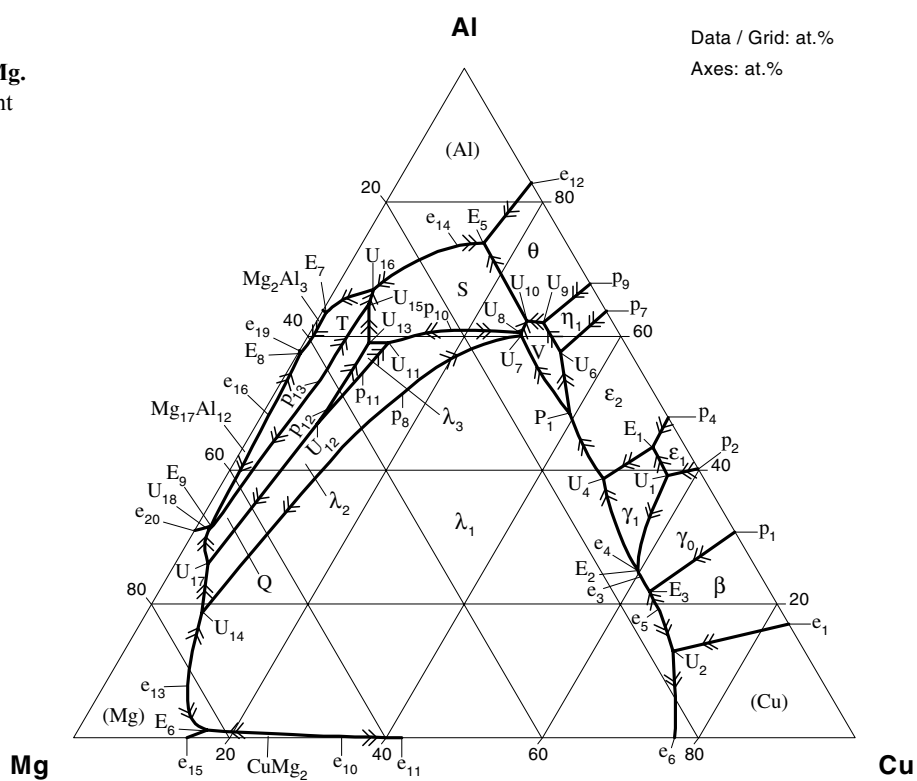
Fig. 2a: Al-Cu-Mg.
Enlarged part of the
liquidus projetion
shown in Fig. 2

Mg 20.00
Cu 0.00
Al 80.00

Data / Grid: at.%
Axes: at.%

Mg 80.00
Cu 0.00
Al 20.00

Mg 20.00
Cu 60.00
Al 20.00
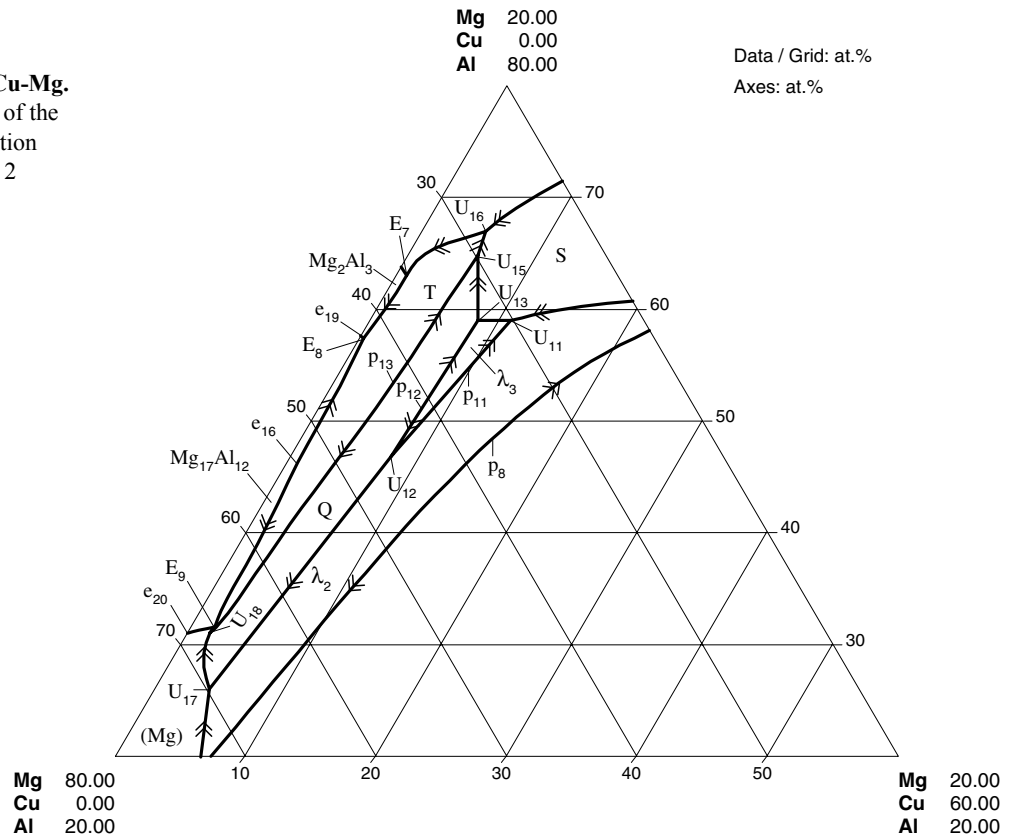
Fig. 2b: Al-Cu-Mg.
Liquidus projection
with liquidus
isotherms

Data / Grid: at.%
Axes: at.%

| Al-Cu | Al-Mg | Al-Cu-Mg | Cu-Mg |

Al-Cu

1036.1	e₁	l ⇌ (Cu) + β
1020	p₁	l + β ⇌ γ₀
959	p₂	l + γ₀ ⇌ ε₁
880.7	p₃	γ₀ + ε₁ ⇌ γ₁
850.9	p₄	l + ε₁ ⇌ ε₂
837	e₂	ε₁ ⇌ γ₁ + ε₂
781.3	p₅	β + γ₀ ⇌ γ₁
690.2	p₆	γ₁ + ε₂ ⇌ δ

Al-Cu-Mg

- 876.4 | U_1 | $\gamma_0 + \varepsilon_1 \rightleftharpoons \gamma_1 + L$
- $\gamma_1 + \gamma_0 + L$
- 804.4 | e_3 | $L \rightleftharpoons \gamma_0 + \lambda_1$
- 804 | E_2 | $L \rightleftharpoons \gamma_0 + \gamma_1 + \lambda_1$
- 827.6 | E_1 | $\varepsilon_1 \rightleftharpoons \gamma_1 + \varepsilon_2 + L$
- 804.0 | e_4 | $L \rightleftharpoons \gamma_1 + \lambda_1$
- 800.4 | e_5 | $L \rightleftharpoons \beta + \lambda_1$
- 800.3 | E_3 | $L \rightleftharpoons \beta + \gamma_0 + \lambda_1$
- 782.1 | U_3 | $\gamma_0 + \lambda_1 \rightleftharpoons \beta + \gamma_1$
- 782.8 | U_2 | $L + \beta \rightleftharpoons (Cu) + \lambda_1$
- 739.9 | U_4 | $L + \gamma_1 \rightleftharpoons \varepsilon_2 + \lambda_1$
- 690.2 | D_1 | $\varepsilon_2 + \gamma_1 \rightleftharpoons \delta, \lambda_1$

Reaction labels: $\varepsilon_1 + \gamma_1 + L$; $\gamma_1 + \varepsilon_2 + L$; $\gamma_0 + \gamma_1 + \lambda_1$; $\beta + \gamma_1 + (Cu)$; $\varepsilon_2 + \lambda_1 + \gamma_1$; $\varepsilon_2 + \lambda_1 + L$ | P_1; $\beta + \gamma_1 + \lambda_1$; $\beta + \gamma_0 + \lambda_1$; $\varepsilon_2 + \delta + \lambda_1$ | U_5; $\gamma_1 + \delta + \lambda_1$; E_4 E_4

Cu-Mg

| 725 | e₆ | l ⇌ (Cu) + λ₁ |

Fig. 3a: Al-Cu-Mg. Reaction scheme, part 1.

Al-Cu | **Al-Mg** | **Al-Cu-Mg** | **Cu-Mg**

Cu-Mg:

552 e_{11} — $l \rightleftharpoons \lambda_1 + CuMg_2$

Al-Cu-Mg:

683.9 P_1 — $\varepsilon_2 + \lambda_1 + V$, $L + \varepsilon_2 + \lambda_1 \rightleftharpoons V$, U_4

$L + \lambda_1 + V$

$L + \varepsilon_2 + V$

601.5 U_6 — $L + \varepsilon_2 \rightleftharpoons \eta + V$

588 d(max) — $\varepsilon_2 \rightleftharpoons \zeta, V$

$V + \eta + \varepsilon_2$

U_3 U_2

566.5 e_{10} — $L \rightleftharpoons \lambda_1 + CuMg_2$

564.6 E_4 — $\beta \rightleftharpoons (Cu) + \gamma_1 + \lambda_1$, $(Cu) + \gamma_1 + \lambda_1$

559.4 U_9 — $L + \eta \rightleftharpoons \theta + V$, $V + \eta + \theta$, $L + V + \theta$

543.8 U_{10} — $L + V \rightleftharpoons \theta + S$, $V + S + \theta$, $V + S \rightleftharpoons$

534.7 U_{11} — $L + \lambda_2 \rightleftharpoons \lambda_3 + S$, $L + \theta + S$, $L + S + \lambda_3$, U_{13}, $S + \lambda_2 + \lambda_3$

641.8 D_1 U_5 — $\varepsilon_2 + \lambda_1 \rightleftharpoons \delta + V$, $\lambda_1 + \delta + V$, $\varepsilon_2 + \delta + V$

601.6 p_8 — $L + \lambda_1 \rightleftharpoons \lambda_2$

582.7 D_2 — $\varepsilon_2 \rightleftharpoons \delta + \zeta, V$, $\zeta + \delta + V$

579.3 D_3 — $\varepsilon_2 \rightleftharpoons \eta + \zeta, V$, $\zeta + \eta + V$

570.9 p_{10} — $L + \lambda_2 \rightleftharpoons S$

U_7 — $L + \lambda_1 \rightleftharpoons \lambda_2 + V$, $V + \lambda_1 + \lambda_2$, $L + \lambda_2 + V$

562 U_8 — $L + \lambda_2 \rightleftharpoons S + V$, $L + V + S$

561.2 — $V + S + \lambda_2$

537.8 p_{11} — $L + \lambda_2 \rightleftharpoons \lambda_3$

E_5 E_6 U_{12} U_{14}

Al-Cu:

624.9 p_7 — $l + \varepsilon_2 \rightleftharpoons \eta$

595.8 p_9 — $l + \eta \rightleftharpoons \theta$

582.7 e_7 — $\varepsilon_2 \rightleftharpoons \delta + \zeta$

579.3 e_8 — $\varepsilon_2 \rightleftharpoons \eta + \zeta$

566.9 e_9 — $\beta \rightleftharpoons (Cu) + \gamma_1$

547.6 e_{12} — $l \rightleftharpoons (Al) + \theta$

Fig. 3b: **Al-Cu-Mg.** Reaction scheme, part 2

| Cu-Mg | Al-Cu-Mg | Al-Mg | Al-Cu |

Cu-Mg:

485 | e_{15} | $l \rightleftharpoons CuMg_2 + (Mg)$

Al-Cu-Mg:

528.2 | e_{13} | $L \rightleftharpoons \lambda_1 + (Mg)$ — p_{11}

527.5 | p_{12} | $L + \lambda_3 \rightleftharpoons Q$

524.9 | U_{12} | $L + \lambda_3 \rightleftharpoons \lambda_2 + Q$ — $\underline{\lambda_2 + \lambda_3 + Q}$ — U_{11}

513.2 | U_{13} | $L + \lambda_3 \rightleftharpoons Q + S$ — $\underline{\lambda_3 + Q + S}$ — e_{12}

505.5 | e_{14} | $L \rightleftharpoons (Al) + S$

502.1 | E_5 | $L \rightleftharpoons \theta + (Al) + S$ — $\underline{(Al) + S + \theta}$ — U_{10}

497.3 | U_{14} | $L + \lambda_1 \rightleftharpoons \lambda_2 + (Mg)$ — $\underline{(Mg) + \lambda_1 + \lambda_2}$ — p_8

$L + \lambda_2 + (Mg)$ — e_{10}

495.4 | p_{13} | $L + Q \rightleftharpoons T$

481.2 | E_6 | $L \rightleftharpoons \lambda_1 + CuMg_2 + (Mg)$ — $\underline{(Mg) + CuMg_2 + \lambda_1}$

479 | U_{15} | $L + Q \rightleftharpoons T + S$ — $\underline{Q + S + T}$ — $L + T + S$

$L + Q + S$

469.2 | U_{16} | $L + S \rightleftharpoons T + (Al)$ — $\underline{(Al) + S + T}$ — $L+T+(Al)$

457.2 | e_{16} | $L \rightleftharpoons Mg_{17}Al_{12} + T$

454.6 | U_{17} | $L + \lambda_2 \rightleftharpoons Q + (Mg)$ — $L + \lambda_2 + Q$

$\underline{(Mg) + Q + \lambda_1}$ — $L + Q + (Mg)$

449.3 | e_{19} | $L \rightleftharpoons Mg_2Al_3 + T$

447.6 | E_8 | $L \rightleftharpoons T + Mg_2Al_3 + Mg_{17}Al_{12}$ — $\underline{Mg_{17}Al_{12} + T + Mg_2Al_3}$ — D_4

447.6 | E_7 | $L \rightleftharpoons T + Mg_2Al_3 + (Al)$ — $\underline{(Al) + T + Mg_2Al_3}$ — U_{18}

E_9

Al-Mg:

450.5 | e_{17} | $l \rightleftharpoons (Al) + Mg_2Al_3$

449.5 | e_{18} | $l \rightleftharpoons Mg_2Al_3 + Mg_{17}Al_{12}$

U_{18}

Fig. 3c: **Al-Cu-Mg.** Reaction scheme, part 3

Al-Cu **Al-Mg** **Al-Cu-Mg** **Cu-Mg**

E_8 e_{16} p_{13} U_{17}

436 | e_{20}
$l \rightleftharpoons (Mg)+Mg_{17}Al_{12}$

424.7 | $L \rightleftharpoons (Mg)+T+Mg_{17}Al_{12}$ | E_9
$(Mg)+T+Mg_{17}Al_{12}$

426.8 | $L+T+(Mg)$
$L+Q \rightleftharpoons T+(Mg)$ | U_{18}
$T+Q+(Mg)$

410 | p_{14}
$Mg_2Al_3+Mg_{17}Al_{12} \rightleftharpoons Mg_{23}Al_{30}$

409.8 | $Mg_2Al_3+Mg_{17}Al_{12} \rightleftharpoons Mg_{23}Al_{30}$, T | D_4
$T+Mg_{17}Al_{12}+Mg_{23}Al_{30}$
$Mg_{23}Al_{30}+Mg_2Al_3+T$

250 | e_{21}
$Mg_{23}Al_{30} \rightleftharpoons Mg_2Al_3+Mg_{17}Al_{12}$

250.1 | $Mg_{23}Al_{30} \rightleftharpoons Mg_2Al_3+Mg_{17}Al_{12}$; T | D_5
$T + Mg_{17}Al_{12} + Mg_2Al_3$

Fig. 3d: Al-Cu-Mg. Reaction scheme, part 4

Fig. 4: **Al-Cu-Mg.**
Calculated isothermal
section at 400°C

Data / Grid: at.%

Axes: at.%
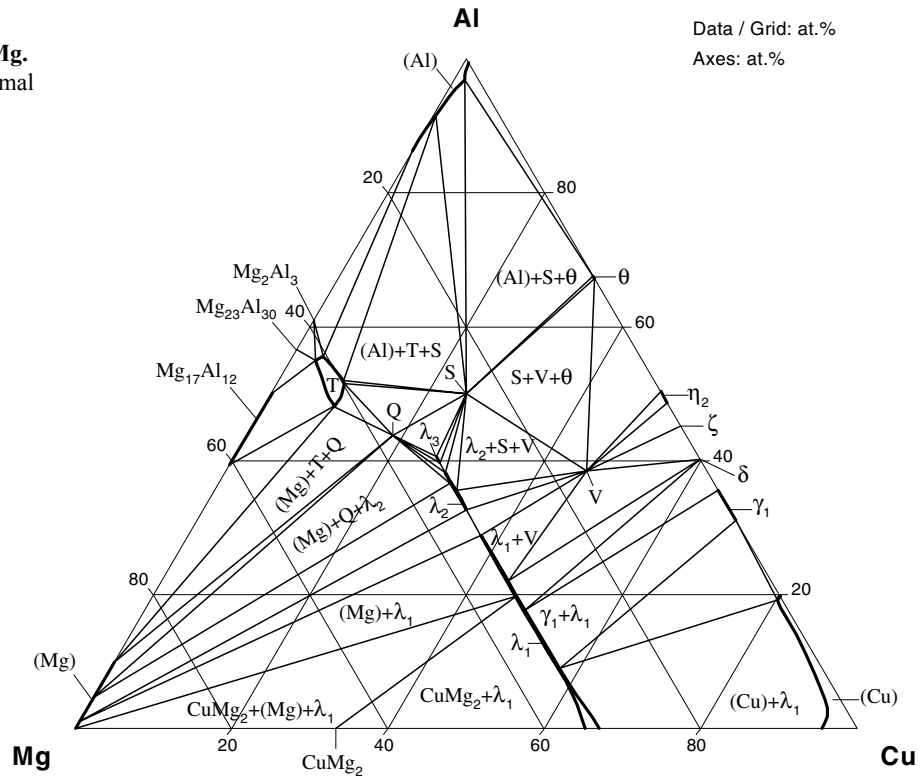
Fig. 5: **Al-Cu-Mg.**
Isothermal sections in
the Al-rich corner at
460 and 375°C

Data / Grid: at.%

Axes: at.%

Mg	20.00
Cu	0.00
Al	80.00

Mg	0.00
Cu	20.00
Al	80.00

Al

Data / Grid: at.%

Axes: at.%
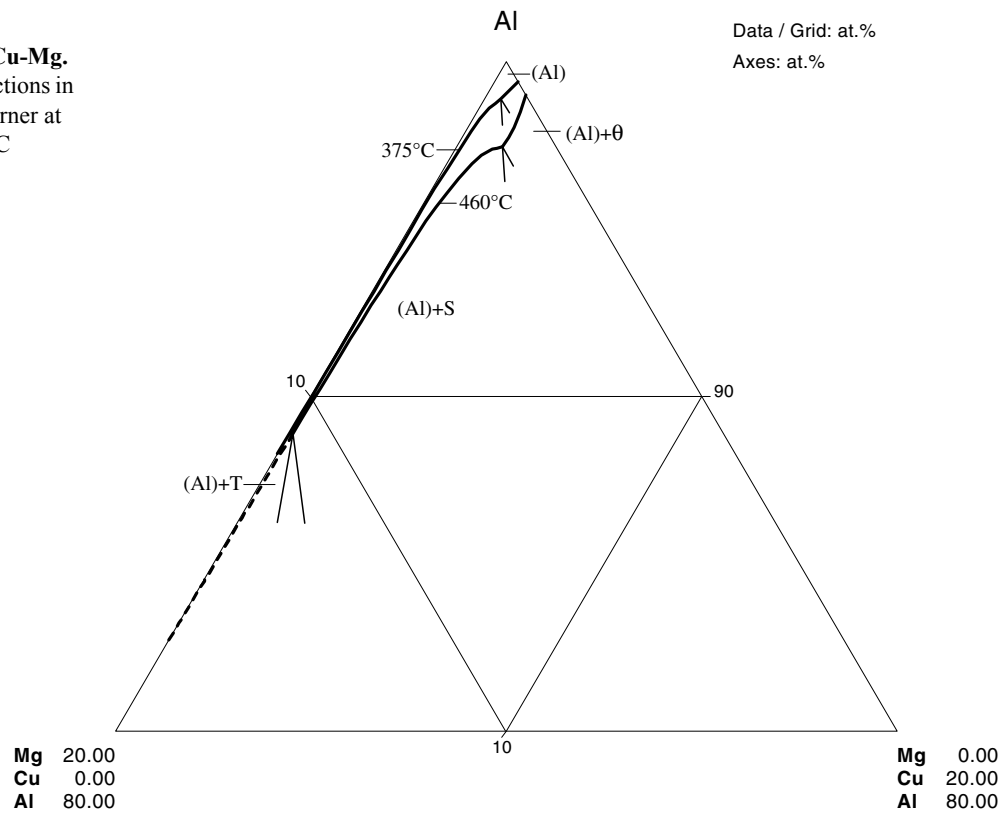
Fig. 6: Al-Cu-Mg.
Isotherms of the
(Al)-solvus and
phases in equilibrium
with (Al)

300
325
350
375

400

425

450

Q

475

525

S

500

T

Mg 5.00	**Mg** 0.00
Cu 0.00	**Cu** 5.00
Al 95.00	**Al** 95.00

Mg 0.00
Cu 80.00
Al 20.00

Data / Grid: at.%

Axes: at.%
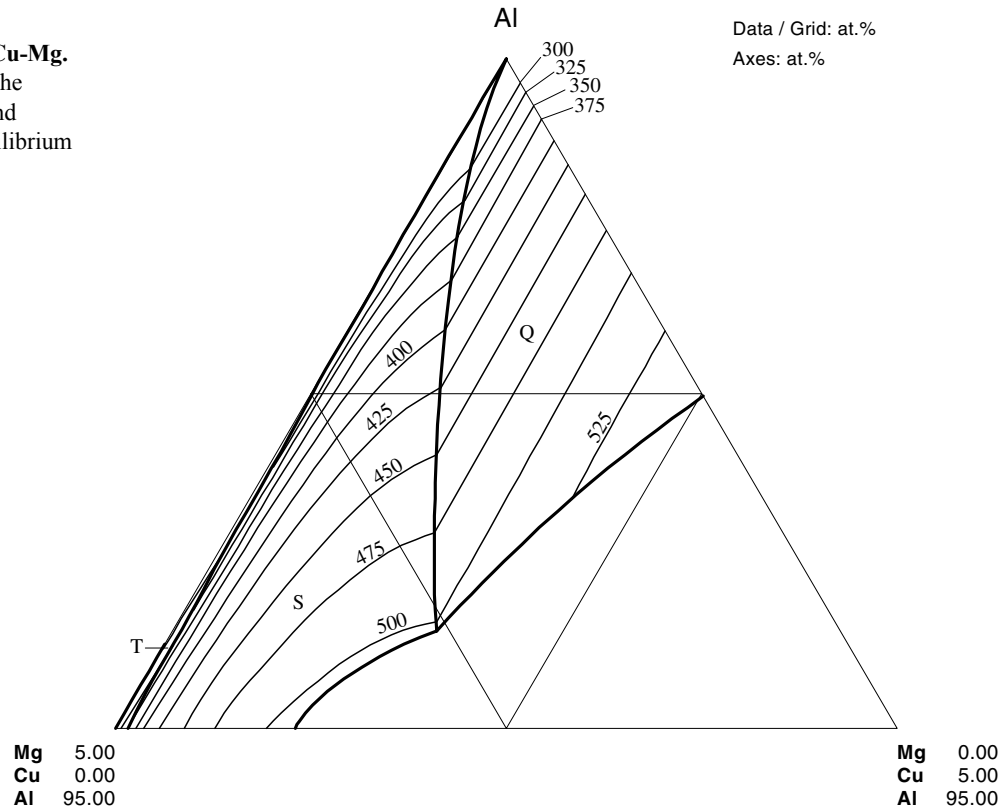
Fig. 7: Al-Cu-Mg.
Solubility of Al and
Mg in (Cu)

10

10

700

(Cu)

400

25

90

Mg 20.00
Cu 80.00
Al 0.00

Cu

62
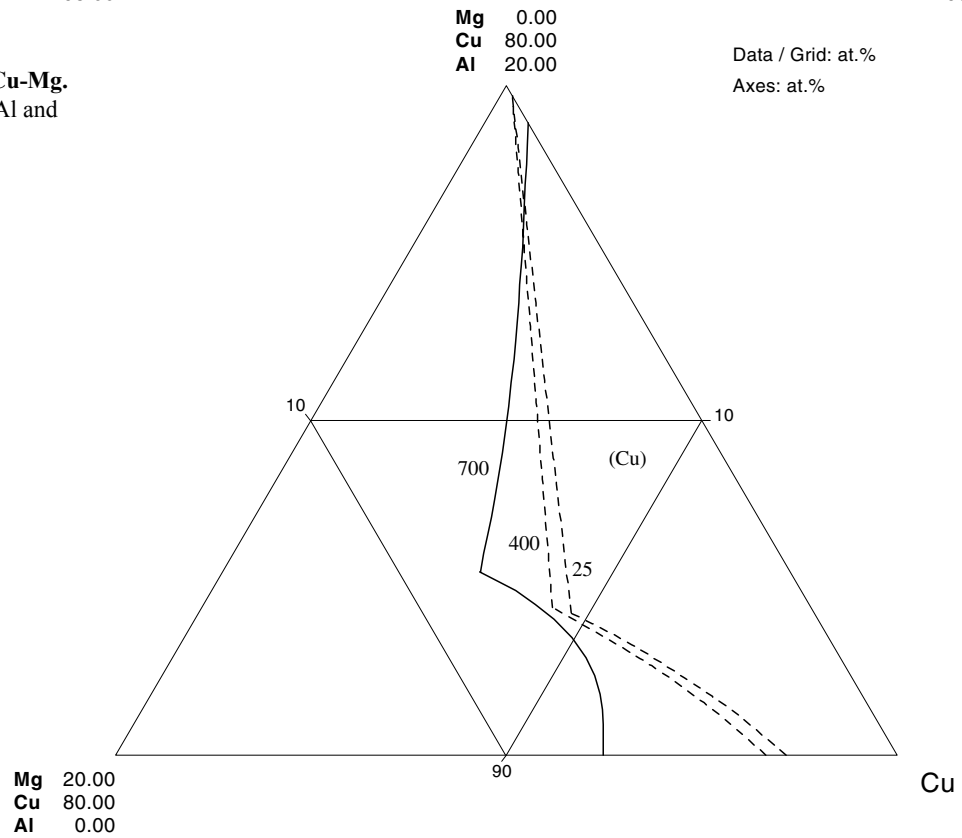
Fig. 8: Al-Cu-Mg.
Isopleth at 33.33 at.%
Mg showing the λ_1
congruent melting
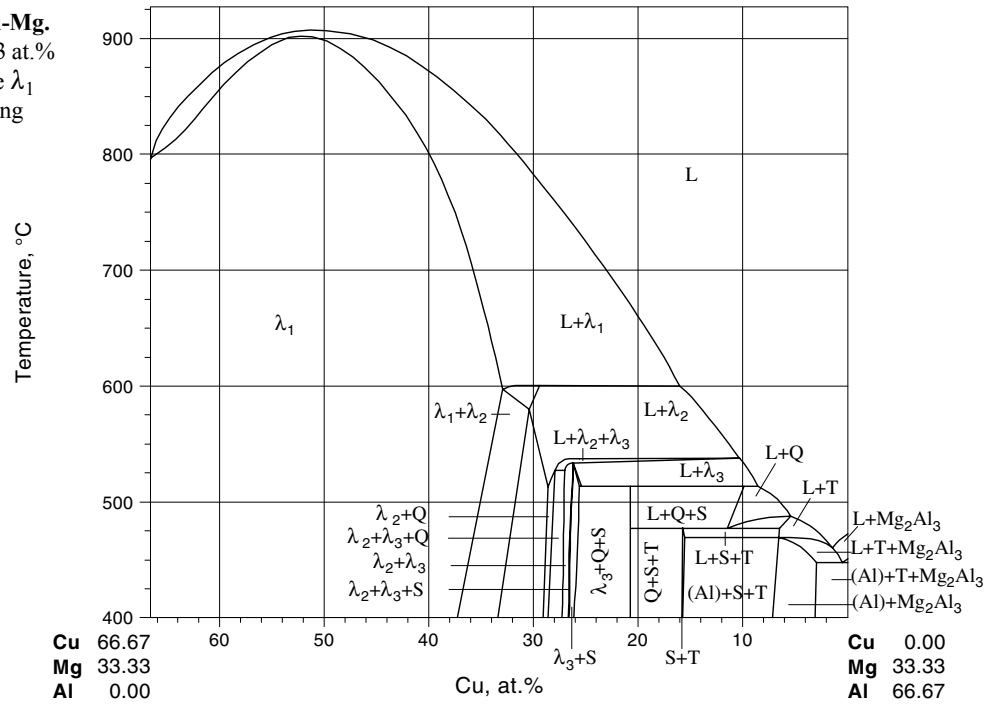
Fig. 9a: Al-Cu-Mg.
Isopleth at 60 mass%
Al
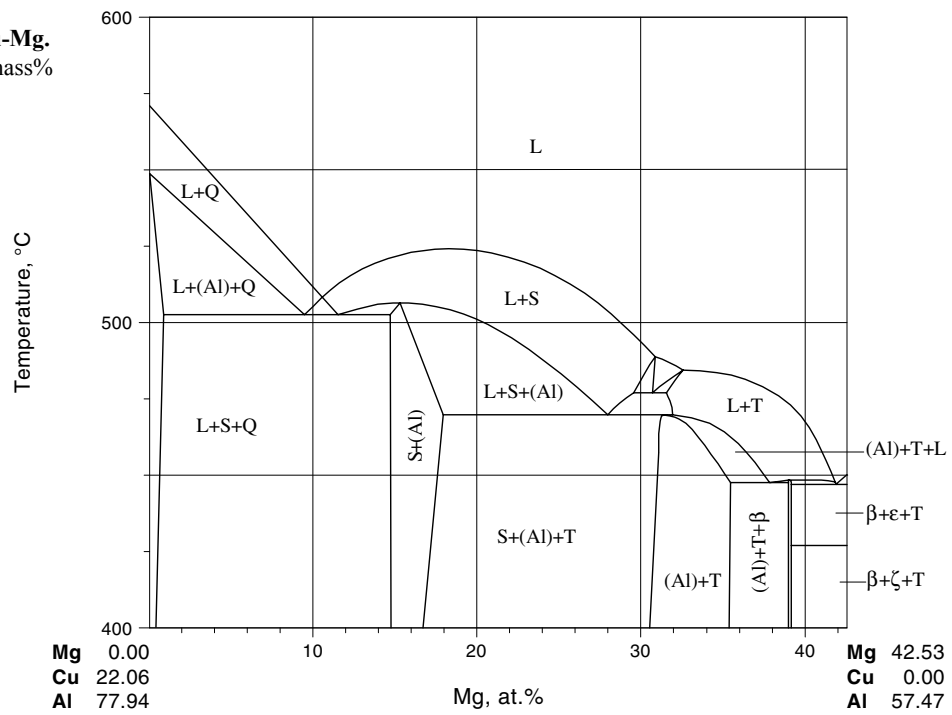
Fig. 9b: Al-Cu-Mg.
Isopleth at 70 mass% Al
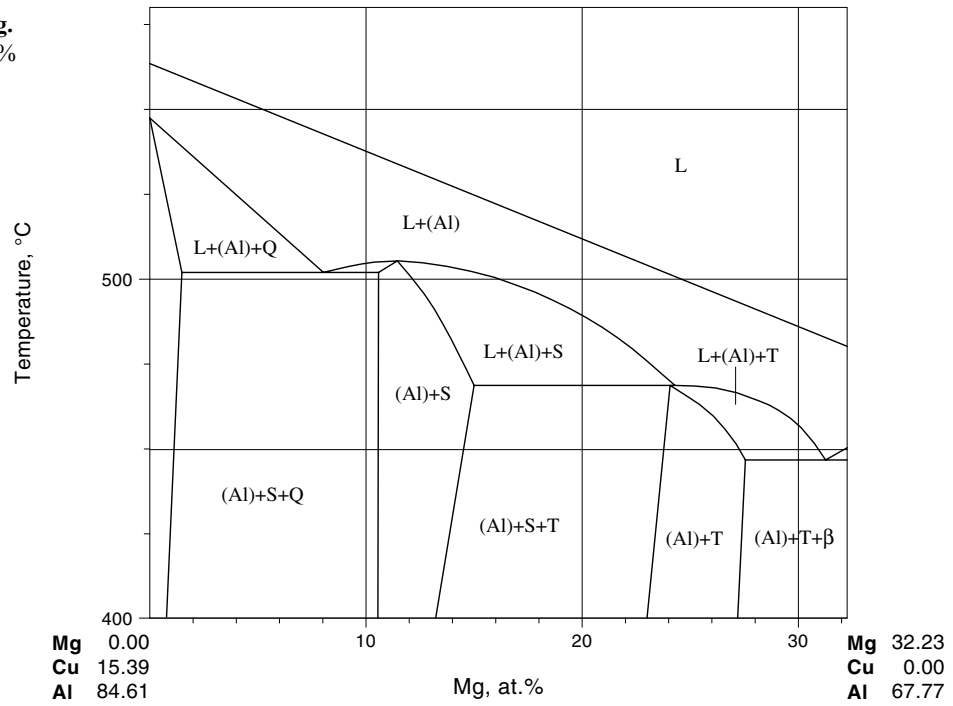
Fig. 9c: Al-Cu-Mg.
Isopleth at 95.5 mass% Al
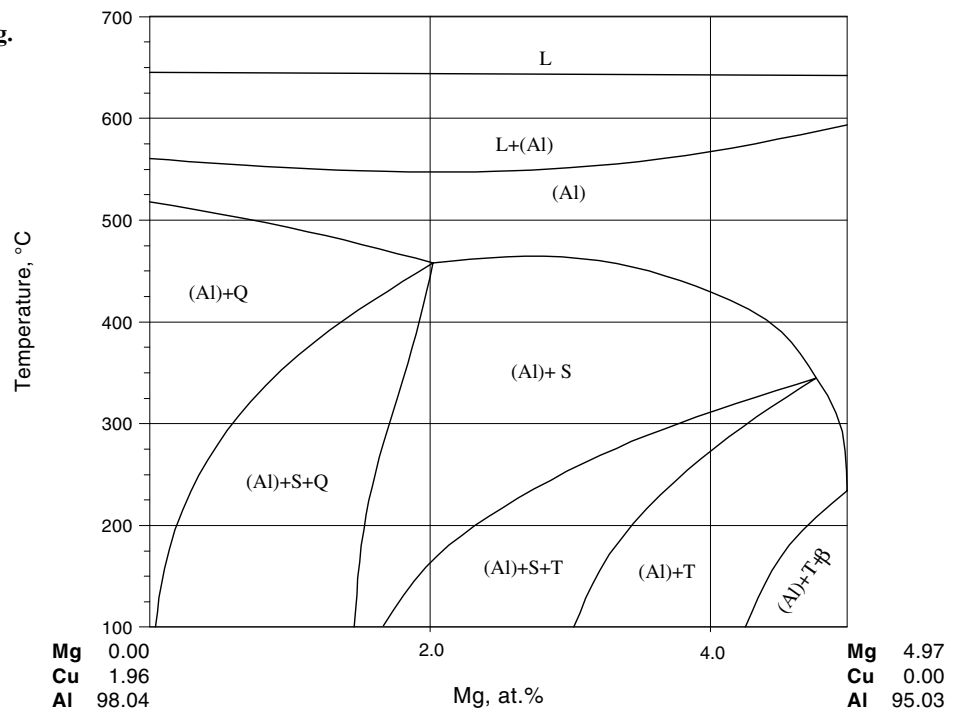
Fig. 10a: Al-Cu-Mg.
Isopleth at 37 at.% Al
showing the λ_2 phase
formation
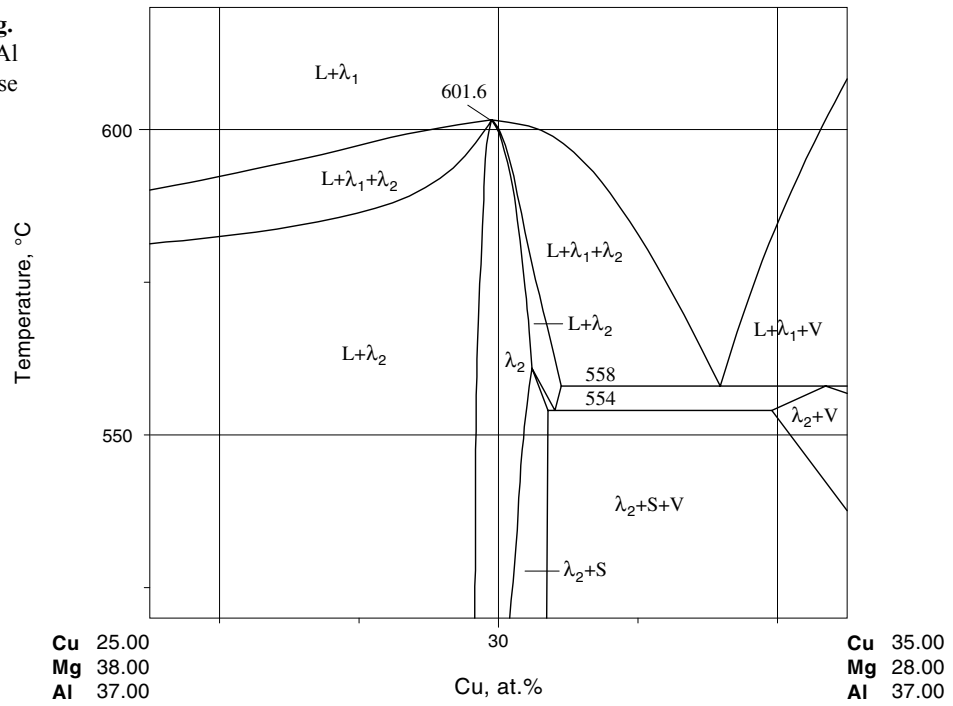
Fig. 10b: Al-Cu-Mg.
Isopleth at 43.75 at.%
Al showing the Q
phase formation
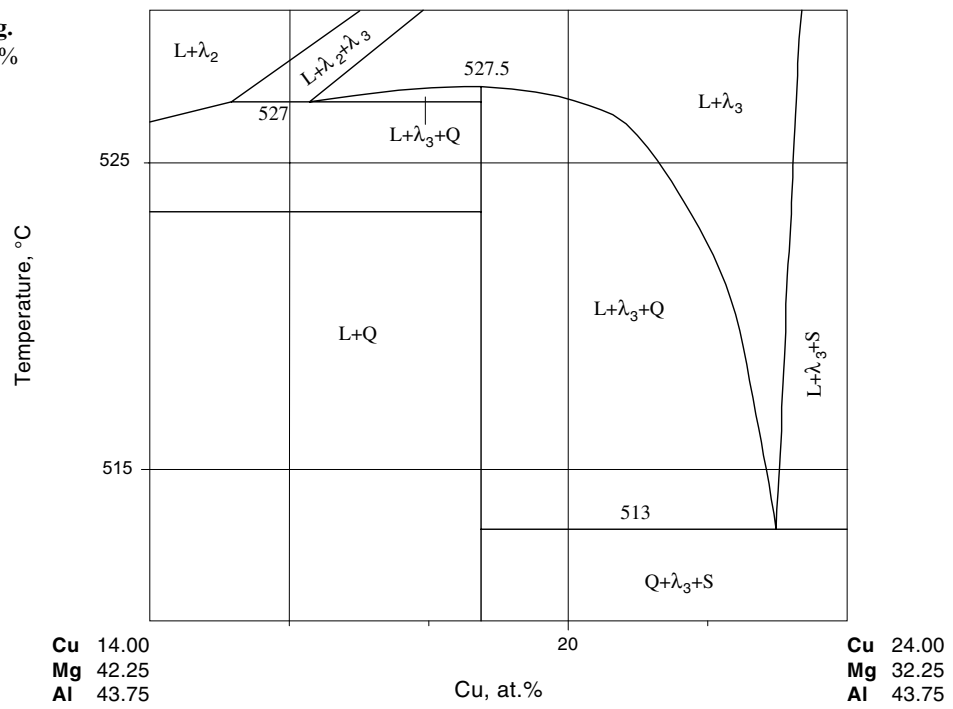
Aluminium – Iron – Nickel

Peter Budberg and Alan Prince,
updated by
Gabriele Cacciamani, Riccardo Ferro, Benjamin Grushko, Pierre Perrot, Rainer Schmid-Fetzer

Introduction

The first extensive investigation of the Al-Fe-Ni ternary system was the determination of the liquidus surface at <50 mass% Al ($\leqslant$75 at.% Al). Since, a critical assessment of the system may be found in [1980Riv] with minor amendments by [1988Ray] and an update by [1992Bud]. [1994Rag] presented isothermal sections at 950 and 1050°C in the Al-rich part of the diagram (> 50 at.% Al), an isothermal section at 1050°C in the Fe-rich part of the diagram (> 50 at.% Fe) and a vertical section along the Ni_3Al-Ni_3Fe join. The first calculations of the whole diagram by the Calphad method has been carried out by [1974Kau] at 1200, 1400, 1600 and 1700 K. The phase diagram calculated at 1200 K looks strongly like the diagram proposed by [1940Bra1] which represents the structures obtained by a slow cooling method. Microstructural observations of [1995Guh] after water quenching $Fe_{30}Ni_{20}Al_{50}$ alloys following annealing at 420, 620 and 820°C does not contradict phase equilibria proposed by [1980Riv]. Experimental work of [1993Pov, 1994Gho, 1994Jia, 1999Dyb, 2000Dyb, 2002Bit] on phase equilibria together with the apparition of quasicrystalline decagonal phases [1989Tsa, 1994Lem, 1996Yam, 1997Sai, 2002Hir, 2003Doe] adds to our knowledge of this ternary system and necessitates an updating of the earlier assessments by [1980Riv] and [1992Bud]. More recent experimental work are summarized in Table 1. This ternary system exhibits a continuous series of solid solutions between β,NiAl and β,FeAl (B2 structure, type CsCl). This fact allows the system to be split into two: the Al-rich portion from 50 to 100 at.% Al and the Fe-Ni rich region from 0 to 50 at.% Al. The solidus temperatures in the β (50 at.% Al) solid solution has been experimentally determined by [2002Bit].

The Al-rich region has been studied by [1934Fus, 1938Bra, 1940Bra1, 1942Phi, 1943Sch, 1947Ray, 1981Kha, 1982Kha, 1986Sei, 1993Pov, 2000Dyb]. Reviews have been published by [1943Mon, 1952Han, 1961Phi, 1976Mon, 1992Bud, 1994Rag].

The data on the possible constitution of liquidus surfaces in the Al-Fe_3Al-Ni_3Al field are given in [1934Fus, 2000Dyb]. According to [1938Bra], however, two ternary phases are formed in the composition field mentioned above: τ_1(FeNiAl$_9$) and τ_2(Fe$_3$NiAl$_{10}$). These data were confirmed by [1940Bra1]. The conditions of the τ_1 formation were established by [1943Sch, 2000Dyb]; it crystallizes by a peritectic reaction (P):

L + Fe$_4$Al$_{13}$ + NiAl$_3$ $\rightleftharpoons$ τ_1 at 809°C.

This temperature was confirmed by [1981Kha, 1982Kha, 1986Sei, 2000Dyb].

The data on the presence of two invariant transformations in the Al-rich alloys

(E$_2$): L $\rightleftharpoons$ (Al) + τ_1 + NiAl$_3$ and
(U$_2$): L + Fe$_4$Al$_{13}$ $\rightleftharpoons$ (Al) + τ_1
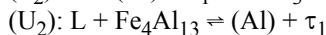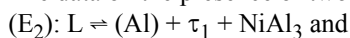
previously obtained by [1942Phi] were also confirmed. These reactions take place at 640 and 650.2°C, respectively [1943Sch] or at 638 [1942Phi, 1981Kha, 1982Kha, 1986Sei, 2000Dyb] and 649°C [1942Phi], respectively.

The phase field boundaries in the Al-rich portion of the diagram at 620°C were constructed by [1943Sch] and isothermal sections at 500 and 550°C by [1947Ray]. These data are in good agreement with each other. [1938Bra, 1940Bra1] cooled homogenized and afterwards powdered alloys, which were then held at different temperatures with 10 K·min^{-1} in vacuum. The authors suggest that the section obtained probably represents a 500°C isothermal.

The phase τ_1(FeNiAl$_9$) has a homogeneity range from 4.42 to 11.11 at.% Fe and from 7.01 to 13.5 at.% Ni at 620°C [1943Sch]. By precipitation from liquid Al-rich alloys, [1996Zho] obtains a τ_1 phase whose chemical composition lies in the range Fe$_x$Ni$_{2-x}$Al$_9$ ($1 \leq x \leq 1.6$). The τ_1 phase is also easily observed by reacting Fe-Ni alloys with liquid Al at 700°C [1999Dyb].

In the reviews [1952Han, 1961Phi] the previously obtained data were generalized though [1961Phi] virtually followed [1942Phi]. According to [1976Mon], the reactions P, E_2 and U_2 occur at 809, 639 and 649°C, respectively. The solubility of Ni in Fe_3Al is 1.4 to 1.9 at.% and that of Fe in Ni_3Al, up to 0.5 at.%. The $FeNiAl_9$ compound (τ_1) has been given a homogeneity range from 3.0 at.% Fe and 17 at.% Ni to 7.5 at.% Fe and 11.5 at.% Ni by [1976Mon].

Using precise investigation techniques, in particular electro-magnetic separation of phases in the liquid-solid state after annealing at 1050, 950 and 750°C for 3 h, [1981Kha, 1982Kha] established the position of tie lines between the equilibrium phases. Isothermal sections at 750, 950 and 1050°C were constructed after prolonged exposures for 40, 15 and 3 d, respectively. These heat treatments allowed establishment of the formation of a new ternary phase, $FeNi_3Al_{10}$, besides two previously known (τ_1 and τ_2). This phase, according to [1981Kha, 1982Kha], exists in a narrow temperature range and decomposes at slow cooling so that it has not been found by [1938Bra, 1940Bra1, 1947Ray] and others. The solubility, at room temperature, of Fe in Ni_2Al_3 and $NiAl_3$ is 2 and 4 at.%, respectively and that of Ni in $FeAl_2$, Fe_2Al_5 and Fe_4Al_{13} at 1050°C is up to 2, 2 and 10 at.%, respectively [1982Kha].

Between 1050 and 950°C an invariant reaction $L + \tau_2 \rightleftharpoons Fe_4Al_{13} + Ni_2Al_3$ takes place [1981Kha, 1982Kha]. The formation of ternary $FeNiAl_5$ was found in a powder sample (composition $Fe_{14.3}Ni_{14.3}Al_{71.4}$) annealed at 720°C for 3 h and water quenched; it has a hexagonal structure of the Co_2Al_5 type [1990Ell]. It is known that τ_2 is also isotypic to Co_2Al_5. According to [1990Ell], the position of homogeneity fields corresponding to ternary phases may be displaced along the Al isoconcentration line (exactly along $Fe_xNi_{0.286-x}Al_{0.714}$), dependent on the heat treatment; during this displacement an Fe to Ni substitution takes place (or a reverse process may occur). This fact may be explained by the ease of the electron exchange between analogous metals. In the case of the alloy quenched from 720°C, the Fe:Ni ratio is equal to 1:1; it corresponds to the $FeNiAl_5$ alloy, so here the $FeNiAl_5$ phase is assumed to lie within the homogeneity range of τ_2.

[1986Sei] used insufficiently prolonged exposures during annealing. 72 h to 200 h were applied to homogenize the alloys at temperatures between 1200 and 600°C followed by annealing for 50 h at 1000, 800 and 600°C and water quenching. [1981Kha, 1982Kha] used 72 h at 1050°C, 360 h at 950°C and 960 h at 750°C, and even then stated that equilibrium was not established at 750°C. This is the reason why the field of the τ_2 existence was not confirmed by [1986Sei]. [1986Sei] did also find a two-phase region NiAl+FeAl at 650, 750, 1000 and 1150°C, which is in contradiction to the results of [1938Bra, 1940Bra1, 1951Bra, 1952Bra], the lattice parameter studies of [1939Lip] and [1972Kot] and the work of [1984Hao]. [1972Kot] found 17 single phase alloys at 950°C with the lattice parameter increasing up to 25 at.% Ni and then constant up to NiAl. [1984Hao] also shows an ordered CsCl type phase to exist between 1150 and 850°C from the Al-Fe to the Al-Ni side.

Alloys with compositions close to the Fe-Ni side were studied in detail by [1938Bra, 1940Bra1, 1949Bra, 1951Bra, 1952Bra]. The features of the crystallization and the phase constitution of these alloys were investigated by DTA, X-ray diffraction and metallographic analysis in a temperature range of 750°C to melting. The position of the phase boundaries in the alloys with < 50 at.% Al is strongly dependent on the invariant four-phase equilibrium U_1 and on the minimum point (point of tangency) of the liquidus and solidus surfaces. The temperature of the reaction:

$U_1: L + \gamma' \rightleftharpoons \gamma + \beta$
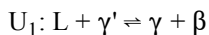
was established to be 1380°C [1949Bra]. Taking into account some new data on the formation of the $\gamma'(Ni_3Al)$ phase in the binary Al-Ni system [1987Hil, 1988Bre], it must be noted that this temperature could not exceed 1365°C. A monovariant order-disorder transformation descends from higher Al contents to the monovariant melting trough p_1-e_2 (see Fig. 3a). The dotted line belongs to the liquidus concentrations corresponding to the solidus intersecting with the order-disorder transformation between $\alpha\delta$ and β as a second order transformation (see Fig. 14). Older publications [1942Dan, 1949Bra] introduced a transition type reaction at 12.5 at.% Al and 67.5 at.% Fe [1949Bra] for the liquid with the equation:

$L + \alpha\delta \rightleftharpoons \gamma + \beta$, 1350°C,
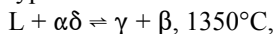
assuming that the two-phase field $\alpha\delta+\beta$ extends up to the liquid, but this has been revised by more recent experiments [1984Hao], Fig. 14. [1984Hao] applied diffusion couple techniques on samples prepared from 99.95% Fe, 99.95% Ni and 99.9% Al and annealed at temperatures between 850 and 1150°C to determine the shape of the miscibility gap between $\alpha\delta$ and β. The exact location of the order-disorder transformation

to higher Al contents is unknown; in Fig. 3a it is assumed that it contacts directly with the same transformation in the Al-Fe binary system.

The decomposition of the ($\alpha\delta$Fe, β) solid solution to a mixture of $\alpha\delta$ and β on cooling was investigated by [1940Kiu, 1941Kiu1, 1941Kiu2, 1941Kiu3, 1942Dan, 1949Bra, 1951Bra, 1952Bra, 1984Hao] in detail. Using X-ray diffraction, [1941Kiu1, 1941Kiu2, 1941Kiu3] investigated both the position of a three-phase field $\alpha\delta+\gamma+\beta$ and possible transformations in the solid state in detail. Unfortunately, this field was incorrectly projected on the composition plane (the phase rule was violated). The position of a three-phase field $\gamma+\gamma'+\beta$ at 1000°C was refined by [1986Bra]; the γ' field at 1000°C stretches to 60.9 at.% Ni though [1949Bra] has supposed that this field stretches to 68 at.% Ni at 1050 and 950°C. The two-phase equilibrium $\gamma+\gamma'$ was calculated by the cluster variation method with the tetrahedron approximation [1991Eno] and the results compared with experimental determinations of [1949Bra, 1951Bra]. Experimental investigations of the γ-γ' and β-γ' equilibria in the Ni rich corner of the diagram were carried out by [1994Jia] at 1100 and 1300°C using diffusion couples and electron microprobe analysis.

The Ni_3Al-$FeNi_3$ section has been studied by [1987Mas] using 99.9 mass% Ni, 99.99 mass% Al and 99.9 mass% Fe, the samples being homogenized at 1050°C for 48 h. Metallographic, X-ray and diffusion couple techniques have been applied to examine the phase boundaries at 75% Ni. Using neutron diffraction, [1998Gom] investigated the $L1_2$ ordering in the Ni_3Al-$FeNi_3$ section at low temperatures.

Binary Systems

The binary boundary systems Al-Ni and Al-Fe are accepted from critical assessments of [2003Sal] and [2003Pis], respectively. The Fe-Ni binary phase diagram is taken from [1982Kub].

Solid Phases

The crystallographic data of the Al-Fe-Ni phases and their temperature ranges of stability are listed in Table 2. In general Fe and Ni are not appreciably dissolved in Al, but form solid solutions which extend significantly into the ternary system.

The Al-Fe based bcc solid solution $\alpha\delta$ extends into the ternary and its Ni concentration increases with the increase of the Al concentration. In the binary Al-Fe system it orders in β by a second order transformation which became first order by adding Ni.

β phase (CsCl-type) forms a continuous range of solid solutions between Al-Fe, Al-Ni and toward Fe. Along the NiAl-Fe direction a miscibility gap is formed between the ordered β and disordered $\alpha\delta$ solid solutions. Lattice parameters and hardness measurements in the β field have been carried out by [2001Tan]. Site occupancies of Fe in NiAl were first investigated by [1994Dun] by using atom-probe field-ion microscopy. Then an exhaustive study of lattice parameters, site occupancies and vacancy concentration, point defects, density and hardness has been carried out by [1997Pik, 2002Pik] over a wide range of compositions and temperatures in the β-region. The triple defect structure was observed across the entire phase field. In all Al-rich compositions constitutional vacancies were observed. Thermodynamic predictions that the Fe anti-sites are more stable than the Ni anti-sites in the Al-poor compositions were qualitatively confirmed. The lattice parameter as a function of composition is reported in Figs. 1a and 1b.

The fcc solid solution γ extends from the Fe-Ni subsystem to more than 20 at.% Al. With decreasing temperature it orders in the γ' structure ($AuCu_3$ type) at about 75 at.% Ni and forms a continuous solid solution with the isostructural Ni_3Al [1986Bra, 1987Mas, 1998Gom]. Iron can occupy both Al and Ni sublattices, 78% of Fe atoms occupy Al sublattice for the Fe concentration of 2.5 at.%, while only 54% for the 9.3 at.% Fe compound [1977Nic]. Dissolution of Fe to at least 7 at.% does not influence the lattice parameter of γ' [1959Gua, 1984Och].

Site occupancies in Fe_3Al and, in particular, the substitution of Fe by Ni (about 3 at.%) have been investigated by neutron diffractometry [1998Sun].

The monoclinic Fe_4Al_{13} phase dissolves up to 12.0 at.% Ni at 800°C and $NiAl_3$ dissolves up to 2.5 at.% Fe [1996Gru1], Ni_2Al_3 can dissolve about 2, 4 and 10 at.% Fe at room temperature, 850 and 1050°C, respectively, Fe_2Al_5 and $FeAl_2$ can dissolve up to 2 at.% Ni at elevated temperatures [1982Kha].

No ternary phases were reported in the Al-poor region. In the Al-rich region three stable ternary phases were revealed. The τ_1 $(Ni,Fe)_2Al_9$ phase isostructural to Co_2Al_9 is formed at almost constant 82 at.% Al between 4.4 to 11.1 at.% Fe [1943Sch, 1999Dyb, 2000Dyb]. The same phase extends from 9 to 14.5 at.% Fe when τ_1 precipitates from melt-spun samples [1996Zho].

The hexagonal τ_2 Fe_3NiAl_{10} phase of the Co_2Al_5 type has been observed at 1050°C in the $Al_{70-72.5}Fe_{18-24.5}Ni_{10.5-4.5}$ composition range [1981Kha]; it has been structurally characterized by [1990Ell].

Quasiperiodic structures to which higher dimensional crystallography is applicable were discovered in Al-Fe-Ni alloys since 1989. A number of different decagonal diffraction patterns have been first observed [1989Tsa] in Al-Fe-Ni alloys prepared by melt quenching. After that decagonal phases have been studied by several authors [1989Tsa, 1993Tan, 1994Lem, 1996Gru1, 1997Sai, 2000Fre, 2001Hir, 2002Yok, 2003Doe]. The best known is the phase τ_3 (periodicity of about 0.4 nm), stable between 930 and 847°C in a range of less than 1 at.% around the $Al_{71}Ni_{24}Fe_5$ composition [1994Gru, 1994Lem, 1996Gru1, 2000Dro, 2003Doe]. It probably corresponds to an unidentified phase $FeNi_3Al_{10}$ previously observed by [1982Kha]. The diffraction patterns of the τ_3-phase are very similar to those of the Ni-rich decagonal phase found in the more extensively studied Al-Co-Ni alloy system [1996Gru2]. It was argued by [1996Gru1] that the stable ternary τ_3 phase is an extension of a metastable isostructural Al-Ni phase.

Two more metastable D-phases with slightly different diffraction properties were observed by [1993Tan, 1997Sai, 2001Qia] at higher Fe content. Structural models belonging to the space groups $P\overline{10}m2$ and $P10_5/mmc$ (or $P10/mmm$, according to [1993Tan]) were found to approximate the HRTEM images of quasicrystals at $Fe_{30-x}Ni_xAl_{70}$ with $10 < x < 17$ and $17 < x < 20$, respectively [1997Sai]. Disorder in these phases has been studied by X-ray (synchrotron) and neutron diffraction experiments [2000Fre]. [2001Hir] found that large columnar clusters of atoms with a decagonal section of about 3.2 nm in diameter exist as a basic structural unit.

It may be noticed that owing to the experimental and interpreting difficulties, also connected to the dependence of the sample structures on the preparation procedures, the reported description of the Al-Fe-Ni decagonal phases may be considered still incomplete but representative of a more complex situation.

Quasibinary Systems

It may be supposed that a quasibinary section exists in the system. It occurs between FeAl and NiAl which possess isotypic structures. A series of continuous solid solutions β is formed of the CsCl structure type; the melting point of the alloys decreases monotonically from NiAl to FeAl. However, the tie lines L+β are essentially perpendicular to that section, which renders it non-quasibinary. A miscibility gap develops in β at lower temperatures [1986Sei]. These tie lines are again off-section and essentially in the NiAl-Fe direction as described in more detail under Isothermal Sections.

Invariant Equilibria

The data on the invariant equilibria are given in Table 3 according to [1949Bra] (U_1) and [1943Sch] (P, E_2, U_2). The U_1 temperature was corrected according to [1987Hil, 1988Bre]. The data on the eutectic decomposition, E_1, of the ternary decagonal phase τ_3 are accepted from [1996Gru1]. A partial reaction scheme is given in Fig. 2.

Liquidus Surface

The projection of liquidus surfaces of portions of the ternary diagram investigated by [1949Bra] (0 to 50 at.% Al) and [1943Sch] (100 to 88 at.% Al), adapted to the accepted binaries, are given in Fig. 3a, and a more detailed view of the Al-corner [1942Phi] in Fig. 3b. It should be noted that the position of the minimum point of the peritectic/eutectic line, e_2, at 50 at.% Fe must be above 1350°C, see Fig. 4, and below the 1365°C of U_1. It is assessed at 1360°C. The liquidus surface of β is extremely flat in that range. In the alloys with 85 to 50 at.% Al additional invariant transformations must occur in the range 850 to 1340°C (besides the four-phase reactions already investigated) where the reactions p_3, p_4, p_5, p_6, p_7, e_3 and e_4 of the

corresponding binary systems enter the ternary. The U-type reaction suggested at ~840°C with a liquid at about 82 at.% Al [1992Bud] cannot be accepted in view of the firmly established three-phase equilibrium $Fe_4Al_{13} + Ni_2Al_3 + NiAl_3$ formed in the reaction E_1 at 847°C [1996Gru1].

Isothermal Sections

Isothermal sections between 1350 and 750°C, Figs. 4 - 10, were constructed on the basis of the data obtained by [1949Bra, 1951Bra, 1981Kha, 1982Kha, 1984Hao, 1986Bra, 1996Gru1]. The location of the order-disorder transition between β and αδ at 1350°C in Fig. 4 is not known but must occur inside the ternary since in the binary Al-Fe that transition ends at 1310°C. This line is shown dotted in Figs. 5 and 6. At even lower temperature, Figs. 7 - 10, the peculiar horn-shape develops. This indicates the change from the second order transition along a single line to the first order transition with a two-phase field αδ+β, that exists only in the ternary. This miscibility gap, taken essentially from [1984Hao] is in qualitative agreement with the data of [1941Kiu3]. The plotted phase boundaries of [1941Kiu3], however, do not show the horn-shape with the necessary tricritical point and are therefore not reproduced.

The position of the three-phase field β+γ+γ' at 1050 and 950°C in Figs. 7 and 8 was refined based on the data of [1986Bra] at 1000°C. The data obtained by diffusion couple technique at 1300 and 1100°C [1994Jia] essentially agree with that, although they show a somewhat different curvature of the phase boundaries. The γ'/β+γ' and β/β+γ' boundaries of [1994Jia] are curved towards higher Al-content. All sources agree on the important distribution of Fe in the three phases, showing a decreasing Fe-content in the phase sequence β-γ'-γ [1949Bra, 1986Bra, 1994Jia].

The position of phase fields in the Al-rich alloys are given according to [1981Kha, 1982Kha, 1996Gru1]. At 1050 and 950°C, the τ_2 phase field can be seen; the decagonal phase τ_3, stable between 930 and 847°C [1996Gru1], is given in Fig. 9 with other partial equilibria; at 750°C, the τ_1 phase already exists. The isothermal section at 620°C of the Al-rich portion of the diagram is shown in Fig. 11 [1943Sch].

The general distribution of phase fields in the whole composition triangle is given in Fig. 12; the data were obtained by cooling the alloys with a rate of $10°C·h^{-1}$ from 900°C (for Al-rich alloys, from 600°C) in [1938Bra, 1940Bra1, 1940Bra2]. Early calculations of isothermal sections for 927, 1127, 1327 and 1427°C are given by [1974Kau], at that time without modeling the bcc ordering. The γ-γ' phase boundaries have been calculated in [1991Eno] by cluster variation method using tetrahedron approximation and the phenomenological Lennard-Jones pair potentials. The results are in a fair agreement with the experimental data from [1949Bra, 1951Bra].

Temperature – Composition Sections

Two vertical sections parallel to the Fe-NiAl section with some Ni-excess are shown in Figs. 13 and 14, and the Fe-NiAl section in Fig. 15. The Ni-excess sections may be approximately considered as quasibinary sections. By contrast, Fig. 15 is absolutely not quasibinary with the γ+αδ tie lines virtually perpendicular to the section. It is important to note that minute changes of the phase limits in the isothermal sections correspond to drastic changes in these vertical sections. In this context, the agreement between the sections reported by [1951Bra, 1984Hao] for Fig. 14 or [1951Bra, 1951Iva] may be considered to be fair. As an example in Fig. 15, [1951Bra] reports a small three-phase field αδ+β+γ around 80 at.% Fe and 750-850°C, whereas [1951Iva] reports a continuous single phase field αδ connecting (αFe) and (δFe), as shown dashed in Fig. 15. These alternatives are probably within the experimental error of the phase limit in the corresponding isothermal sections. It is thus not considered helpful to reproduce the additional vertical sections reported by [1951Bra] for the Al-excess sections or by [1952Bra] for the sections parallel to Al-Fe. A similar reasoning applies to the vertical sections reported in the early work of [1933Koe, 1941Kiu3].

The vertical section Ni_3Al-Fe_3Al [1987Mas] displayed in Fig. 16 is also supported by the data of [1994Jia] on the Fe-poor γ+γ' equilibrium. The data of [1998Gom] indicate a lower γ/γ+γ' boundary but are unacceptably low for the Ni_3Al limit.

The αδ+β miscibility gap is due to both chemical and magnetic ordering effects. It has been tried to separate these effects in a Calphad-type calculation, suggesting that the (metastable) miscibility gap in the

magnetically and chemically disordered state is at much lower temperature compared to the stable gap along a vertical section Fe97.5Al2.5 - Ni49.5Al50.5 [1994Gho].

Thermodynamics

The temperature and the enthalpy of fusion of the decagonal phase $Fe_5Ni_{24}Al_{71}$ prepared by inductively melting the pure metals, water cooling, then annealing 300h at 880°C has been respectively determined in 967 ± 5°C and 13.0 ± 0.4 kJ·mol^{-1} of atoms [1999Hol]. The standard enthalpy of formation of the β phase at different compositions has been measured by Al solution calorimetry by [1993Zub] and, with very good reproducibility, by [2001Bre]. Their results are reported in Table 4.

Notes on Materials Properties and Applications

Fe is one of the most important constituent of Ni-base superalloys because the B2-type of NiAl phase has a high melting temperature, high thermal conductivity and high resistance to oxidation. The lack of high temperature strength may be overcome by the use of Fe or other minor additions such as Ga or Mo [2002Alb] and a systematic study of correlation between point defects and Fe precipitates has been undertaken [1998Ko, 2002Alb], together with the influence of iron on physical, mechanical (grain size, yield strength) and magnetic properties of NiAl [2002Ban, 2002Mun]. Indeed, these compounds would be of higher practical interest if their attractive high temperature behavior could be combined with good room temperature formability. This aim may be achieved by introducing a substantial amount of disorder in their crystal lattice. Several techniques have been proposed like melt spinning, ion irradiation, mechanical alloying [1991Kos, 1995Gaf, 2001Sur] or introduction of dopants such as carbon [2002Kim]. Nanostructured materials show significant kinetics of reordering even at 300°C. However, complete reordering could not be achieved, even after long annealing time at 600°C [2002Joa]. Al-Fe-Ni alloys are good precursors for the preparation of Fe-Ni powders with high surface area and interesting catalyst properties [1981Kha]. Ternary alloys with nominal compositions $Ni_{30}Fe_5Al_{65}$ and $Ni_{15}Fe_{10}Al_{75}$ prepared by mechanical alloying were used to obtain Fe-Ni Raney-type catalysts by leaching aluminium with an alkaline aqueous solution [2000Zei].

New materials may be obtained through thermal explosion reaction as an alternative to combustion synthesis. The order of reaction n and the activation energy E of thermal explosive reaction for Fe30Ni50Al20 (in mass%) has been respectively measured as $n = 0.37$ and $E = 152$ kJ·mol^{-1} [2002He]. The maximum reaction temperature is 657°C, higher than eutectic temperature between Al and $NiAl_3$, so that the thermal explosion consists of both liquid and solid state reactions.

Al-Fe-Ni alloys present a shape memory effect in the β+γ field [1992Kai]. The control of the Ms (Martensite start) temperature, difficult to achieve in Al-Ni alloys because of the very sensitive dependence on the Al content, is, on the other hand, very easily achieved in the ternary two-phase alloy by manipulating the composition of the β phase through appropriate choice of annealing temperatures.

Miscellaneous

Crystallographic features of decagonal structures are presented in [1996Yam, 2002Hir] and formation rules for Al-Fe-Ni quasicrystals were pointed out in [2001Qia]. A number of different decagonal diffraction patterns have been first observed [1989Tsa] in Al-Fe-Ni alloys prepared by melt quenching in the composition ranges from 9 to 16 at.% Ni, 9 to 21 at.% Fe, in good agreement with the composition range $Fe_{20-x}Ni_{10+x}Al_{70}$ ($0 \leq x \leq 10$) more recently proposed by [1993Tan, 1997Sai]. However, more precise investigations show the possible existence of at least 3 decagonal phases. Quasicrystals $Fe_{20-x}Ni_{10+x}Al_{70}$ were found by the convergent-beam electron diffraction (CBED) method to belong to the noncentrosymmetric space group $P\overline{10}m2$ for $0 \leq x \leq 7$ [1993Tan, 1997Sai] and to the centrosymmetric group $P10/mmm$ for $7 \leq x \leq 10$ [1993Tan] and to present periods along the tenfold axis which are multiple of 0.4 nm [1997Yam]. It is probable that these structures correspond actually to the phases D_1, $Fe_{14.5}Ni_{13}Al_{72.5}$ and D_2, $Fe_{9.83}Ni_{19.34}Al_{70.83}$ whose structure has been described by [2001Qia]. D_1, $Fe_{14.5}Ni_{13}Al_{72.5}$ is observed to coexist with τ_2, $FeNiAl_5$. Decagonal phases reveal higher positron

lifetime than crystalline compounds [1995Wue], which implies higher concentration of structural vacancies. A characteristic feature of these structures, isotypic with decagonal phases encountered in Al-Co-Ni and Al-Co-Cu systems [1994Gru] is that they consist of 2 nm clusters with pentagonal symmetry. The superstructure is due to chemical ordering in the central part of the 2 nm clusters. Star-shaped and butterfly-shaped tiles observed in quasicrystals are well understood from observations of [2002Yok]. Diffuse scattering from X-rays (synchrotron) and neutrons [2000Fre] shows disordered layers perpendicular to the unique tenfold axis.

The diffusion experiments, carried out at 1002°C in the B2 (βNiAl) domain of the ternary system presents anomalous behavior [1976Moy], the interactions among the various components being strongly composition dependent. This is explained [1997Kai] by the fact that NiAl has a wide composition range and exhibits two types of structural imperfections depending on the nature of deviation from stoichiometry. In NiAl, iron was observed to substitute preferentially aluminium atoms whatever the Al/Ni ratio [1994Dun, 2002Ban]. The substitution (up to 10 at.%) of Al by Fe in NiAl decreases the lattice parameter and increases the Young's modulus [1991Mas]. More generally, the introduction of Fe increases the hardness of the Al rich alloys and decreases the hardness in the Ni rich alloys [1997Pik, 2001Tan]. This softening is attributed to the replacement of Ni anti-site defects with Fe defects on the Al sublattice. On the other hand, the site preference of Ni in β ordered iron aluminide has been determined using ALCHEMI technique (Atom Location by Chaneling-Enhanced Microanalysis), first in the $Fe_{50}Ni_5Al_{45}$ alloy [1997And], then in the whole β domain (40 to 52 at.% Al) [2002Pik]. Ni was found to occupy the Fe sites exclusively, displacing Fe to Al anti-sites [2002Ban, 2002Pik]. The influence of Ni on the formation and growth characteristics of Fe based aluminide diffusion layers has been modelled [1998Akd, 1999Mek] by mean of a quasichemical method combined with an electronic theory in the pseudopotential approximation; the influence of Fe on the lattice parameter and hardening of NiAl has been modelled [2002Liu] by first principle quantum mechanical calculations. The site preference in various β solid solutions ($Fe_xNi_{50-x/2}Al_{50-x/2}$, $Fe_xNi_{50-x}Al_{50}$ $Fe_xNi_{50}Al_{50-x}$) have also been modelled [2002Boz] via Monte-Carlo simulation. A phenomenological model for multicomponent diffusion in the β (B2 ordered) phase was presented by [1999Hel] and calculated diffusion paths were compared with experimental ones given by [1976Moy]. The OTL (ordering tie-line) approach [2000Ama] confirms the preceding observations showing that, while Ni segregates preferentially to the Fe sublattice in Al depleted FeAl, Fe segregates preferentially to the Al sublattice in Al depleted NiAl. The presence of iron improves the fatigue behavior under cyclic accumulated strain [1991Har]. Fracture thoughness and yield strength of β,NiAl and β,$Fe_{20}Ni_{45}Al_{35}$ is improved by mechanical alloying with additions of small amounts of Y_2O_3 which allows the achievement of fine grain sizes [1991Kos].

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Table 1: Recent Investigations of the Al-Fe-Ni System

Reference	Experimental Technique	Temperature/ Composition/ Phase Range Studied
[1989Tsa]	New decagonal phases prepared by liquid quenching	9 to 21 at.% Fe, 9 to 16 at.% Ni,
[1990Ell]	Crystal structure	$FeNiAl_5$
[1991Har]	Texture measurements, cyclic deformation	$Fe_{60}Al_{40}$ and $Fe_{20}Ni_{50}Al_{30}$
[1991Kos]	Fracture toughness, grain size effects, strain-stress measurements	$Fe_{20}Ni_{45}Al_{35}$
[1991Pat]	Transition in Burgers' vector	$(Fe_xNi_{1-x})_{60}Al_{40}$ $(0 \leq x \leq 1)$
[1991Mas]	Crystal structure, Hardness, Young's modulus	$Fe_xNi_{50}Al_{50-x}$ $(0 \leq x \leq 10)$
[1991Yav]	Magnetization of γ' alloys obtained by cold working or melt spinning	10 to 13 at.% Fe, 16 to 17.4 at.% Al
[1992Kai]	Shape memory effect, stress-strain curves, Ms temperature	$Fe_{57}Ni_{25}Al_{18}$, 1000-1300°C
[1993Pov]	Phase equilibria, Electron microprobe analysis, X-ray analysis	> 50 at.% Al, 900-1100°C
[1993Zub]	Enthalpies of formation, enthalpies of dilution in liquid Al	0 to 10 at.% Fe, 40 to 50 at.% Ni, 800°C
[1994Dun]	Crystal structure, atom probe field-ion microscope	$Fe_{0.3}Ni_{50}Al_{49.7}$ and $Fe_{2.2}Ni_{47.8}Al_{50}$
[1994Gho]	Spinodal decomposition by transmission electron microscopy, field-ion microscopy	Fe-23.3 mass% Ni-9.4 mass% Al, water quenched from 1300°C
[1994Jia]	Equilibria γ-γ' and β-γ', diffusion couples, electron microprobe analysis	< 6 mass% Fe, < 22 mass% Al, 1100-1300°C
[1994Lem]	Stability of the decagonal phase	23 to 24.6 at.% Ni, 4.3 to 5.3 at.% Fe, 800 to 940°C (τ_3 phase)
[1995Gaf]	Mechanical alloying, crystal structure	NiAl-Fe join, room temperature
[1995Wue]	Structural vacancies, positron lifetimes measurements	< 25 at.% Fe, 20-25 at.% Ni
[1996Gru1]	Decagonal phase, Stability	$Fe_5Ni_{24}Al_{71}$, inductive melting then annealing 340h at 880°C (τ_3 phase)
[1996Zho]	Crystal structure, Mössbauer	$Fe_xNi_{2-x}Al_9$ $(1 \leq x \leq 1.6)$ (τ_1 phase)
[1997Pik]	Lattice parameters, bulk density, hardness measurements	0 to 12 at.% Fe, 40 to 52 at.% Al water quenched from 1000°C
[1997Sai]	Decagonal phases, Crystal Structure, Convergent-beam electron diffraction	$Fe_{30-x}Ni_xAl_{70}$ $(10 \leq x \leq 17)$ (D_1 phase)
[1998Gom]	Neutron diffraction, Order-disorder equilibrium	$FeNi_3$-Ni_3Al join, 500-1000°C
[1998Sun]	Crystal structure, neutron diffraction study	$Fe_{72}Ni_3Al_{25}$
[1999Dyb]	Interface Al-intermetallic layers by electron probe microanalysis	Reaction between liquid Al and Fe-Ni alloys at 700°C

Reference	Experimental Technique	Temperature/ Composition/ Phase Range Studied
[1999Hol]	DTA investigation, Melting point and enthalpy of fusion of quasicrystals	$Fe_5Ni_{24}Al_{71}$ quenched from the melt then annealed 300h at 880°C (τ_3 phase)
[2000Dro]	Scanning electron microscopy, atomic force microscopy	$Fe_5Ni_{23.5}Al_{71.5}$ quenched from the melt, then annealed 51 h at 900°C (τ_3 phase)
[2000Dyb]	Liquidus surfaces, phase field in the solid state	> 60 mass% Al, < 800°C
[2000Fre]	Diffuse scattering of X-rays and neutrons in decagonal phase	$Fe_5Ni_{23.5}Al_{71.5}$ (τ_3 phase)
[2001Bre]	Enthalpies measurements, differential solution calorimetry	Fe_xAl_{1-x} and $Fe_xNi_yAl_z$ (x = 0-0.6, y = 0-0.55, z = 0.35-0.50), 800°C
[2001Hir]	Crystal structure, atomic scale observation by scanning transmission electron microscopy	4.7 at.% Fe, 23.7 at.% Ni,
[2001Sav]	Crystal structure, Order-disorder transition, electrical resistivity	$Fe_8Ni_{71}Al_{21}$, 1000-1850°C
[2001Tan]	Crystal parameters and hardness measured in the β domain	< 60 at.% Al, powder homogenized 1h at 850°C
[2002Bit]	Solidus determination, high temperature differential thermal analysis	Ni_xAl_{100-x} (45 < x < 47) and $Fe_yNi_{50-y}Al_{50}$ (0 < y < 50), 1259-1681°C
[2002Joa]	Nanostructured alloy, kinetics of reordering	$Fe_{20}Ni_{40}Al_{40}$, 300-600°C
[2002Mun]	Microstructure, tensile and compressive strength, hardness and wear tests	Fe-NiAl join (0 to 44 at.% Fe), 500-900°C
[2002Pik]	Hardness, Vacancy concentration, Atomic site occupancy in the β domain, ALCHEMI technique	40 to 52 at.% Al, samples quenched from 700 and 1000°C
[2001Qia]	Decagonal phases, crystal structures	$Fe_{14.5}Ni_{13}Al_{72.5}$ and $Fe_{12}Ni_{17.5}Al_{70.5}$ (D_1 and D_2 phases)
[2002Yok]	Crystal structure of decagonal phase, high-angle annular dark-field scanning transmission electron microscope	$Fe_{15}Ni_{15}Al_{70}$, prepared with a single roller melt-spinning apparatus (D_1 phase)

Table 2: Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	References/Comments
(Al) < 660.452	$cF4$ $Fm\overline{3}m$ Cu	$a = 404.96$	dissolves 0.03 at.% Fe at 652°C and 0.025 at.% Ni at 640°C [L-B]
γ, $Fe_{1-x-y}Ni_xAl_y$	$cF4$ $Fm\overline{3}m$ Cu		at $x = 0$, $0 \leq y \leq 0.013$ at $y = 0$, $0 \leq x \leq 1$ at $x + y = 1$, $0 \leq y \leq 0.02$
(γFe) 1394 - 912		$a = 352.40$	at $x = 0$, $y = 0$ and 915°C [V-C2, Mas2]
(Ni) < 1455		$a = 364.67$	at $x = 1$, $y = 0$ and 20°C [V-C2, Mas2] (at $y = 0$ and 20°C a vs x is not linear and has a maximum for $x \approx 0.4$)
αδ, $Fe_{1-x-y}Ni_xAl_y$	$cI2$ $Fm\overline{3}m$ W		at $x = 0$, $0 \leq y \leq 0.045$ at $y = 0$, $0 \leq x \leq 0.055$ (αFe) at $y = 0$, $0 \leq x \leq 0.035$ (δFe)
(δFe) 1538 - 1394		$a = 286.65$	at $x = 0$, $y = 0$ and 25°C [V-C2]
(αFe) <912		$a = 293.22$ $a = 286.64$ to 289.59 $a = 286.60$ to 289.99 $a = 286.60$ to 290.12	at $x = 0$, $y = 0$ and 1394°C [V-C2] at $x = 0$, $0 \leq y \leq 0.019$, 20°C [1958Tay] at $x = 0$, $0 \leq y \leq 0.019$, 20°C [1961Lih] at $x = 0$, $0 \leq y \leq 0.010$, 20°C [1999Dub]
β, $(Fe_{1-x}Ni_x)_{1+y}Al_{1-y}$	$cP2$ $Pm\overline{3}m$		at $x = 0$, $0.10 \leq y \leq 0.54$ (FeAl) at $x = 1$, $0.16 \leq y \leq 0.38$ (NiAl)
FeAl < 1310	CsCl	$a = 290.90$ $a = 290.17$ $a = 289.77$ $a = 289.66$ $a = 289.53$	at $x = 0$, $y = 0$ (50 at.%Al) at $x = 0$, $y = 0.124$ (43.8 at.%Al) at $x = 0$, $y = 0.182$ (40.9 at.%Al) at $x = 0$, $y = 0.234$ (38.3 at.%Al) $x = 0$, $y = 0.276$ (36.2 at.%Al) [1958Tay]
NiAl < 1638		$a = 288.7$ $a = 288.0$	at $x = 1$, $y = 0$ (50 at.% Al) at $x = 1$, $y = 0.08$ (46 at.%Al) [1996Pau] (see also Figs. 1a and 1b)
Fe_4Al_{13} < 1157	$mC102$ $C2/m$ Fe_4Al_{13}	$a = 1549.2(2)$ $b = 807.8(2)$ $c = 1247.1(1)$ $\beta = 107.69(1)°$ $a = 1543.7$ $b = 810.9$ $c = 1243.0$ $\beta = 107,66°$	74.5-76.6 at.% Al at 0 at.% Ni [2003Pis] at 76.0 at.% Al [1994Gri] [1982Kha] at 10 at.% Ni dissolves 12 at.% Ni at 800°C [1996Gru1] 10 at.% Ni at 950°C [1982Kha] 6 at.% Ni at 1050°C [1982Kha]
Fe_2Al_5 < 1169	$oC24$ $Cmcm$ Fe_2Al_5	$a = 765.59$ $b = 641.54$ $c = 421.84$	70-73 at.% Al at 0 at.% Ni [1993Kat] at 71.5 at.% Al [1994Bur] dissolves 2 at.% Ni at 1050°C [1982Kha, 1993Pov]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	References/Comments
FeAl$_2$ < 1156	aP18 P1 FeAl$_2$	a = 487.8 b = 646.1 c = 880.0 α = 91.75° β = 73.27° γ = 96.89°	66-66.9 at.% Al at 0 at.% Ni [1993Kat] at 66.9 at.% Al [1973Cor] dissolves 2.5 at.% Ni at 1050°C [1982Kha]
ε 1102 - 1232	cI16?	a = 578.0	at 61 at.% Al [1933Osa]
Fe$_3$Al < 547	cF16 Fm$\bar{3}$m BiF$_3$	a = 579.98 a = 579.30 to 578.86 a = 579.98 a = 579.30 to 578.92	~24 - ~37 at.% Al in Al-Fe [2001Ike] Extends less than 10 at.% Ni into the ternary [1940Bra2] at 24.35 at.% Al [1998Sun] 23.1-35.0 at.% Al [1958Tay] at 25 at.% Al and 3 at.% Ni neutron diffr. [1998Sun] 24.7-31.7 at.% Al [1961Lih]
O-Fe$_4$Al$_{13}$	oC~50 Cmmm Fe$_4$Al$_{13}$	a = 2377.1 b = 775.10 c = 403.36	Metastable (?) Described by the authors in terms of the Bmmm group. It was suggested that multiple twinning of this structure exhibits decagonal pseudo-symmetry [1995Ell]
Fe$_2$Al$_9$	mP22 P2$_1$/a Co$_2$Al$_9$	a = 869 b = 635 c = 632 β = 93.4°	Metastable [1977Sim]
FeAl$_6$	oC28 Cmc2$_1$ MnAl$_6$	a = 646.4 b = 744.0 c = 877.9	Metastable [1965Wal]
FeAl$_{4+x}$	t**	a = 884 c = 2160	(0 < x < 0.4) metastable [1998Ali]
I(Al-Fe)			Icosahedral, Metastable [1984She]
γ',(Ni$_3$Al) < 1372 (FeNi$_3$) < 517	cP4 Pm$\bar{3}$m AuCu$_3$	a = 358.9 a = 356.32 a = 357.92 a = 355.25	73 to 76 at.% Ni at 0 at.% Fe [Mas2] dissolves up to 15 at.% Fe [1986Bra, 1993Pov] 63-85 at.% Ni at 0 at.% Al and 350°C [1982Kub] complete solid solution with FeNi$_3$ at T<500°C [1987Mas] at 75 at.% Ni, 0 at.% Fe [1993Kha] disordered [1998Rav] ordered [1998Rav] at 75 at.% Ni, 0 at.% Al, 20°C [L-B]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	References/Comments
Ni_3Al_4 < 580	$cI112$ $Ia\overline{3}d$ Ni_3Ga_4	$a = 1140.8$	[1989Ell, V-C]
Ni_2Al_3 < 1138	$hP5$ $P\overline{3}m1$ Ni_2Al_3	$a = 402.8$ $c = 489.1$	36.8 to 40.5 at.% Ni at 0at.% Fe [Mas2] [1997Bou, V-C] dissolves 2 at.% Fe at 20°C and 10 at.% Fe at 1050°C [1982Kha]
$NiAl_3$ < 856	$oP16$ $Pnma$ $NiAl_3$	$a = 661.3$ $b = 736.7$ $c = 481.1$	[1996Vik] dissolves 4 at.% Fe [1982Kha]
Ni_2Al	$hP3$ $P\overline{3}m1$ CdI_2	$a = 407$ $b = 499$	Metastable [1993Kha]
Ni_xAl_{1-x} martensite	$tP4$ $P4/mmm$ AuCu	$a = 383.0$ $c = 320.5$ $a = 379.5$ $c = 325.6$ $a = 375.1$ $c = 330.7$ $a = 379.9$ to 380.4 $c = 322.6$ to 323.3 $a = 371.7$ to 376.8 $c = 335.3$ to 339.9	Metastable $0.60 < x < 0.68$ [1993Kha] at 62.5 at.% Ni [1991Kim] at 66.0 at.% Ni [1991Kim] at 64 at.% Ni [1997Pot] at 65 at.% Ni [1997Pot]
	m^{**}	$a = 418$ $b = 271$ $c = 1448$ $\beta = 93.4°$	[1992Mur]
Ni_2Al_9	$mP22$ $P2_1/a$ Co_2Al_9	$a = 868.5$ $b = 623.2$ $c = 618.5$ $\beta = 96.50°$	Metastable [1997Poh]
FeNi	$tP4$ $P4/mmm$ CuAu	$a = 358.23$ $c = 358.22$	Metastable (?) [L-B]
Fe_3Ni	c^{**}	$a = 357.5$	Metastable(?) [L-B]
D_1, $Fe_{14.5}Ni_{13}Al_{72.5}$	$P\overline{10}m2$	$a_D = 713.4$ $c_D = 818$	Metastable in the ternary at $Al_{70}Ni_{10-17}Fe_{20-13}$ [1997Sai, 2001Qia] Metastable in the Al-Fe binary [1986Fun]
D_2, $Fe_{9.83}Ni_{19.34}Al_{70.83}$	$P10/mmm$ or $P10_5mc$	$a_D = 712$ $c_D = 409$	Metastable in the ternary at $Al_{70}Ni_{17-20}Fe_{13-10}$ [1997Sai, 2001Qia]
*τ_1, $FeNiAl_9$ forms between 850 and 750°C	$mP22$ $P2_1/a$ Co_2Al_9	$a = 859.8$ $b = 627.1$ $c = 620.7$ $\beta = 94.66°$	at $Al_{82}Ni_{11.7}Fe_{6.3}$ [1982Kha] 7.3 to 12.7 at.% Ni, 10.4 to 4.7at.% Fe at 620°C [1943Sch], confirmed by [1999Dyb, 2000Dyb]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	References/Comments
*τ_2, FeNi$_3$Al$_{10}$ $\sim$850 < T < 1110	$hP28$ $P6_3/mmc$ Co$_2$Al$_5$	a = 770.3 c = 766.8	[1990Ell] at FeNiAl$_5$ Al$_{70\text{-}72.5}$Fe$_{18\text{-}24.5}$Ni$_{10.5\text{-}4.5}$ at 1050°C [1981Kha]
*τ_3, Fe$_5$Ni$_{24}$Al$_{71}$ 847 < T < 930		$a_D \approx$ 378 $c_D \approx$ 411	Decagonal phase with small solubility range [1994Lem, 1996Gru]. Diameter of the decagonal section $\sim$3200 pm [2001Hir]
		a_D = 373.3 c_D = 407.3	Metastable in Al-Ni binary system at 24-30 at.% Ni [1997Poh]

Table 3: Invariant Equilibria

Reaction	T (°C)	Type	Phase	Composition (at.%)		
				Al	Fe	Ni
L + γ' ⇌ γ + β	$\sim$1365	U$_1$	L	23	4	73
τ_3 ⇌ Fe$_4$Al$_{13}$ + Ni$_2$Al$_3$ + NiAl$_3$	847	E$_1$	τ_3 Fe$_4$Al$_{13}$ Ni$_2$Al$_3$ NiAl$_3$	$\sim$71 $\sim$75 $\sim$61 75	$\sim$5 $\sim$15 $\sim$2 $\sim$2	$\sim$24 $\sim$10 $\sim$37 $\sim$23
L + Fe$_4$Al$_{13}$+ NiAl$_3$ ⇌ τ_1	809	P	L	87.06	2.11	10.83
L + Fe$_4$Al$_{13}$ ⇌ (Al) + (τ_1)	650	U$_2$	L	98.42	0.795	0.786
L ⇌ (Al) + NiAl$_3$ + τ_1	638	E$_2$	L	96.72	0.105	3.175

Table 4: Thermodynamic Data

Reaction or Transformation	Temperature (°C)	Quantity per Reaction (J, mol, K)	Comments
xFe(α) + yNi(γ) + zAl(liq) ⇒ Fe$_x$Ni$_y$Al$_z$(β)	800	$\Delta_f H$ = –42780 ± 280 $\Delta_f H$ = –48730 ± 220 $\Delta_f H$ = –54420 ± 240 $\Delta_f H$ = –60860 ± 230 $\Delta_f H$ = –65740 ± 270 $\Delta_f H$ = –39870 ± 230 $\Delta_f H$ = –45740 ± 050 $\Delta_f H$ = –51920 ± 140 $\Delta_f H$ = –58070 ± 110 $\Delta_f H$ = –63110 ± 060 $\Delta_f H$ = –65380 ± 100 $\Delta_f H$ = –30920 ± 240 $\Delta_f H$ = –35460 ± 310 $\Delta_f H$ = –51520 ± 290	x = 0.42, y = 0.08, z = 0.50 x = 0.34, y = 0.16, z = 0.50 x = 0.25, y = 0.25, z = 0.50 x = 0.16, y = 0.34, z = 0.50 x = 0.08, y = 0.42, z = 0.50 x = 0.46, y = 0.09, z = 0.45 x = 0.37, y = 0.18, z = 0.45 x = 0.275, y = 0.275, z = 0.45 x = 0.18, y = 0.37, z = 0.45 x = 0.09, y = 0.46, z = 0.45 x = 0.0, y = 0.55, z = 0.45 x = 0.59, y = 0.06, z = 0.35 x = 0.53, y = 0.12, z = 0.35 x = 0.145, y = 0.505, z = 0.35 Al solution calorimetry [2001Bre]
xFe(α) + yNi(γ) + zAl(liq) ⇒ Fe$_x$Ni$_y$Al$_z$(β)	25	$\Delta_f H$ = –58000 ± 3000 $\Delta_f H$ = –56800 ± 2300 $\Delta_f H$ = –54100 ± 2100 $\Delta_f H$ = –48400 ± 2400	x = 0.0, y = 0.50, z = 0.50 x = 0.02, y = 0.50, z = 0.48 x = 0.05, y = 0.50, z = 0.45 x = 0.10, y = 0.40, z = 0.50 Al solution calorimetry [1993Zub]

Fig. 1a: Al-Fe-Ni.
Lattice parameter of
β-phase, (Fe,Ni)Al as
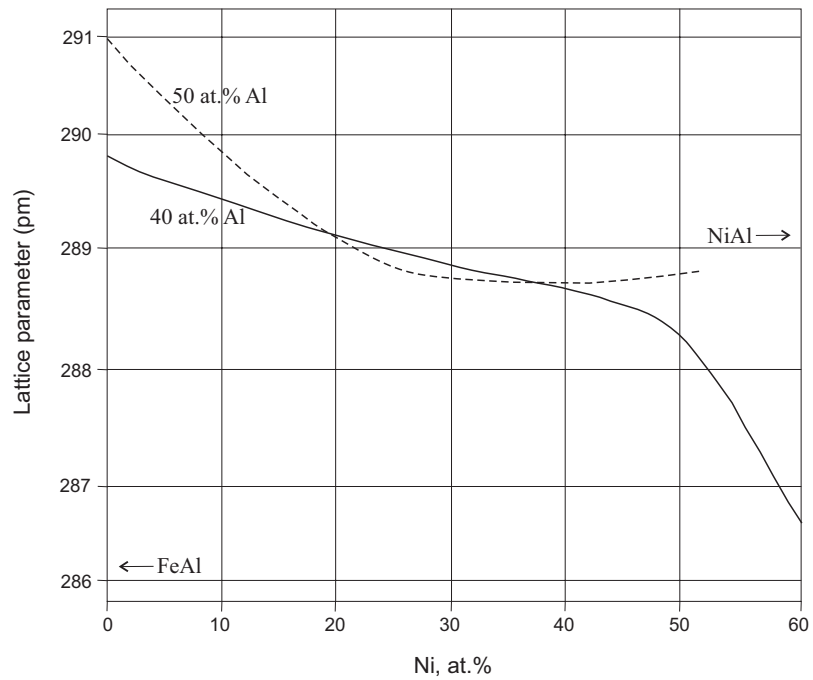a function of
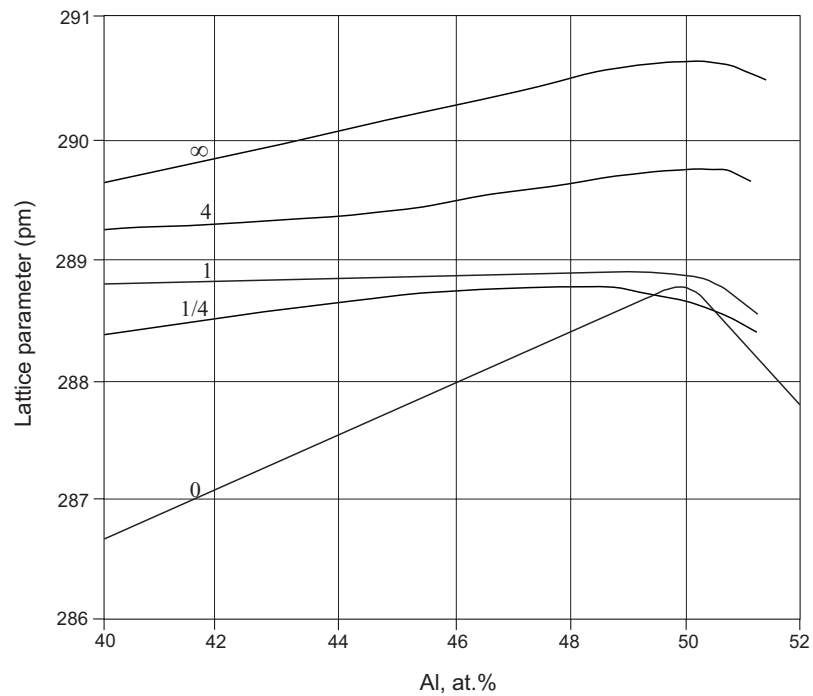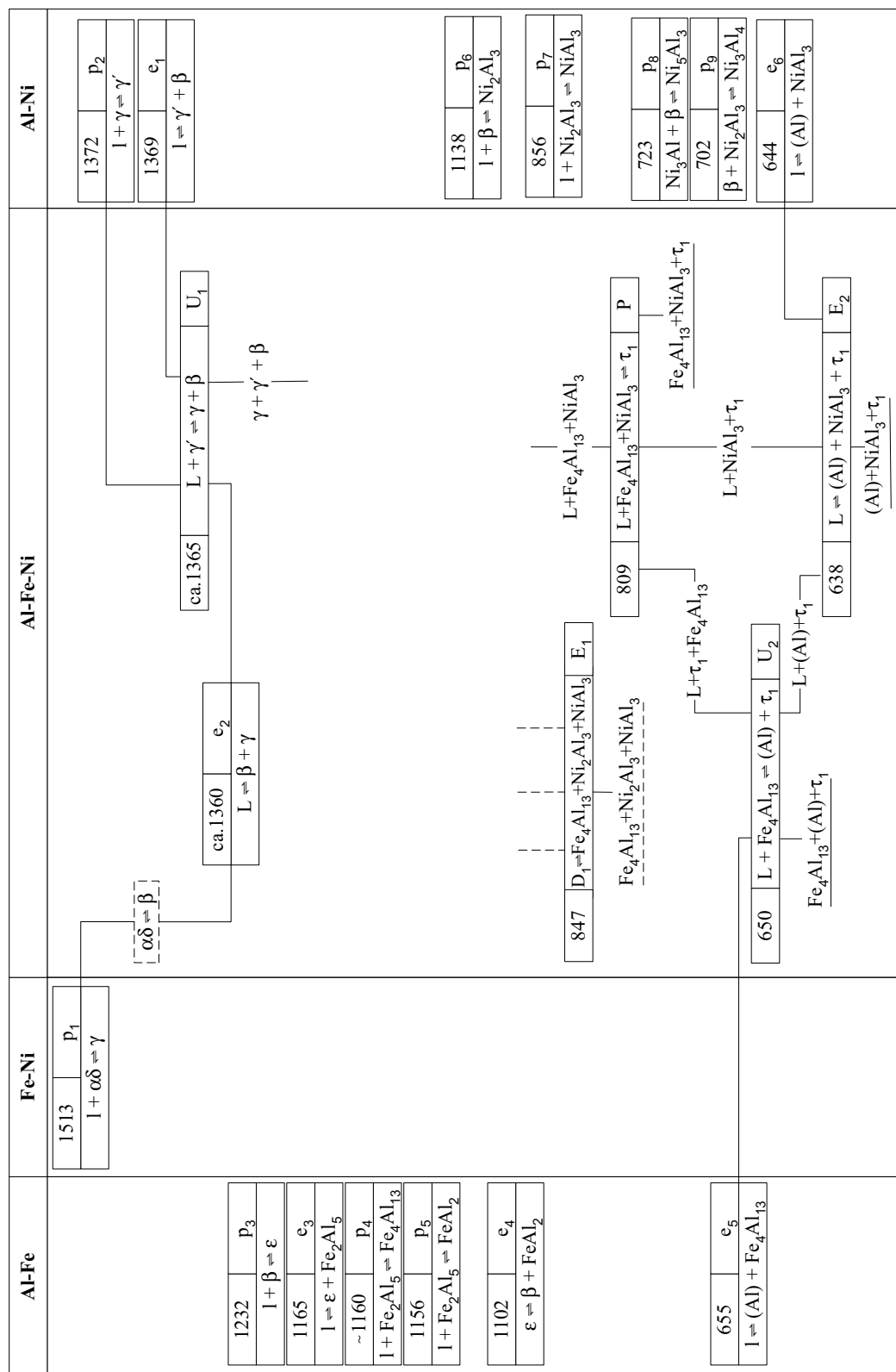composition at
constant Al contents

Fig. 1b: Al-Fe-Ni.
Lattice parameter of
β-phase, (Fe,Ni)Al as
a function of
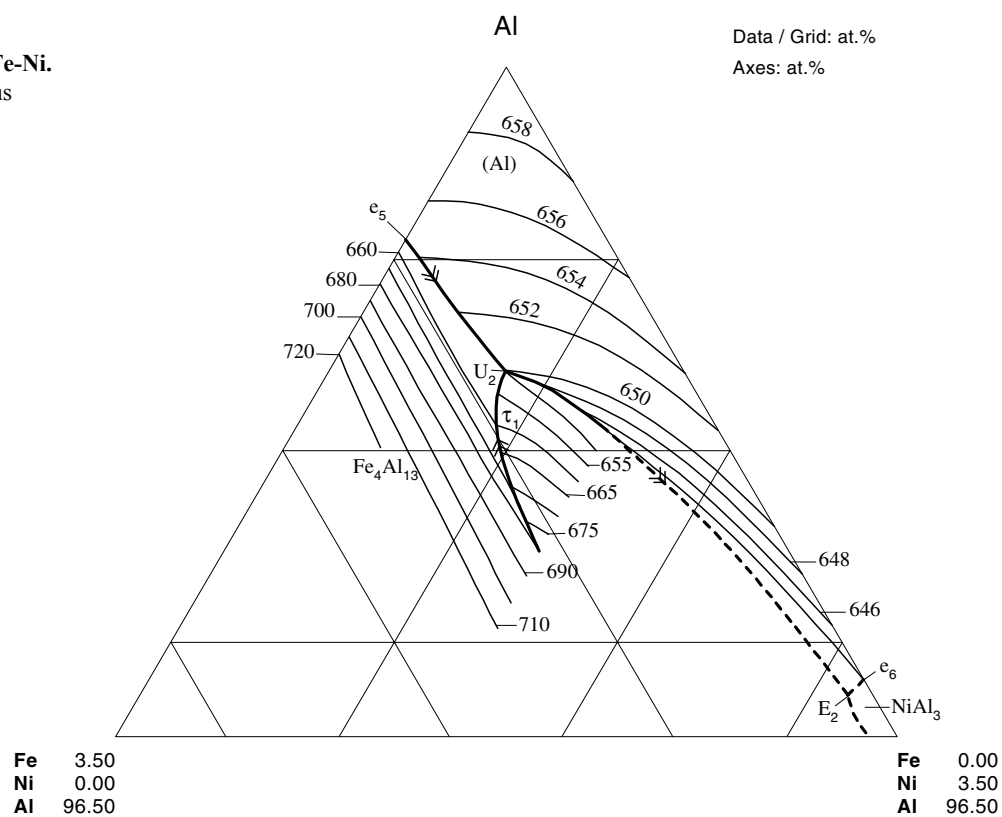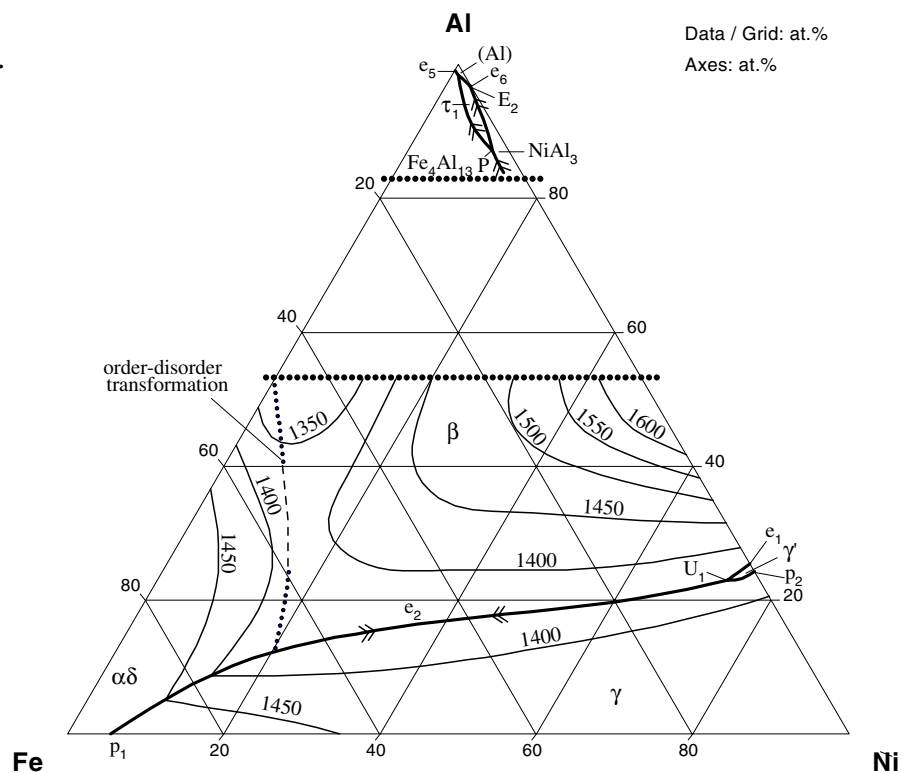composition at
constant Fe:Ni ratio
(0 - for NiAl, ∞- for
FeAl)

Al-Fe	Fe-Ni	Al-Fe-Ni	Al-Ni

Al-Ni

1372	p$_2$
l + γ ⇌ γ′	

1369	e$_1$
l ⇌ γ′ + β	

1138	p$_6$
l + β ⇌ Ni$_2$Al$_3$	

856	p$_7$
l + Ni$_2$Al$_3$ ⇌ NiAl$_3$	

723	p$_8$
Ni$_3$Al + β ⇌ Ni$_5$Al$_3$	

702	p$_9$
β + Ni$_2$Al$_3$ ⇌ Ni$_3$Al$_4$	

644	e$_6$
l ⇌ (Al) + NiAl$_3$	

Al-Fe-Ni

[αδ ⇌ β]

ca.1365		U$_1$
L + γ′ ⇌ γ + β		

γ + γ′ + β

ca.1360	e$_2$
L ⇌ β + γ	

847	D$_1$ ⇌ Fe$_4$Al$_{13}$ + Ni$_2$Al$_3$ + NiAl$_3$	E$_1$

Fe$_4$Al$_{13}$ + Ni$_2$Al$_3$ + NiAl$_3$

809	L + Fe$_4$Al$_{13}$ + NiAl$_3$ ⇌ τ$_1$	P

L + Fe$_4$Al$_{13}$ + NiAl$_3$

Fe$_4$Al$_{13}$ + NiAl$_3$ + τ$_1$

L + τ$_1$ + Fe$_4$Al$_{13}$

650	L + Fe$_4$Al$_{13}$ ⇌ (Al) + τ$_1$	U$_2$

Fe$_4$Al$_{13}$ + (Al) + τ$_1$

L + (Al) + τ$_1$

L + NiAl$_3$ + τ$_1$

638	L ⇌ (Al) + NiAl$_3$ + τ$_1$	E$_2$

(Al) + NiAl$_3$ + τ$_1$

Fe-Ni

1513	p$_1$
l + αδ ⇌ γ	

Al-Fe

1232	p$_3$
l + β ⇌ ε	

1165	e$_3$
l ⇌ ε + Fe$_2$Al$_5$	

~ 1160	p$_4$
l + Fe$_2$Al$_5$ ⇌ Fe$_4$Al$_{13}$	

1156	p$_5$
l + Fe$_2$Al$_5$ ⇌ FeAl$_2$	

1102	e$_4$
ε ⇌ β + FeAl$_2$	

655	e$_5$
l ⇌ (Al) + Fe$_4$Al$_{13}$	

Fig. 2: Al-Fe-Ni. Partial reaction scheme

Fig. 3a: Al-Fe-Ni.
Partial liquidus
surface

Al

Data / Grid: at.%

Axes: at.%

e_5 (Al)
e_6
τ_1 E_2
Fe$_4$Al$_{13}$ P NiAl$_3$
20 80

40 60

order-disorder
transformation

1350 β
1500 1550 1600
60 40
1400
1450
1450 1400
e_1 γ′
U$_1$ p_2
20
e_2
1400
αδ 1400
1450 γ
Fe p_1 20 40 60 80 **Ni**

Al

Data / Grid: at.%

Axes: at.%

Fig. 3b: Al-Fe-Ni.
Partial liquidus
projection of
Al-corner

658
(Al)
656
e_5
654
660
680 652
700
720
650
U$_2$
τ_1
Fe$_4$Al$_{13}$ 655
665
675
648
690
646
710
e_6
E$_2$ NiAl$_3$

Fe	3.50		**Fe**	0.00
Ni	0.00		**Ni**	3.50
Al	96.50		**Al**	96.50

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Fig. 4: Al-Fe-Ni. Isothermal section at 1350°C. Note that order-disorder limit between αδ+β is not shown and must occur inside the ternary

Data / Grid: at.%
Axes: at.%
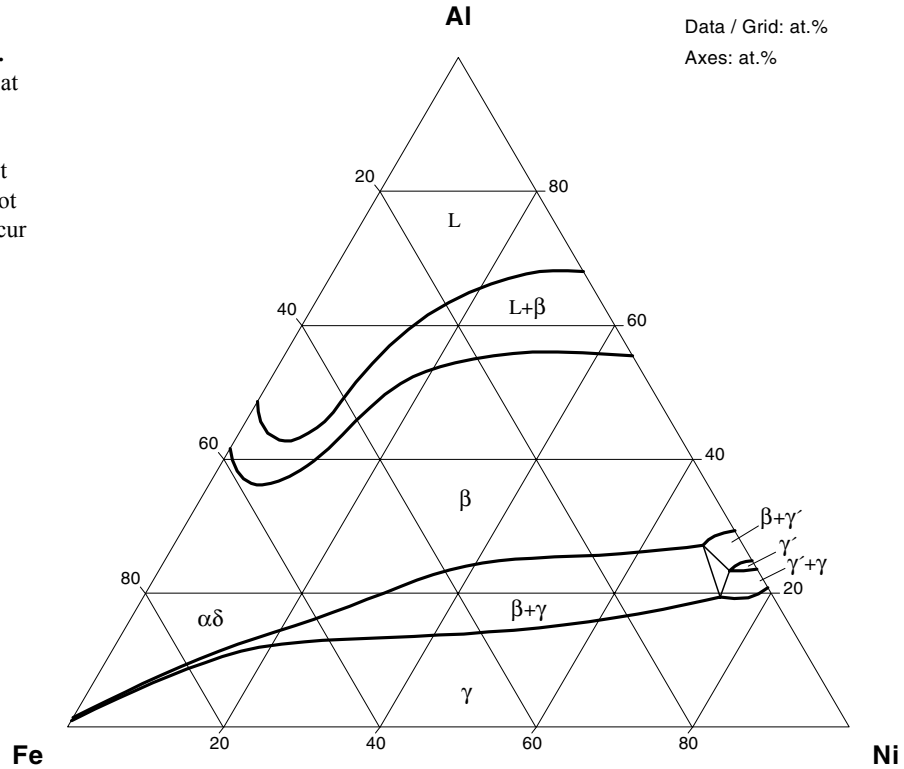
Fig. 5: Al-Fe-Ni. Isothermal section at 1250°C. The dotted order-disorder line is added

Data / Grid: at.%
Axes: at.%
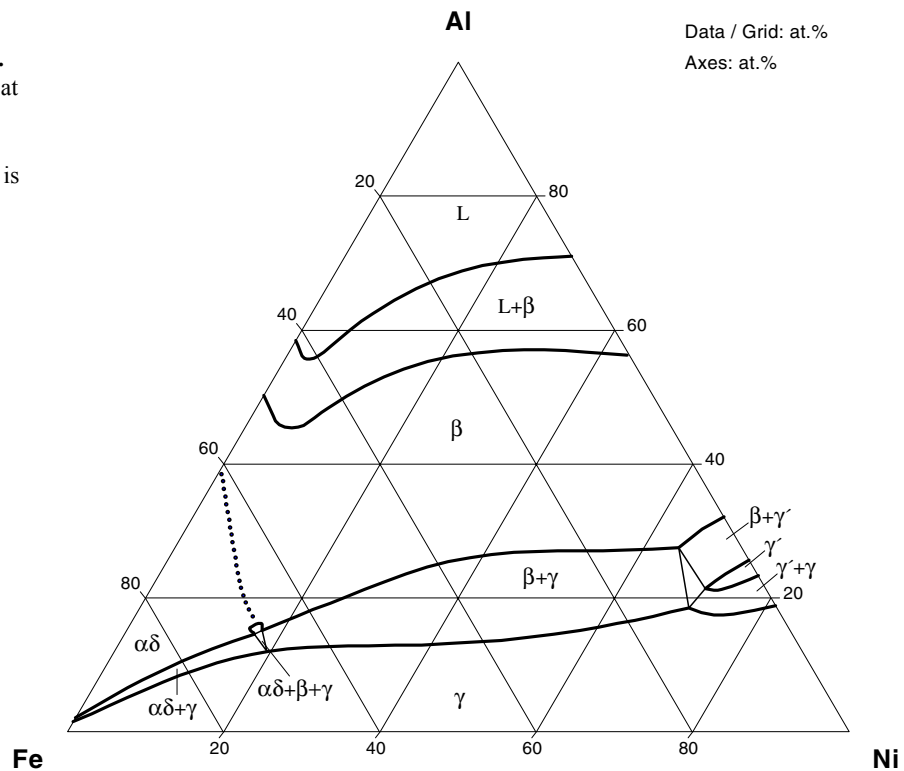
Fig. 6: **Al-Fe-Ni.**
Isothermal section at
1150°C [1949Bra]
below 50 at.% Al

Data / Grid: at.%
Axes: at.%

Al

Fe

Ni

β

β+γ+γ´

β+γ´

γ´

β+γ

γ´+γ

αδ

αδ+γ

αδ+β+γ

γ
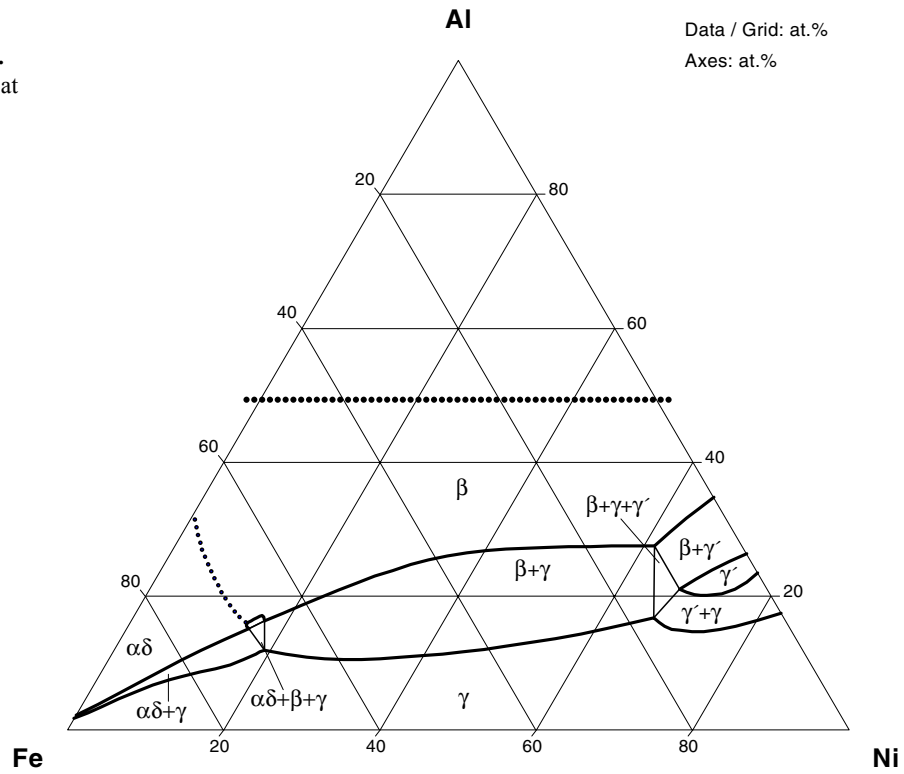
Fig. 7: **Al-Fe-Ni.**
Isothermal section at
1150°C
below 50 at.% Al

Data / Grid: at.%
Axes: at.%

Al

Fe

Ni

L

Fe$_4$Al$_{13}$

Fe$_2$Al$_5$

FeAl$_2$

τ$_2$

Ni$_2$Al$_3$

β

αδ+β

β+γ´

γ´

β+γ+γ´

αδ

β+γ

γ+γ´

αδ+γ+β

γ

90
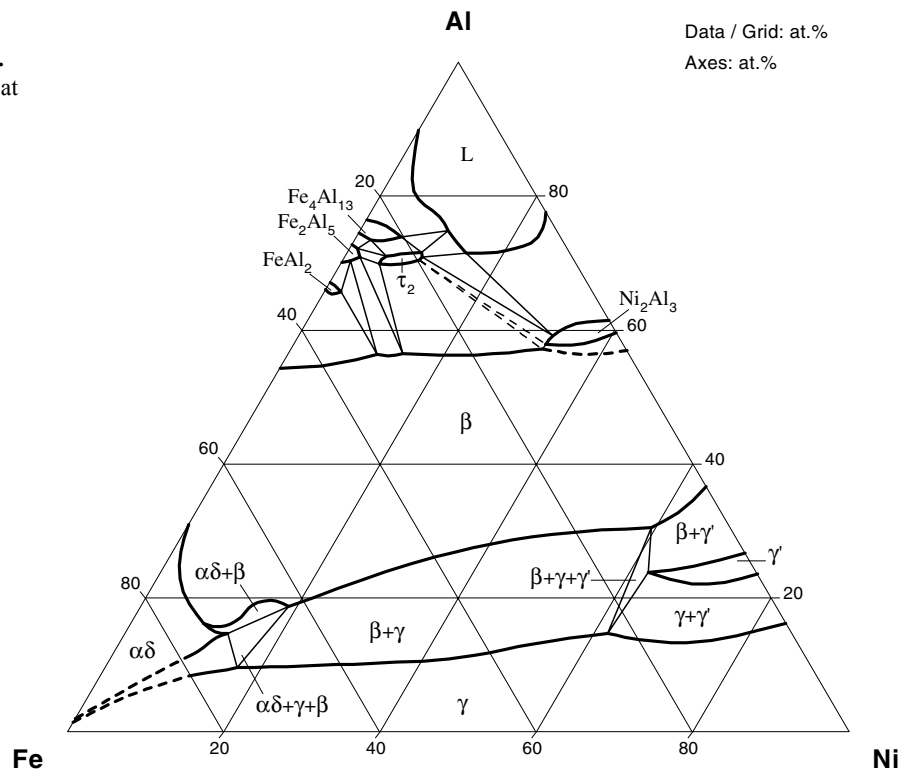
Fig. 8: Al-Fe-Ni.
Isothermal section at
950°C, Al-rich
[1982Kho], Al-poor
[1951Bra, 1984Hao]

Al

Data / Grid: at.%

Axes: at.%

L

Fe$_4$Al$_{13}$
Fe$_2$Al$_5$
FeAl$_2$

20

80

τ_2

Ni$_2$Al$_3$

40

60

β

60

40

β+γ´

γ

80

20

αδ+β

β+γ

γ+γ´

αδ

γ

Fe

20

40

60

80

Ni
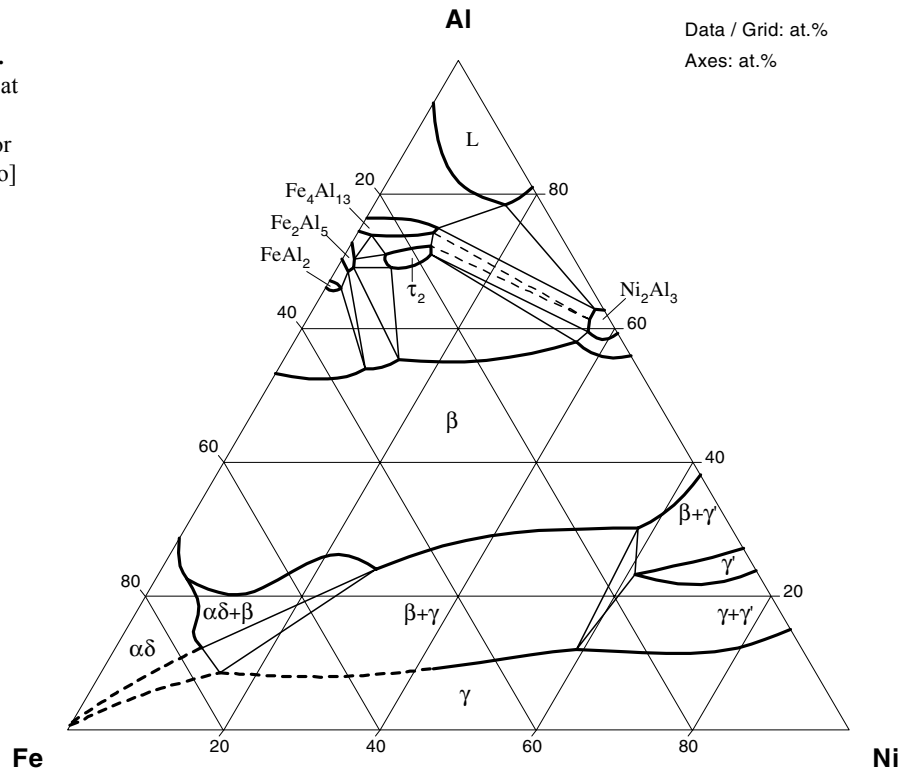
Fig. 9: Al-Fe-Ni.
Partial isothermal
section of Al-Fe-Ni at
850°C

Al

Data / Grid: at.%

Axes: at.%

L

20

80

Fe$_4$Al$_{13}$

NiAl$_3$

τ_2

τ_3

Ni$_2$Al$_3$

40

60

60

40

β

αδ+β

β+γ´

γ´

80

20

αδ

β+γ

γ+γ´

αδ

γ

Fe

20

40

60

80

Ni
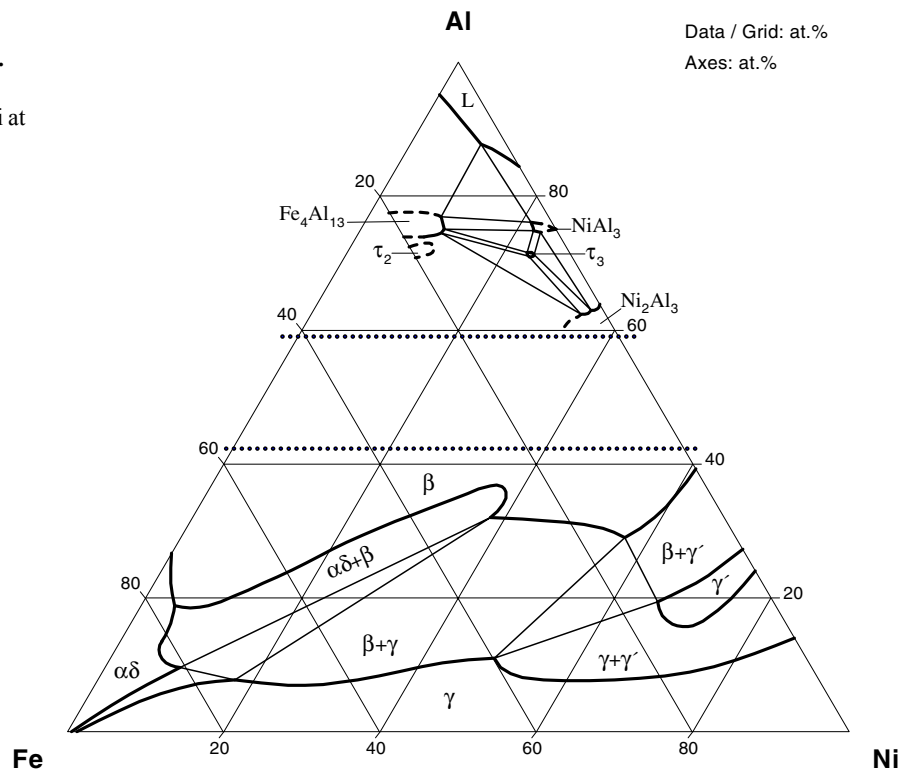
Fig. 10: Al-Fe-Ni.
Partial isothermal
section at 750°C:
Al-rich [1982Kho],
Al-poor [1951Bra]

Data / Grid: at.%

Axes: at.%

Al

Fe

Ni

L

τ_1

Fe_4Al_{13}

$NiAl_3$

20

80

40

60

60

40

80

20

20

40

60

80

?

β

β+γ'

γ'

αδ+β

β+γ+γ'

αδ

β+γ

γ+γ'

γ

Fig. 11: Al-Fe-Ni.
Partial isothermal
section at 620°C

Data / Grid: at.%

Axes: at.%

Al

(Al)

10

90

20

80

10

20

(Al)+τ_1

(Al)+Fe_4Al_{13}+τ_1

$(Al)+NiAl_3+\tau_1$

τ_1

Fe_4Al_{13}+$NiAl_3$+τ_1

Fe_4Al_{13}

$NiAl_3$

Fe	30.00
Ni	0.00
Al	70.00

Fe	0.00
Ni	30.00
Al	70.00
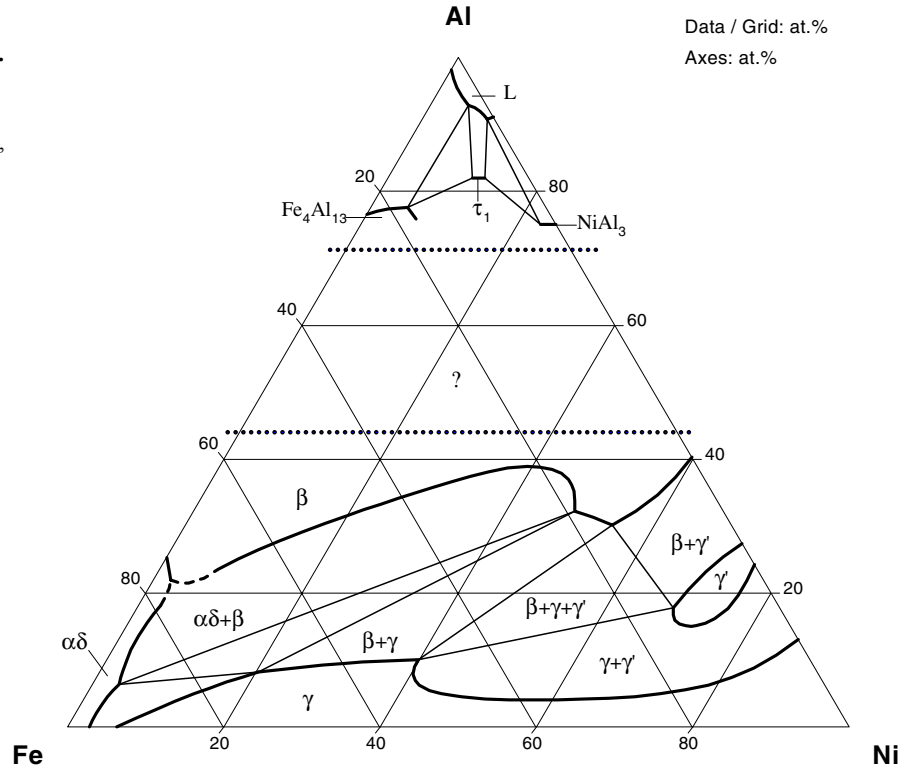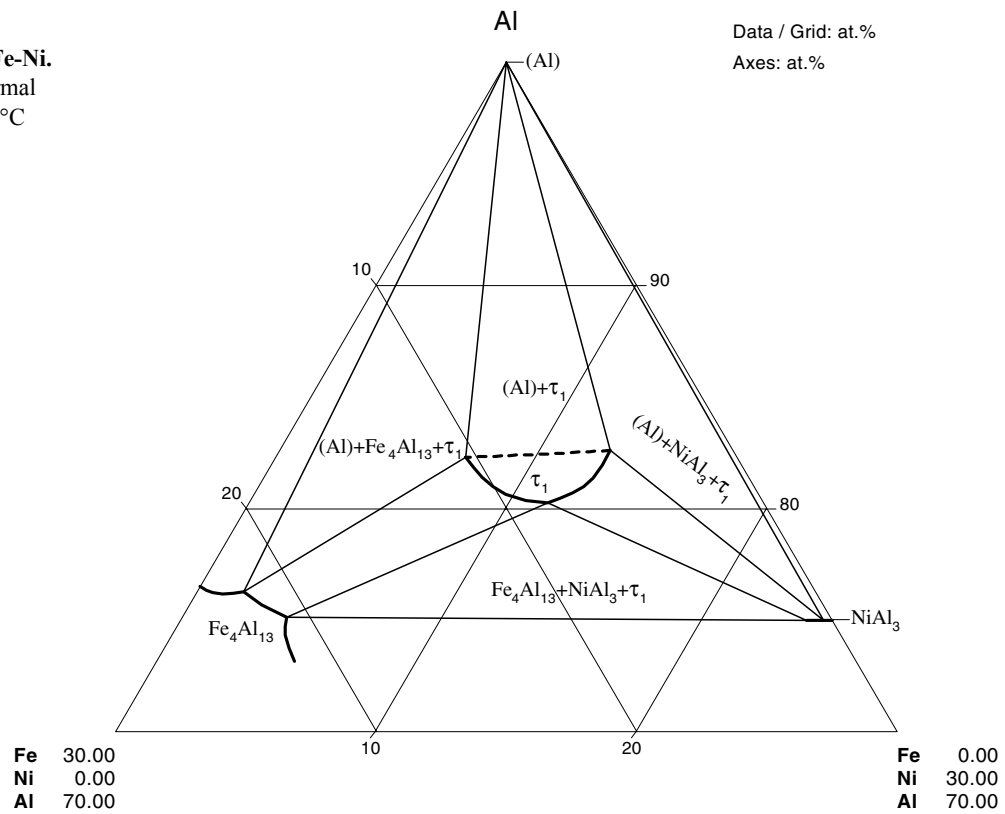
Fig. 12: Al-Fe-Ni.
Solid phases in alloys
cooled at 10 K/h

Data / Grid: at.%

Axes: at.%

Al

τ_1

Fe$_4$Al$_{13}$ 20

80

NiAl$_3$

Fe$_2$Al$_5$

FeAl$_2$

τ_2

Ni$_2$Al$_3$

40

60

β

60

40

Fe$_3$Al

$\beta+\gamma$

80

20

$\alpha\delta+\beta$

$\gamma+\gamma'$

$\alpha\delta$

$\alpha\delta+\gamma$

γ

Fe

20

40

60

80

Ni
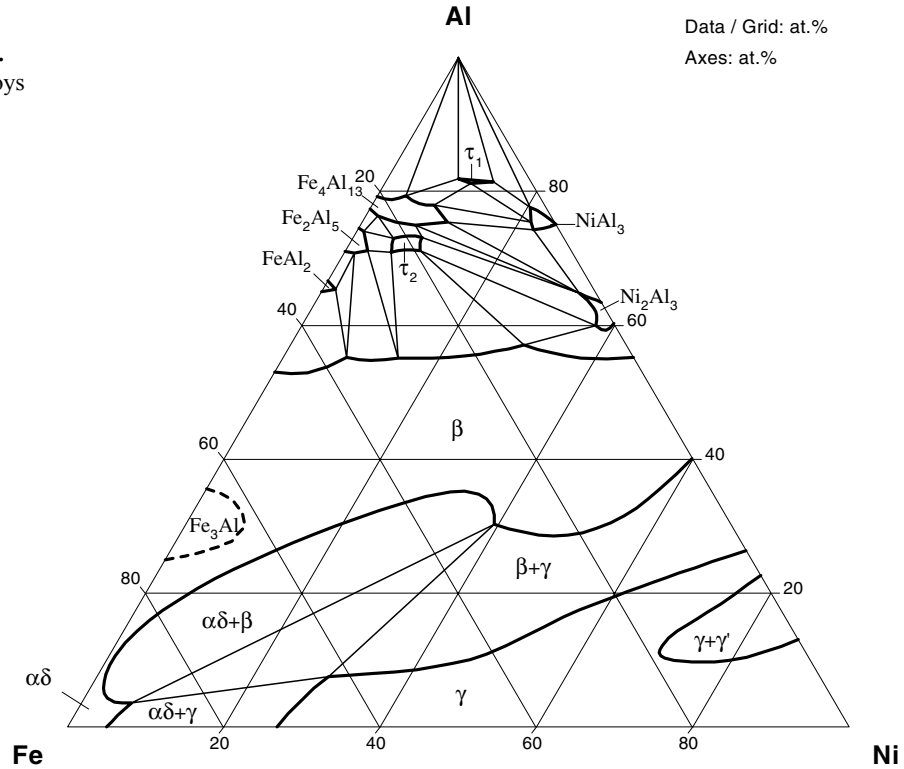
Fig. 13: Al-Fe-Ni.
Vertical section
parallel to Fe-NiAl,
Fe$_{95}$Al$_5$-Ni$_{47.5}$Al$_{52.5}$

L

L+$\alpha\delta$

L+β

$\alpha\delta$

β

$\alpha\delta+\beta$

Temperature, °C

Fe, at.%

Fe 95.00	90	80	70	60	50	40	30	20	10	**Fe** 0.00
Ni 0.00										**Ni** 47.50
Al 5.00										**Al** 52.50
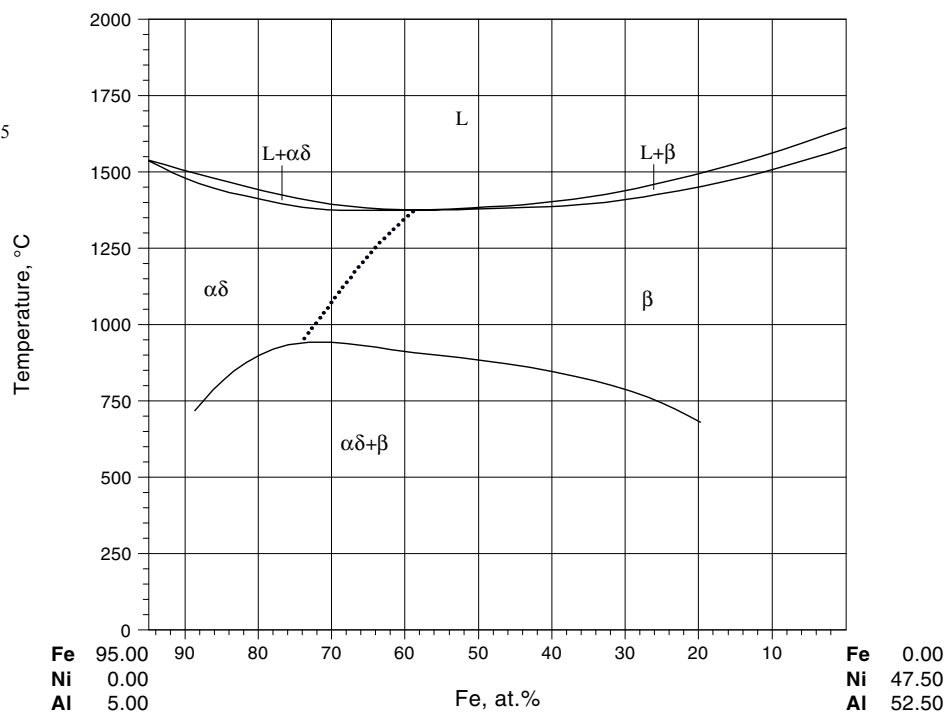
Fig. 14: Al-Fe-Ni.
Vertical section parallel to Fe-NiAl, Fe$_{97.5}$Al$_{2.5}$ - Ni$_{48.75}$Al$_{51.25}$
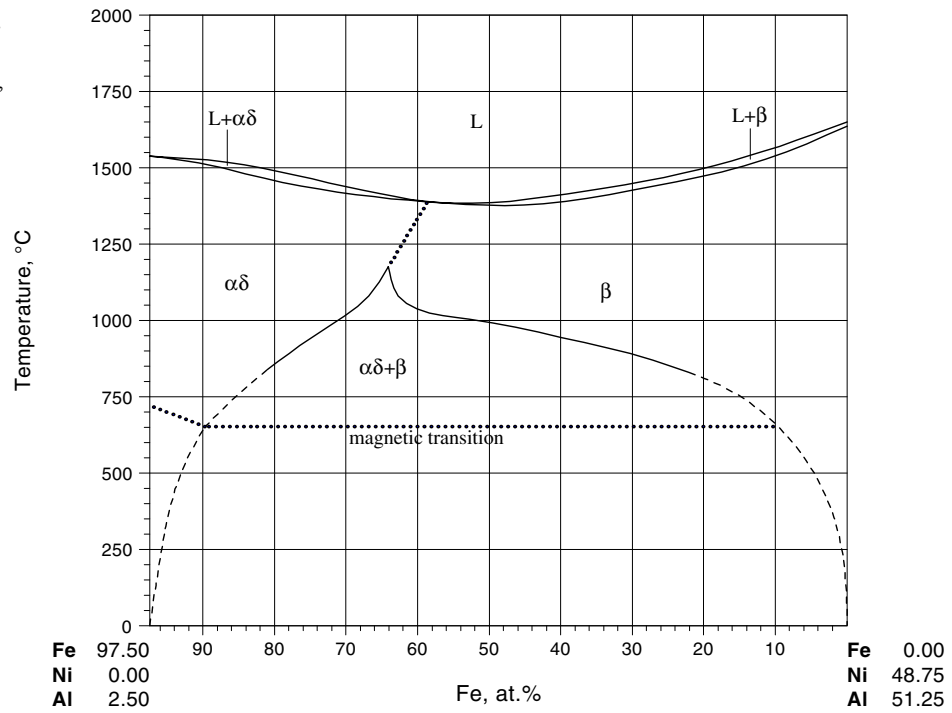
Fig. 15: Al-Fe-Ni.
Vertical section Fe-NiAl
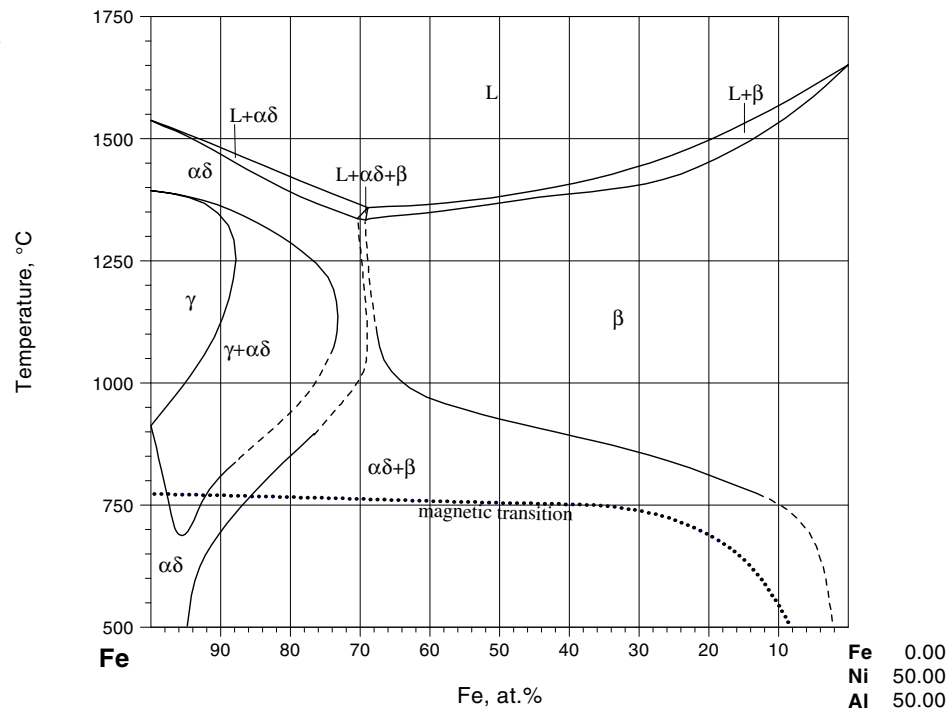
Fig. 16: Al-Fe-Ni.
Vertical section
Ni$_3$Al-FeNi$_3$
The tiny
L+γ'+β around
1369°C close to
Ni$_3$Al is not shown
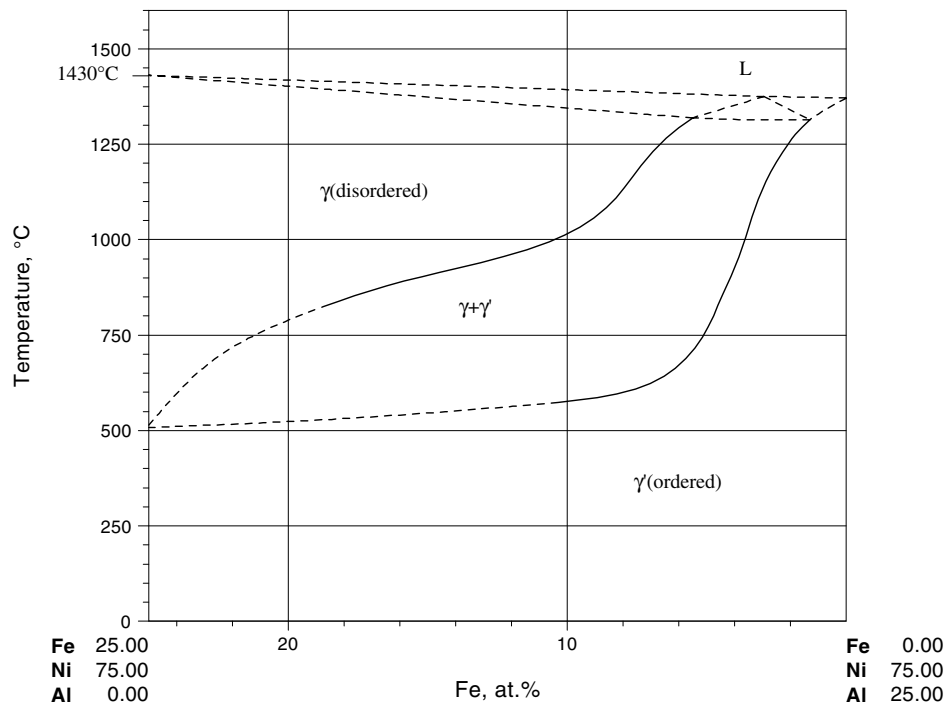
Cerium – Copper – Silicon

Oksana Bodak[t], Peter Rogl

Introduction

Although phase relations in the ternary system have been established in form of isothermal sections by several research groups [1965Gla, 1966Bod, 1967Ram, 1969Rie, 1974Bod], the discovery of $CeCu_2Si_2$ as the first superconducting heavy fermion system [1979Ste], made the Ce-Cu-Si system and particularly $CeCu_2Si_2$ the subject of intensive experimental and theoretical investigations because of the unusual interplay between superconducting and magnetic interactions at low temperature [1980Ste]. A summary of the physical properties is given below in section "*Notes on Materials Properties and Applications*". Most of the ternary compounds in the Ce-Cu-Si system are now well characterized with respect to region of existence and their crystal structures [1965Gla, 1966Bod, 1967Ram, 1969Rie, 1974Bod, 1983Jar, 1983Ian, 1983Kle, 1985Bra, 1985Neu, 1986Gig, 1986Spa, 1987Boe, 1988Neu, 1992Lev, 1996Hwa, 2004Ish]. Information on phase relations, structures and thermodynamics is summarized in Table 1.

Binary Systems

The Ce-Si system was adopted from a recent investigation by [2002Bul]. There is no doubt about the formation of the phase, $Ce_2Si_{3-x}(CeSi_{1.34})$, for which crystal and magnetic structures were determined by [1993Sch]. The Ce-Cu system is accepted from [1994Sub] and [2002Per]. The Cu-Si binary is taken from a recent MSIT assessment [2002Leb]. Crystallographic and melting data pertinent to the compounds of the Ce-Cu-Si system are given in Table 2.

Solid Phases

Crystallographic data of the binary and ternary compounds are listed in Table 2. Of all compounds the heavy fermion superconductor, $CeCu_2Si_2$ with the $ThCr_2Si_2$ structure type, has attracted most attention. Although unnoticed in earlier studies, it was found to exhibit a small homogeneity range at 750°C, which extends for about 3 at.% in the Cu/Si direction, $CeCu_{2-x}Si_{2+x}$ [1985Bra]. However, the ground state in $CeCu_2Si_2$ depends very delicately on the actual composition. Thus, Cu rich samples exhibit only superconductivity, Si rich show a magnetically ordered phase called A phase, while in stoichiometric samples (A/S type) a complex interaction between superconductivity (S) and magnetic order occurs [2001Ste].

Single-crystals of $CeCu_2Si_2$ have been investigated by [1983Jar]. The temperature dependence of lattice parameters for $CeCu_2Si_2$ was studied by [1985Neu] and pressure dependence of lattice parameters for $CeCu_2Si_2$ was reported by [1985Neu, 1986Spa] and for $CeCu_{1.8}Si_2$ by [1986Spa]. Two samples of $CeCu_xSi_2$ with $x = 1.8$ (non superconducting) and $x = 2.2$ (superconducting) have been investigated by neutron powder diffraction [1988Neu]. A crystallographic investigation of two $CeCu_xSi_2$ samples with $x = 1.8$ and $x = 2.2$ shows that the $CeCu_2Si_2$ structure is formed in both cases but with some differences in the degree of disorder of Cu and Si as well as in the composition of the impurity phases. [1992Lev] emphasized that $CeCu_{2-x}Si_{2+x}$ is a compound of variable composition with lattice parameters and electronic structure depending on Cu and Si content. Anisotropic vibration is detected for the Cu and Si atoms in both phases showing that the lattice degrees of freedom are important in $CeCu_2Si_2$ [1988Neu]. [2000Lou] found that the local atomic structure for a superconducting sample with $x = 0.33$ is fundamentally different from a nonsuperconducting sample with $x = -0.08$, and that superconducting, magnetic and non-Fermi-liquid-like ground states evolve in $CeCu_{2+x}Si_2$ with small changes in the Ce/Cu ratio that leave the average crystal structure unchanged. The $CeCu_2Si_2$ compound has $4f^2$ final-state amplitudes with formally $4f^1$ initial state configurations [1981Bia]. A valence transition would presumably result from transfer of the $4f^1$ electron to a conduction band state. The proximity of the f-electron to the Fermi level is consistent with the normal and superconducting properties [1986Spa]. The tetragonal ambient pressure

phase was at room temperature found to be stable up to 60 GPa: from the equation of state data a bulk modulus of 112.0(5.1) GPa was derived for $CeCu_2Si_2$ [2005Tsu].

The energy band structures and Fermi surfaces are calculated for $CeCu_6$ in [1992Har]. 4f-electrons of Ce in $CeCu_2Si_2$ are well localized and do not affect the Fermi surface significantly in an applied magnetic field [1992Har].

[2004Ish] synthesized a new ternary compound $Ce_2Cu_3Si_5$ (with orthorhombic $U_2Co_3Si_5$ structure type), which was not included in the phase triangulation of [1974Bod] at 600°C.

The phases τ_2 and τ_3 show a close crystallographic relationship: although unit cell, crystal symmetry and atom sites are identical, both compounds differ with respect to atom occupation. As a consequence the two structures may be considered as type (τ_3-$CeCuSi_2$) and inverse type (τ_2-$CeCu_2Si$). It shall be noted that both compounds are not in equilibrium but separated by foreign two phase regions. A similar situation is met with the phases τ_4 and τ_5, which both adopt the AlB_2 type structure separated by a two-phase field between the two phases. In this case a miscibility gap is conceivable suggesting a critical point at higher temperatures.

Liquidus Surface

[2000Nue1, 2000Nue2] performed a systematic investigation to determine the primary solidification area of the heavy fermion system $CeCu_2Si_2$ examining the liquidus surface by differential scanning calorimetric analysis in a special crucible system. Using the Nacken-Kyropoulos technique crystal growth experiments from a levitated melt within the primary solidification area yielded high quality single crystals of $CeCu_2Si_2$ with dimensions up to 7 mm [2000Nue2].

Invariant Equilibria

The phase $CeCu_2Si_2$ with the $ThCr_2Si_2$ structure type forms peritectically at (1545 ± 15)°C without evidence for a high temperature polymorphic transformation: $L + Ce_2CuSi_3 + CeSi_2 \rightleftharpoons CeCu_2Si_2$ [1984Bra, 1985Bra].

Isothermal Sections

The isothermal section of the Ce-Cu-Si system at 600°C, as shown in Fig. 1, is based on an early investigation by [1974Bod, 1985Bra] with amendments to comply with the accepted binary systems as well as with the findings concerning the extension of the homogeneity region for $CeCu_2Si_2$ (see details in Fig. 2). The location of the ternary compound $Ce_2Cu_3Si_5$ found by [2004Ish] is indicated by a filled circle. It may be a high temperature phase. Cerium solubility in copper silicides is generally below ca. 1 at.% Ce. Mutual solubility among cerium silicides and cerium copper phases, however, is significant. The essentially random substitution of the almost equally sized atom species copper and silicon is also reflected in extended homogeneous regions for some ternary compounds such as for τ_4-$Ce(Pt_xSi_{1-x})_2$ and τ_5-$Ce(Pt_{1-x}Si_x)_2$.

Thermodynamics

[1985Bre, 1998Geg] studied the low temperature specific heat and the entropy changes for $CeCu_xSi_2$, $x = 1.9, 2.0, 2.2$.

Notes on Materials Properties and Applications

Physical property data are known for $CeCu_2Si_2$, $CeCuSi$, $CeCu_{0.5}Si_{1.5}$, $CeCu_{0.24}Si_{1.76}$, $Ce_2Cu_3Si_5$ and are discussed below.

$CeCu_2Si_2$:
Since the observation of superconductivity in $CeCu_2Si_2$ [1979Ste], much work has been devoted to understand the unusual properties of this prototypical heavy-fermion superconductor. Particularly the unusual type of magnetic order in the so-called ''A phase'' [1994Bru], discovered about ten years after the superconductivity by NMR [1988Nak] and muon spin rotation (mSR) [1989Uem], has attracted much

interest. From thermodynamic and transport measurements a complex magnetic (B,T) phase diagram was constructed with superconducting and magnetically ordered phases and a ground state depending very delicately on the actual stoichiometry [1994Bru]. The ground state was claimed to be (i) the A phase, sometimes coexisting with superconductivity, A+S where superconductivity expels the A phase, or (ii) the superconducting S phase [2001Ste]. Doping experiments (Ge substituting for Si) as well as experiments under hydrostatic pressure indicated that $CeCu_2Si_2$ is near a quantum critical point in line with the disappearance of the A phase. In the vicinity of the quantum critical point Non-Fermi-liquid behavior (in the specific heat and the electrical resistivity) was reported. A detailed investigation of the A phase in order to detect magnetic order by neutron diffraction failed, but measurements of the electrical resistivity revealed a spin-density wave (SDW), with an opening of a gap below the ordering temperature in certain directions [1998Geg], and μSR experiments gave a rough estimation of the ordered moment of ~0.1 μB [1989Uem]. Below T_N ~0.8 K the A phase exhibits long-range antiferromagnetic order derived from neutron diffraction experiments on a magnetically ordered $CeCu_2Si_2$ single crystal (see also Fig. 3) [2004Sto]. The propagation vector, $\mathbf{T}$ = (0.215 0.215 0.530) at T = 50 mK, of the magnetic order appears to be determined by the topology of the Fermi surface of heavy quasiparticles as indicated by renormalized band-structure calculations. The absence of magnetic Bragg peaks in the superconducting phase gives evidence that antiferromagnetism and superconductivity seem to exclude each other on a microscopic scale. The observed instability of the Fermi liquid was reported to be related to the fact that the Fermi surface exhibits parallel flat parts separated by the measured propagation vector. These results suggest that a spin-density-wave instability is the origin of the quantum critical point observed in $CeCu_2Si_2$. However, the discrepancy between the small ordered moment and the observed large anomalies in the thermal expansion as well as the elastic constants [1994Bru] demand further examination. The existence of long-range incommensurate antiferromagnetic order in the A phase suggests that the origin of the quantum critical point arises from a spin-density-wave instability. The strong electron correlations in $CeCu_2Si_2$ show up *e.g.* in a huge linear coefficient to the electronic specific heat at low temperatures, γ = C/T ~1 J·mol^{-1}·K^{-2}, indicative of a largely enhanced effective electron mass (heavy-fermion system).

The description of the physical behavior of $CeCu_2Si_2$ given above is rather short. For detailed information the reader may be transferred to a series of reviews on the subject given in [1980Ste, 1984Bra, 1998Geg, 2001Ish, 2001Ste, 2002Kit, 2004Sto, 2005Ste1, 2005Ste2, 2005Ste3, 2005Sto].

CeCuSi:
CeCuSi exhibits a ferromagnetic ordering below T_c = 15.5 K, with a magnetic moment of 1.25 μ_B at 2.5 K, perpendicular to the *c*-axis [1983Kid, 1986Gig]. Neutron scattering measurements on the heavy fermion system $CeCu_{0.24}Si_{1.76}$ confirm a phase transition to ferromagnetic order below T_c = 8 K. The ordered moment μ = 0.62 ± 0.05 μ_B [1987Boe].

CeCu$_{0.5}$Si$_{1.5}$:
Temperature dependences of specific heat, electrical resistivity and magnetic susceptibility of $CeCu_{0.5}Si_{1.5}$ with AlB_2 structure type are reported on polycrystalline samples [1996Hwa] as well as on single crystals [2000Nak] revealing complex magnetic properties with strong anisotropy. $CeCu_{0.5}Si_{1.5}$ orders antiferromagnetically at 2.1 K. The magnetic susceptibility exhibits a maximum at 2 K only along the hexagonal *c*-axis at low magnetic fields [2000Nak]. Electrical resistivity shows the typical behavior of a Kondo compound with crystalline electric field effect [1996Hwa].

Ce$_2$Cu$_3$Si$_5$:
Magnetization measurements up to 30 T at 1.5 K in the temperature range from 2.0 to 300 K showed that $Ce_2Cu_3Si_5$ undergoes a transition to the antiferromagnetic state at T_N = 4.4 K. The highest magnetization values per Ce atom of $Ce_2Cu_3Si_5$ is 0.92 μ_B at B = 30 T [2004Ish].
Microhardness was reported for $CeCu_2Si_2$ (394), $CeCu_{1.6}Si_{1.4}$ (464), $CeCuSi_2$ (613), $CeCu_{1.19-1.10}Si_{0.8-0.90}$ (446), and for $CeCu_{0.78-0.44}Si_{1.24-1.56}$ (634 kg·mm^{-2}) [1974Bod].

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Table 1: Investigations of the Ce-Cu-Si Phase Relations, Structures and Thermodynamics

Reference	Method/Experimental Technique	Temperature/Composition/Phase Studied
[1965Gla]	X-ray diffraction (XPD)	formation, structure of AlB_2 type $Ce(Cu,Si)_2$ at 800°C
[1966Bod]	XPD	formation, structure of $CeCu_2Si_2$
[1967Ram]	XPD	formation, structure of AlB_2 type Ce_2CuSi_3, Ce_2Cu_3Si
[1969Rie]	XPD	formation, structure of $CeCu_{0.67}Si_{1.33}$, $CeCuSi$, $CeCu_{0.5}Si_{1.5}$, $CeCu_{1.5}Si_{0.5}$
[1974Bod]	XPD; X-ray single crystal photographs	formation, structure of $CeCu_{1.6}Si_{1.4}$, $CeCuSi_2$, $CeCu_{0.78-0.44}Si_{1.24-1.56}$

Reference	Method/Experimental Technique	Temperature/Composition/Phase Studied
[1981Bia]	synchrotron radiation	formation, structure of γ-Ce, $CeCu_2Si_2$
[1983Jar]	X-ray single-crystal four-circle data	structure of $CeCu_2Si_2$
[1983Kid]	XPD	formation, structure of CeCuSi
[1983Kle]	Bridgman single-crystal growth, XPD, X-ray single crystal photographs	structure of $CeCu_2Si_2$
[1983Ian]	XPD	formation, structure of CeCuSi
[1984Kit]	nuclear quadrupole resonance	$CeCu_2Si_2$
[1984Onu]	Czochralski single-crystal growth, XPD, X-ray single crystal photographs	structure of $CeCu_2Si_2$
[1985Neu]	XPD	formation, structure of $CeCu_2Si_2$
[1985Bra]	XPD, metallography and differential thermal analysis (DTA), microprobe analysis (EMPA)	partial isothermal section
[1986Gig]	neutron powder diffraction	structure of CeCuSi
[1986Spa]	XPD	formation, structure of $CeCu_2Si_2$, $CeCu_{1.8}Si_2$
[1986Lev]	XPD	formation, structure of $CeCu_2Si_2$
[1987Boe]	neutron powder diffraction	structure of $CeCu_{0.24}Si_{1.76}$
[1988Neu]	neutron powder diffraction	structure of $CeCu_xSi_2$; x = 1.8, 2.2
[1992Lev]	XPD	formation, structure of $CeCu_{2-x}Si_{2+x}$ at 1000 K; x = -0.20, -0.15, -0.10, -0.05, 0.005, 0.10, 0.15, 0.20
[1996Hwa]	XPD	formation, structure of Ce_2CuSi_3
[1997Mor]	XPD, DTA	formation, structure of $CeCu_2Si_2$
[1997Nue]	Nacken Kyropoulos technique, microscopy	$CeCu_2Si_2$
[1998Koy]	scattering technique	900°C; $CeCu_{2.2}Si_2$
[1999Ish]	XPD	formation, structure of $CeCu_{2.05}Si_2$, $Ce_{1.025}Cu_2Si_2$, $Ce_{0.99}Cu_{2.02}Si_2$, $Ce_{0.975}Cu_2Si_2$
[2000Nue1] [2000Nue2]	DSC measurements, Nacken Kyropoulos technique, scanning electron microscopy (SEM), X-ray analysis (EDX), XPD, metallography	partial isothermal section
[2000Nak]	Czochralski single-crystal growth, XPD, X-ray single crystal photographs	formation, structure of Ce_2CuSi_3, 800°C
[2000Lou]	neutron pair density function analysis, (GLAD) of the Intense pulsed neutron source (IPNS), powder diffractometer (GPPD) of IPNS, Rietveld refinement method	formation, structure of $CeCu_{2+x}Si_2$ at 900°C, x = 0.33, 0.08
[2001Kaw]	Cu-NQR measurements, EPMA	$Ce_{0.99}Cu_{2.02}Si_2$, $CeCu_{2.05}Si_2$

Reference	Method/Experimental Technique	Temperature/Composition/Phase Studied
[2001Ish]	XPD	750°C; samples with 20 different compositions near $CeCu_2Si_2$ compound
[2002Ish]	XPD	750°C; samples with 20 different compositions near $CeCu_2Si_2$ compound
[2003Tay]	X-ray diffraction	formation, structure of $CeCu_2Si_2$
[2004Ish]	XPD	formation, structure of $Ce_2Cu_3Si_5$ at 900°C

Table 2: Crystallographic Data of Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
(Cu) < 1084.62	$cF4$ $Fm\bar{3}m$ Cu	$a = 361.46$	at 25°C [Mas2] 0 to 11.3 at.% Si [Mas2]
(δCe) 798 - 726	$cI2$ $Im\bar{3}m$ W	$a = 412$	0 to 0.55 at.% Cu at 708°C [1994Sub] 0 to 2.5 at.% Al at 720°C [2000Oka]
(γCe) 726 - 61	$cF4$ $Fm\bar{3}m$ Cu	$a = 516.10$	0 to 0.37 at.% Cu at 708°C [1994Sub]
(βCe) 61 -(−177)	$hP4$ $P6_3/mm$ La	$a = 308.10$ $c = 1185.7$	at 24°C [1994Sub]
(αCe) < −177	$cF4$ $Fm\bar{3}m$ Cu	$a = 485$	at −196°C [1994Sub]
(Si) < 1414	$cF8$ $Fd\bar{3}m$ $C_{diam.}$	$a = 543.09$	[V-C2] 0-0.002 at.% Cu [Mas2]
CeCu < 516	$oP8$ $Pnma$ FeB	$a = 737.0$ $b = 462.3$ $c = 564.8$	[1994Sub], [2002Per]
$CeCu_{2-x}Si_x$ $CeCu_2$ < 817	$oI12$ $Imma$ KHg_2 ($CeCu_2$)	$a = 442.9$ $b = 706.1$ $c = 747.4$	$0 < x < 0.15$ at $x = 0$ [1994Sub], [2002Per]
$CeCu_4$ < 796	$oP20$ $Pnnm$ $CeCu_4$	$a = 458$ $b = 810$ $c = 935$	[1994Sub], [2002Per]
$CeCu_{5-x}Si_x$ $CeCu_5$ < 798	$hP6$ $P6/mmm$ $CaCu_5$	$a = 514.8$ $c = 410.8$	$0 < x < 0.54$ [Mas2, 1994Sub]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
$\beta CeCu_6$ 938 - (−43)	$oP28$ $Pnma$ $\beta CeCu_6$	$a = 810.88$ $b = 510.04$ $c = 1016.21$	at 22°C [1990Vrt]
		$a = 810.09$ $b = 509.78$ $c = 1015.48$	at −23°C [1990Vrt] [1994Sub], [2002Per]
$\alpha CeCu_6$ < −43	$mP28$ $P2_1/c$ $LaCu_6$	$a = 509.5$ $b = 1014.66$ $c = 809.31$ $\beta = 90.485°$	at −73°C [1990Vrt]
		$a = 508.92$ $b = 1013.26$ $c = 807.89$ $\beta = 91.148°$	at −173°C [1990Vrt]
		$a = 508.41$ $b = 1012.79$ $c = 807.31$ $\beta = 91.442°$	at −263°C [1990Vrt] [1994Sub], [2002Per]
Cu_7Si (K) 842 - 552	$hP2$ $P6_3/mmc$ Mg	$a = 256.05$ $c = 418.46$	at 730°C, 12.75 at.% Si [Mas2] 11.05 to 14.5 at.% Si [1994Ole]
Cu_6Si (β) 853 - 787	$cI2$ $Im\bar{3}m$ W	$a = 285.4$	14.2 to 16.2 at.% Si [1994Ole] at 14.9 at.% Si [1994Ole]
Cu_5Si (γ) < 729	$cP20$ $P4_132$ βMn	$a = 619.8$	17.15 to 17.6 at.% Si [1994Ole]
Cu_5Si (δ) 824 - 711	t^{**}		17.6 to 19.6 at.% Si [1994Ole]
		$a = 881.5$ $c = 790.3$	sample annealed at 700°C [V-C2]
$Cu_{15}Si_4$ (ε) < 800	$cI76$ $I\bar{4}3d$ $Cu_{15}Si_4$	$a = 961.5$	21.2 at.% Si [1994Ole, V-C2]
Cu_3Si (η) 859 - 558	hR^* $R\bar{3}m$	$a = 247$ $\alpha = 109.74°$	23.4 to 24.9 at.% Si [1994Ole]
	or t^{**}	$a = 726.7$ $c = 789.0$	[V-C2, Mas2]
Cu_3Si (η′) 620 - 467	hR^* $R\bar{3}$	$a = 472$ $\alpha = 95.72°$	23.2 to 25.2 at.% Si [1994Ole]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
Cu_3Si (η'') < 570	o^{**}	$a = 676$ $b = 700$ $c = 2194$	23.3 to 24.9 at.% Si [1994Ole]
Ce_5Si_3 < 1260	$tI32$ $I4/mcm$ Cr_5B_3	$a = 789$ $c = 1377$	[2002Bul]
		$a = 786.8$ $c = 1373$	[V-C2]
Ce_3Si_2 < 1335	$tP10$ $P4/mbm$ U_3Si_2	$a = 778.0$ $c = 436.7$	[2002Bul]
Ce_5Si_4 < 1500	$tP36$ $P4_12_12$ Zr_5Si_4	$a = 793.6$ $c = 1502.9$	[2002Bul]
$CeSi$ < 1630	$oP8$ $Pnma$ FeB	$a = 828.8$ $b = 396.4$ $c = 595.2$	[2002Bul]
$CeSi_{1.34}$	$oC20 - x$ $Cmcm$ V_2B_3 (Nd_2Si_{3-x})	$a = 440.35$ $b = 2483.89$ $c = 395.17$	[1993Sch]
$CeSi_{1.67}$ < 1725	$oI12$ $Imma$ $GdSi_{2-x}$	$a = 411.3$ $b = 419.0$ $c = 1390.6$	[2002Bul]
		$a = 410.0$ $b = 418.0$ $c = 1382.0$	[V-C2]
$CeSi_{2-y}Cu_y$	$tI12$ $I4_1/amd$ $ThSi_2$	$a = 417.1$ $c = 1394$	$0 < y < 0.27$ [V-C2] at $y = 0.24$; [1987Boe]
		$a = 415.4$ $c = 1382.2$	at $x = 0.214$
$CeSi_{2-x}$ < 1575		$a = 419.2$ $c = 1391.3$	at $x = 0$ [2002Bul]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
* τ_1, CeCu$_2$Si$_2$	tI10 $I4/mmm$ ThCr$_2$Si$_2$ (CeGa$_2$Al$_2$) or BaAl$_4$	$a = 419.3$ $c = 998.6$	[1966Bod]
		$a = 409.4 \pm 0.1$ $c = 993.0 \pm 0.2$	[1983Jar]
		$a = 411.0 \pm 0.1$ $c = 994.8 \pm 0.1$	[1983Kle]
		$a = 411.2$ $c = 994.6$	[1983Kle] single crystal with an excess of 21.5 mass% Cu
		$a = 409.7$ $c = 991.8$	[1984Onu]
		$a = 410.0 \pm 0.1$ - 410.8 ± 0.3 $c = 992.1 \pm 0.3$ - 993.1 ± 0.6	[1985Bra]
			for "CeCu$_{1.8}$Si$_2$"
		$a = 408.63 \pm 0.01$ $c = 991.15 \pm 0.01$	at 1.5 K [1988Neu]
		$a = 408.64 \pm 0.01$ $c = 991.15 \pm 0.01$	at 10 K [1988Neu]
		$a = 408.91 \pm 0.01$ $c = 991.16 \pm 0.01$	at 100 K [1988Neu]
			for "CeCu$_{2.2}$Si$_2$" at
		$a = 408.25 \pm 0.01$ $c = 991.03 \pm 0.01$	at 1.5 K [1988Neu]
		$a = 408.26 \pm 0.01$ $c = 991.00 \pm 0.02$	at 10 K [1988Neu]
		$a = 408.56 \pm 0.01$ $c = 991.01 \pm 0.02$	at 100 K [1988Neu]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
$CeCu_{2-x}Si_{2+x}$		$a = 409.8 \pm 0.1$ $c = 987.2 \pm 0.3$	at 1000 K $x = -0.20$ [1992Lev]
		$a = 409.4 \pm 0.2$ $c = 986.8 \pm 0.6$	at 1000 K $x = -0.15$ [1992Lev]
		$a = 409.6 \pm 0.2$ $c = 989.0 \pm 0.4$	at 1000 K $x = -0.10$ [1992Lev]
		$a = 410.0 \pm 0.1$ $c = 991.8 \pm 0.3$	at 1000 K $x = -0.05$ [1992Lev]
		$a = 409.3 \pm 0.1$ $c = 990.3 \pm 0.3$	at 1000 K $x = 0.005$ [1992Lev]
		$a = 409.6 \pm 0.1$ $c = 991.2 \pm 0.3$	at 1000 K $x = 0.10$ [1992Lev]
		$a = 409.5 \pm 0.1$ $c = 990.8 \pm 0.3$	at 1000 K $x = 0.15$ [1992Lev]
		$a = 409.6 \pm 0.3$ $c = 990.9 \pm 0.3$	at 1000 K $x = 0.20$ [1992Lev]
		$a = 408.599 \pm 0.013$ $c = 991.49 \pm 0.03$	$CeCu_{1.92}Si_2$ at 20 K [2000Lou]
		$a = 408.441 \pm 0.013$ $c = 990.99 \pm 0.07$	$CeCu_{2.23}Si_2$ at 13 K [2000Lou]
		$a = 410.6 \pm 0.1$ $c = 993.6 \pm 0.9$	$CeCu_2Si_2$ [1997Nue]
* τ_2, $CeCu_{2-x}Si_{1+x}$	$oS16$ $Cmcm$ invers $CeNiSi_2$	$a = 416$ $b = 1721$ $c = 417$	at $x = 0.4$ [1974Bod]
* τ_3, $CeCu_{1+x}Si_{2-x}$	$oS16$ $Cmcm$ $CeNiSi_2$	$a = 412$ $b = 1648$ $c = 416$	at $x = 0$ [1974Bod]

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments/References
* τ_4, Ce(Cu$_{1-x}$Si$_x$)$_2$	hP3 P6/mmm AlB$_2$	a = 423.1 to 423.8 c = 398.9 to 403.0	0.405 < x < 0.45 [1974Bod]
		a = 423.8 c = 403.0	at x = 0.25 [1967Ram]
	hP6 P6$_3$/mmc Ni$_2$In	a = 423.3 c = 798.1	at x = 0.50; 750°C [1986Gig]
		a = 423.9 ± 0.2 c = 798.0 ± 0.4	for x = 0.50 [1983Ian]
* τ_5, Ce(Cu$_x$Si$_{1-x}$)$_2$	hP3 P6mmm AlB$_2$	a = 410.3 to 407.0 c = 424.4 to 429.1	0.22 < x < 0.38 [1974Bod]
		a = 405.9 ± 0.2 c = 429.4 ± 0.5	[1996Hwa]
		a = 406.5 c = 430.2	CeCu$_{0.5}$Si$_{1.5}$ [1967Ram] Si rich
		a = 413.6 c = 423.7	CeCu$_{0.5}$Si$_{1.5}$ [1967Ram] Cu rich
		a = 412.4 c = 421.4	at x = 0.50 [1969Rie]
		a = 407.5 c = 428.0	at x = 0.333 [1969Rie]
		a = 407.7 c = 431.4	for Ce(Cu,Si)$_2$ [1965Gla]
Ce$_2$Cu$_3$Si$_5$	oI40 Ibam U$_2$Co$_3$Si$_5$	a = 997.4 b = 1158 c = 584.4	900°C [2004Ish]

Si

Data / Grid: at.%

Axes: at.%

τ_1 - CeCu$_2$Si$_2$
τ_2 - CeCu$_{2-x}$Si$_{1+x}$
τ_3 - CeCu$_{1+x}$Si$_{2-x}$
τ_4 - Ce(Cu$_{1-x}$Si$_x$)$_2$
τ_5 - Ce(Cu$_x$Si$_{1-x}$)$_2$

Fig. 1: Ce-Cu-Si.
Isothermal section at
600°C (0 - 33.3
at.% Ce) and 400°C
(> 33.3 at.% Ce)

CeSi$_2$
CeSi$_{2-x}$
CeSi$_{1.34}$
CeSi
Ce$_5$Si$_4$
Ce$_3$Si$_2$
Ce$_5$Si$_3$
τ_4
τ_3
Ce$_2$Cu$_3$Si$_5$
τ_1
τ_2
τ_5
η, Cu$_3$Si
Cu$_{15}$Si$_4$
Cu$_5$Si
γ, Cu$_5$Si
(Cu)

Ce
(γCe)
CeCu
CeCu$_2$
CeCu$_4$
CeCu$_5$
CeCu$_6$
Cu

Ce	19.50
Cu	39.00
Si	41.50

Data / Grid: at.%

Axes: at.%
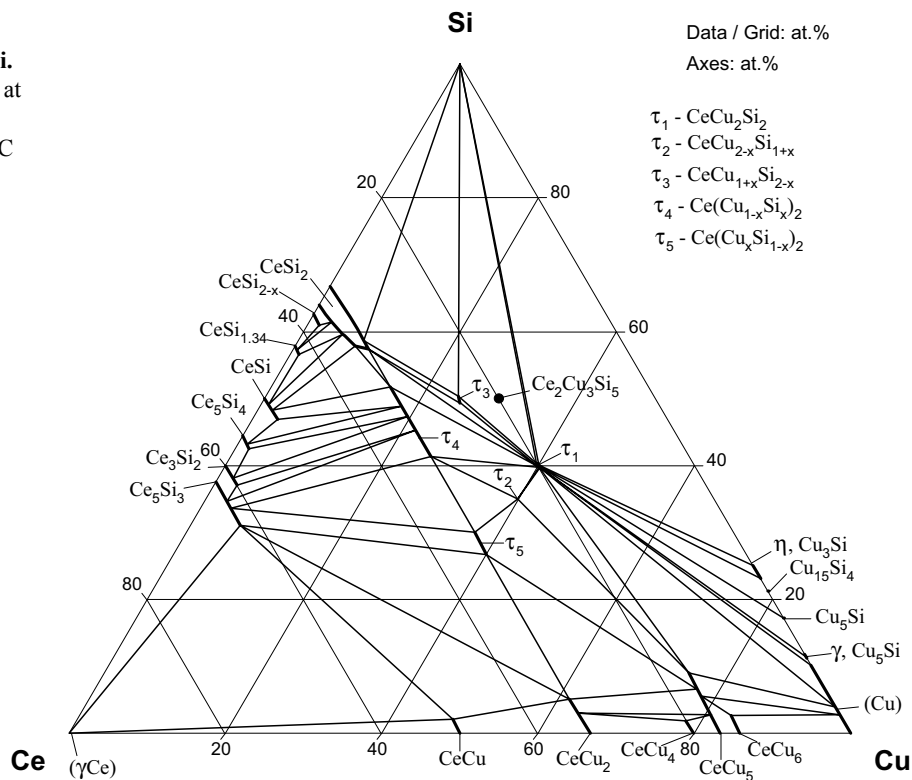
Fig. 2: Ce-Cu-Si.
Phase relations
around τ_1 at about
600°C

$\tau_1+\tau_3$
τ_1+(Si)$+\tau_3$
$\tau_1+\tau_4+$CeSi$_2$
τ_1+(Si)$+\eta$
$\tau_1+\tau_4$
τ_1
$\tau_1+\eta$
$\tau_1+\tau_2+\tau_4$
τ_1+Cu$_{15}$Si$_4+\eta$
τ_1+Cu$_{15}$Si$_4+$Cu
τ_1+(Cu)$+\gamma$
τ_1+Cu$_5$Si$+\gamma$
$\tau_1+\tau_2$
$\tau_1+\tau_2+$CeCu$_5$
τ_1+(Cu)
τ_1+CeCu$_5+$(Cu)

Ce	22.00
Cu	39.00
Si	39.00

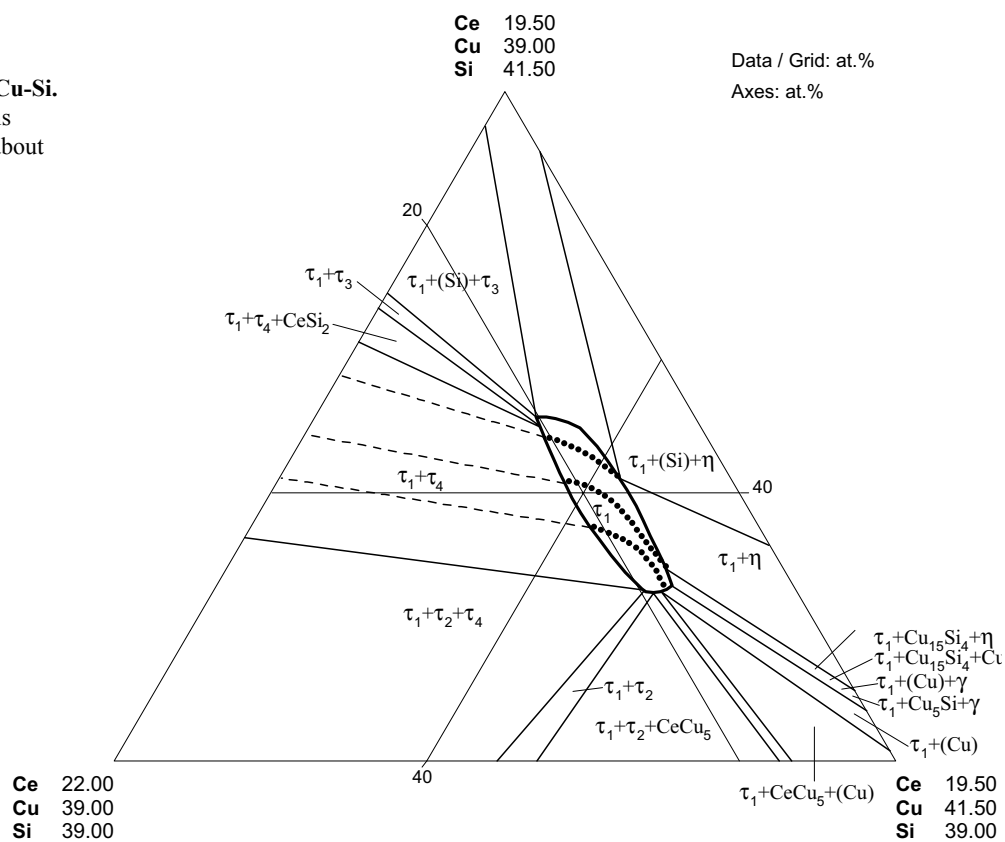| Ce	19.50
Cu	41.50
Si	39.00

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Fig. 3: Ce-Cu-Si.
Schematic magnetic
(B,*T*) phase diagram
of CeCu$_2$Si$_2$ with
different magnetically
ordered phase
(A-,B-phase)
paramagnetic region
PM, and the
superconducting
phase SC

B, T

B

PM

A

SC

Temperature, K